

Model Developer Guide

Release v3.5

June 2012



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June 2012

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Chapter 1. gPROMS Fundamentals

gPROMS process models are built from a number of fundamental building blocks or *Entities* (see also: Entities). A gPROMS process model (for a Simulation activity) consists of the following entities:

- **Variable Types**
- Connection Types
- **Models**
- Tasks
- **Processes**
- Saved Variable Sets

Note that the entities required as a minimum are highlighted in bold.

In addition

- To execute Optimisation activities, **Optimisation** entites are required. For details on solving Optimisation problems in gPROMS refer to the *gPROMS Advanced Users Guide* - included in the gPROMS installation.
- To execute Model Validation activities (Parameter Estimation and Experiment Design), **Parameter Estimation**, **Experiment Design** and **Experiment** Entites are required. For details on solving Parameter Estimation and Experiment Design problems in gPROMS refer to the Model Validation Guide

Variables and Variable Types

See also: Declaring Variable Types

In gPROMS, all quantities calculated by Model Equations are Variables; Variables are always *Real* (continuous) numbers and must always be given a Variable Type.

Variable Types have the following information,

- A *name*, to which the type may be referred globally.
- A *default value* for Variables of this type. This value will be used as an initial guess for any iterative calculation involving Variables of this type, unless it is overridden for individual Variables or a better guess is available from a previous calculation.
- *Upper and lower bounds* on the values of Variables of this type. Any calculation involving Variables of this type must give results that lie within these bounds. These bounds can be used to ensure that the results of a calculation are physically meaningful. Again, these bounds may be overridden¹for individual Variables of this type.
- An optional *unit of measurement*. Users are encouraged to provide this in order to aid Model readability.

¹It is possible to override the bounds on certain Variables. This is done using in PRESET section of the Process entity.

Figure 1.1. Variable Types declared in the gPROMS Process Model Library

Name	Lower bound	Default value	Upper bound	Units
activation_energy	-1E12	10000.0	1E12	J/mol
area	0.0	1.0	100000.0	m ²
diameter	0.0	1.0	100000.0	m
differential_pressure	-1E20	1000.0	1E20	Pa
differential_temperature	-50000.0	0.0	50000.0	K
dynamic_viscosity	1E-10	0.001	1000000.0	Pa.s
efficiency	-1.0	50.0	101.0	
elevation	0.0	1.0	100000.0	m
energy	-1E20	1000.0	1E20	J
energy_holdup	-1E20	1000.0	1E20	J
energy_rate	-1E50	1.0	1E50	J/s
Fanning_friction_factor	1E-8	1.0	1E20	10
head	0.0	1.0	100000.0	m
heat_flux	-1E50	1.0	1E50	J/s/metre
heatcapacity_ratio	1.01	1.1	10.0	
height	-1E-6	1.0	100000.0	m
length	0.0	1.0	100000.0	m
linear_flow_coefficient	1E-10	1.0	100000.0	kg/Pa s
mass	-0.001	1.0	1E20	kg
mass_concentration	-1E-10	1.0	1E10	kg/m ³
mass_density	1E-5	1000.0	1E20	kg/m ³
mass_flowrate	-1E20	1.0	1E20	kg/s
mass_fraction	-1E-10	1.0	1.0001	
mass_holdup	-0.001	1.0	1E20	kg
mass_specific_enthalpy	-1E20	10.0	1E20	J/kg
mass_specific_volume	-1.0	0.01	1000000.0	m ³ /kg
molar_concentration	-1E-10	1.0	1E10	mol/m ³
molar_flowrate	-1E20	1.0	1E20	mol/s
molar_fraction	-1E-10	1.0	1.0001	
molar_specific_enthalpy	-1E20	10.0	1E20	J/mol
molar_specific_volume	-1.0	0.01	1000000.0	m ³ /mol
molecular_weight	1E-5	1.0	1E20	
moles	0.0	1.0	1E20	mol
no_type	-1E200	1.0	1E200	
no_type_gezero	0.0	1.0	1E20	
no_type_gbunity	1.01	1.1	10.0	
no_type_gtzero	1E-10	1.0	1E200	
no_type_percentage	-1.0	50.0	101.0	
no_type_positive_fraction	-1E-10	1.0	1.0	
no_type_smallbound	0.0	1.0	1.0	
polytropic_head	-1E20	100.0	1E20	J/kg
power	-1E50	1.0	1E50	watt
pressure	1.0	100000.0	1E20	Pa
protected_velocity	1E-6	1.0	1000.0	m/s
reaction_rate	-1E20	1.0	1E20	mol/s
reynolds_number	-1000.0	30000.0	1E12	
rps_speed	0.0	1.0	1E20	rev per sec
specific_gravity	0.0	1.0	1000000.0	
temperature	10.0	300.0	50000.0	K
torque	-1E50	1.0	1E50	N-m
velocity	-1000.0	1.0	1000.0	m/s
volume	0.0	1.0	100000.0	m ³
volume_energy	-1E10	1000.0	1E10	J/m ³
volume_flowrate	-1E20	1.0	1E20	m ³ /s

Type definitions Properties

When developing gPROMS Models you can either use the existing Variable Types that are found in the gPROMS Process Model Library (PML) (refer to the gPROMS Process Model Library Guide) or define your own Variable Types.

Connection Types

See also: Declaring Connection Types

Connections between different Units in a flowsheet Model are associated with a Connection Type which defines the type of information conveyed by the connection.

A Connection Type definition includes

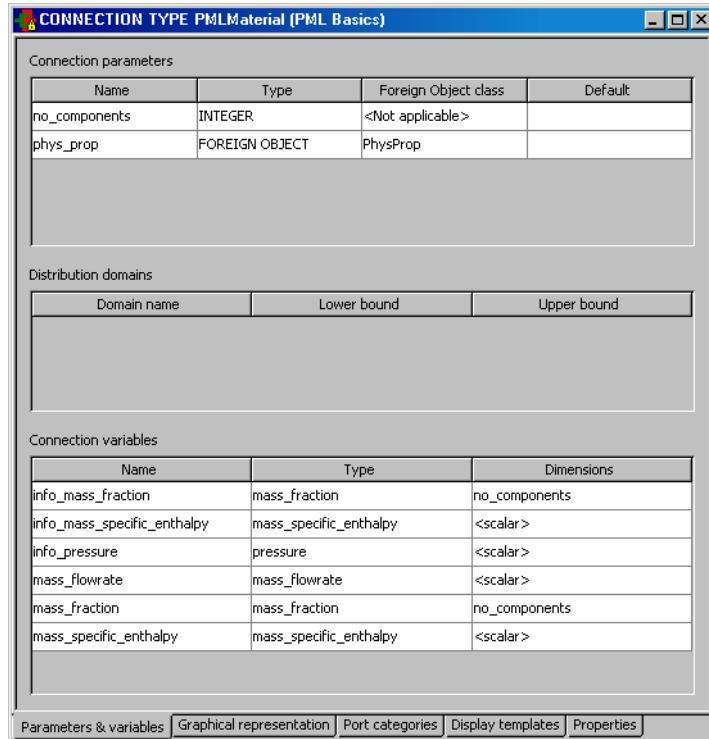
- A declaration of a set of Parameters, Distribution domains and Variables; these are identical to those that are declared in Models.
- A Graphical representation.
- Connectivity rules to allow and forbid connections between Ports of different categories.

- A Display template which specifies how any connection based on this Connection Type appears in results stream tables.

A connections to or from a Unit is made from its Model Port. Model Ports are associated with a Connection Type and all the quantities declared by the Connection Type are automatically included in the Model that declares the Port.

When a connection between two Ports is made in a flowsheet Model; all the Variables, Parameters and Distribution domain are equated.

Figure 1.2. The PMLMaterial Connection Type from the gPROMS Process Model Library - Parameters and Variable declaration tab



When developing gPROMS Models you can either use existing Connection Types such as those that are found in the gPROMS Process Model Library (PML) or you can define your own Connection Types.

Models

See also: Defining a gPROMS Model

A Model provides a description of the physical behavior of a given system in the form of mathematical equations: a gPROMS process model will contain at least one Model. Each Model contains the following information (defined in each of its associated tabs):

- A gPROMS Language declaration: a Model's gPROMS Language tab is where the mathematical equations are provided along with the declaration of the quantities (such as Parameters and Variables) that appear in these equations.
- A Public Interface: a Model interface consists of an icon, Model port declarations and a Specification dialog. The interface captures information explaining how to use the Model within composite or flowsheet Models and to aid in making Model specifications.
- A topology: the topology tab is used for the graphical construction of flowsheet Models. On the topology tab you can drag and drop existing component Models and equate their Model Ports by making graphical connections. Note that these connections are of course represented in the gPROMS language tab as mathematical equations.

gPROMS Language declaration for Models

The gPROMS Language Tab in the Model entity comprises a number of sections, each containing a different type of information regarding the system being Modelled. The minimal information that needs to be specified in any Model is the following:

- A set of constant *Parameters* that characterise the system. These correspond to quantities that will *never* be calculated by any simulation or other type of calculation making use of this Model. Therefore, their values must always be specified before the simulation begins and remain unchanged thereafter. They are declared in the PARAMETER section.
- A set of *Variables* that describe the time-dependent behaviour of the system. These may be specified in later sections or left to be calculated by the simulation. They are declared in the VARIABLE section.
- A set of *Equations* involving the declared Variables and Parameters. These are used to determine the time-dependent behaviour of the system. They are declared in the EQUATION section.

The structure of a simple Model declaration in the gPROMS language is the following:

PARAMETER

... *Parameter declarations* ...

VARIABLE

... *Variable declarations* ...

EQUATION

... *Equation declarations* ...

The general structure that a Model entity may have is shown below.

Please note that the SET, ASSIGN, INITIAL and INITIALSELECTOR sections are also part of a Process and that there are both advantages and disadvantages in using these sections in a Model. This is discussed at the example of Parameter settings for composite Models.

PARAMETER

... *Parameter declarations* ...

DISTRIBUTION_DOMAIN # For distributed Models

... *Distribution domain declarations* ...

UNIT

... *Sub-Model declarations* ...

PART

... *PART declarations* ...

PARTSET

... *PARTSET declarations* ...

Variable

... *Variable declarations* ...

```
SET
... PARAMETER value settings ...

BOUNDARY # For distributed Models
... Boundary conditions for partial differential equations ...

TOPOLOGY
... Equations defining the connection of sub-Models ...

EQUATION
... Equation declarations ...

ASSIGN
... Degrees of freedom assignment ...

PRESET
... PRESET specifications ...

INITIALSELECTOR
... Initial SELECTOR specifications ...

INITIAL
... Initial conditions specifications ...
```

Tasks

See also: Defining a Task

A Task is a Model of an operating procedure. An operating procedure can be considered as a recipe that defines periods of undisturbed operation *along with* specified or conditional external disturbances to the system.

A Process Entity defines an operating procedure for a process model; this is done either with explicit statements in the Process entity or by invoking one or more generic Tasks (or indeed some combination of the two). So typically, a Task defines part of the operating procedure for a whole Process.

A Task

- can be re-used multiple times during a dynamic simulation
- is associated with one or more Models and thus can be used on different Model instances (Units) based on the same Model
- can invoke other Tasks and thus complex operating procedures can be defined in a hierarchical manner.

gPROMS language declaration for Tasks

A Task is defined by three sections: Task Parameter declarations, (optional) Task Variable declarations and a Schedule where the Task's operating procedure is expressed in terms of the Task Parameters and Variables.

Overall, the structure of a Task definition is the following:

```

PARAMETER
... Parameter declarations ...

VARIABLE
... Local Variable declarations ...

SCHEDULE
... Schedule declaration ...

```

Task Parameters may be of any of the following types:

- INTEGER, REAL or LOGICAL constants. These are used to Parameterise a Task with respect to, for instance, controller tuning Parameters, event durations etc.
- INTEGER_EXPRESSION, REAL_EXPRESSION or LOGICAL_EXPRESSION. These are used to parameterise a Task with respect to, for instance, logical conditions for the conditional and iterative structures etc.
- Model. These are used to parameterise a Task with respect to the actual Models on which it acts.

The purpose of Parameters in a Task is to defines the number and type of arguments that a Task accepts as arguments and enables one to write generic reusable tasks. All Task Parameters must be given a value whenever the Task is invoked.

Task Variables are the equivalent of local subroutine Variables and as such are calculated by the Task. They should not be confused with Model Variables and are NOT associated with Variable Types instead they are declared to be of type INTEGER or REAL.

The Schedule section defines the part of the operating procedure implemented by the Task. It is similar to the Schedule section in Processes, the only difference being that it has access to the local Variables declared in the Variable section. The values of the latter can be manipulated by using assignment statements.

Figure 1.3. An example Task used to define change in heat input to the Flash drum Model from the gPROMS Process Model Library

```

1 PARAMETER
2 Drum          AS MODEL Flash_drum
3 Ramp_Time     AS REAL
4 New_Heat_Input AS REAL
5
6
7 SCHEDULE
8   SEQUENCE
9     RESET
10    Drum.input_energy_rate := OLD(Drum.input_energy_rate)
11      + (New_Heat_Input - OLD(Drum.input_energy_rate))
12      * (TIME-OLD(TIME))/Ramp_Time ;
13  END
14  CONTINUE FOR Ramp_Time
15  RESET
16    Drum.input_energy_rate := OLD(Drum.input_energy_rate);
17  END
18 END

```

Processes

See also: Defining a gPROMS Process

A Model can usually be used to study the behaviour of the system under many different circumstances. Each such specific situation is called a *simulation activity*. The coupling of Models with the particulars of a dynamic simulation activity is done in a Process Entity. A Process performs two key roles

- to *instance* a generic Model: this is done by providing specifications for all the Model's Parameters, Input Variables (degrees of freedom), Selectors and Initial Conditions that have not been given values directly in the Model. Any specifications given in Specification dialogs from the topology of a flowsheet Model will appear as un-editable text in the Process Entity
- to define an operating procedure [5] for a process model in the form of a Schedule; a Schedule may simply specify the execution of an undisturbed simulation for a period of time to a more complex scenario such as Modelling the start-up of a complex Process with multiple external disturbances to the system. Complex operating policies will usually make use of Tasks. *Steady-State* simulations require no Schedule.

Solver configuration information for all Model based activities is also specified in Process entities.

gPROMS language for Processes

gPROMS Language declaration for Processes

A gPROMS Project may contain multiple Processes, each corresponding to a different simulation activity (e.g. simulation of system startup, simulation of system shutdown, steady state operation, etc.). A Process is partitioned into sections, each containing information required to define the corresponding dynamic simulation activity:

UNIT

... *Declaration of Model instances*

MONITOR

... *Variable path patterns*

SET

... *Parameter value settings* ...

ASSIGN

... *Degrees of freedom assignment* ...

PRESET

... *PRESET specifications* ...

INITIALSELECTOR

... *Initial SELECTOR specifications* ...

INITIAL

... *Initial conditions specifications* ...

SOLUTIONPARAMETERS

... *Model based activity solver specifications* ...

SCHEDULE

... *Operating procedure specifications* ...

Saved Variable Sets

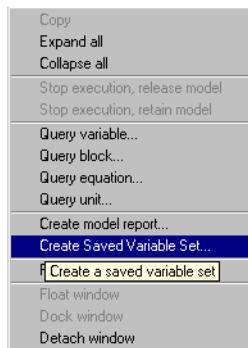
The values of all Model Variable and Selectors at a particular simulation time can be saved for later re-use; these values are stored in *Saved Variable Sets*.

Saved Variable Sets are used

- to provide good initial guesses for initialisation calculations (over-riding the default values for the Variables taken from their Variable Type). This is done in the PRESET section.
- during a simulation to change the values of the Variables and Selectors to those stored in the Saved Variable Set.

Saved Variable Sets are created from a simulation activity either

- using the SAVE elementary task in a Schedule
- right clicking on the Execution Window and selecting Create Saved Variable Set from the short-cut menu.
Note that this is only possible if a license was retained following the execution of the simulation activity:



Any new *Saved Variable Set* created during a simulation activity will be stored in the Results folder of the Execution Case. In order to use it in any subsequent activity the *Saved Variable Set* must be copied into the working project where it will appear in the *Saved Variable Sets* entity group.

Figure 1.4. An example of a Saved Variable Set

SAVED VARIABLE SET column_start (PML Distillation Separation Example)

```

# PROCESS DISTILLATION_COLUMN saved at simulation time 0.000
# The total number of variables in the process
2520
# Note: all variables are saved
# Index : PathName : Value : LowerBound : UpperBound : Type : Units
  1 : PLANT.BOTTOM_PRODUCT.IN.MASS_FRACTION(1) : 1.883279201264309E-001 : -1.00000E-010 : 1.00
  2 : PLANT.BOTTOM_PRODUCT.IN.MASS_FRACTION(2) : 8.116720798735690E-001 : -1.00000E-010 : 1.00
  3 : PLANT.BOTTOM_PRODUCT.IN.MASS_FLOWRATE : 0.000000000000000E+000 : -1.00000E+020 : 1.00000
  4 : PLANT.BOTTOM_PRODUCT.IN.INFO_PRESSURE : 8.00000000000000E+005 : 1.00000E+000 : 1.00000
  5 : PLANT.BOTTOM_PRODUCT.IN.INFO_MASS_SPECIFIC_ENTHALPY : -2.204967486751637E+006 : -1.00000
  6 : PLANT.BOTTOM_PRODUCT.IN.MASS_SPECIFIC_ENTHALPY : -2.40620342307823E+006 : -1.00000E+020
  7 : PLANT.BOTTOM_PRODUCT.IN.INFO_MASS_FRACTION(1) : 9.99999999999998E-002 : -1.00000E-010 :
  8 : PLANT.BOTTOM_PRODUCT.IN.INFO_MASS_FRACTION(2) : 8.99999999999999E-001 : -1.00000E-010 :
  9 : PLANT.BOTTOM_PRODUCT.MASS_FRACTION(1) : 1.00000000000000E-001 : -1.00000E-010 : 1.00010
 10 : PLANT.BOTTOM_PRODUCT.MASS_FRACTION(2) : 9.00000000000000E-001 : -1.00000E-010 : 1.00010
 11 : PLANT.BOTTOM_PRODUCT.PRESSURE : 8.00000000000000E+005 : 1.00000E+000 : 1.00000E+020 : P
 12 : PLANT.BOTTOM_PRODUCT.MASS_SPECIFIC_ENTHALPY : -2.204967486751637E+006 : -1.00000E+020 :
 13 : PLANT.BOTTOM_PRODUCT.NORMALISED_MASS_FRACTION(1) : 9.99999999999998E-002 : -1.00000E-01
 14 : PLANT.BOTTOM_PRODUCT.NORMALISED_MASS_FRACTION(2) : 8.99999999999999E-001 : -1.00000E-01
 15 : PLANT.BOTTOM_PRODUCT.TEMPERATURE : 3.00000000000000E+002 : 1.00000E+001 : 5.00000E+004
 16 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.MASS_FRACTION(1) : 7.50000000000000E-001 : -1.00000E-0
 17 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.MASS_FRACTION(2) : 2.50000000000000E-001 : -1.00000E-0
 18 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.MASS_FLOWRATE : 0.00000000000000E+000 : -1.00000E+020
 19 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.INFO_PRESSURE : 8.00000000000000E+005 : 1.00000E+000 :
 20 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.INFO_MASS_SPECIFIC_ENTHALPY : -1.386242243136098E+006 :
 21 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.MASS_SPECIFIC_ENTHALPY : -1.386242243136098E+006 : -1.0
 22 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.INFO_MASS_FRACTION(1) : 7.50000000000000E-001 : -1.00000E-0
 23 : PLANT.COLUMN.TOP_PRODUCT_PUMP.IN.INFO_MASS_FRACTION(2) : 2.50000000000000E-001 : -1.00000E-0
 24 : PLANT.COLUMN.TOP_PRODUCT_PUMP.FLOW.SIGNAL : 0.00000000000000E+000 : -1.00000E+200 : 1.0
 25 : PLANT.COLUMN.TOP_PRODUCT_PUMP.OUT.MASS_FRACTION(1) : 7.50000000000000E-001 : -1.00000E-0
 26 : PLANT.COLUMN.TOP_PRODUCT_PUMP.OUT.MASS_FRACTION(2) : 2.50000000000000E-001 : -1.00000E-0
 27 : PLANT.COLUMN.TOP_PRODUCT_PUMP.OUT.MASS_FLOWRATE : 0.00000000000000E+000 : -1.00000E+020
 28 : PLANT.COLUMN.TOP_PRODUCT_PUMP.OUT.INFO_PRESSURE : 8.00000000000000E+005 : 1.00000E+000

```

gPROMS language Properties

Chapter 2. Declaring Variable and Connection types

Variable Types are an essential requirement for all gPROMS process models as **all** Variables in a gPROMS Model *must* be associated with a Variable Type.

In a similar way all Model Ports must be associated with a Connection Type.

When developing gPROMS Models you can either use existing Variable or Connection Types, such as those that are found in the gPROMS Process Model Library (PML), or you can define your own:

- Declaring new Variable Types
- Declaring new Connection Types

Declaring Variable Types

Variable Types appear under the first entry in the Project tree. In order to create your own Variable Types; you can *either* select New entity.... from the Entity menu - choosing Variable Type as the Entity type (see also: Entities) or if you open an existing Variable Type it is possible to edit the Variable Types table, shown below, by typing the name in the <new> row and pressing *enter*.

Once the Variable Type has been introduced to the table the following information should be provided

- A *default value* for Variables of this type. This value will be used as an initial guess for any iterative calculation involving Variables of this type, unless it is overridden for individual Variables or a better guess is available from a previous calculation.
- *Upper and lower bounds* on the values of Variables of this type. Any calculation involving Variables of this type must give results that lie within these bounds. These bounds can be used to ensure that the results of a calculation are physically meaningful. Again, these bounds may be overridden¹ for individual Variables of this type.
- An optional *unit of measurement*. Users are encouraged to provide this in order to aid Model readability.

Figure 2.1. An example Variable Types table

Name	Lower bound	Default value	Upper bound	Units
Length	0.0	1.5	100.0	m
Mass	0.0	1.0	100000.0	kg
MassFlowrate	0.0	0.1	100000.0	kg/s

The values of the lower bounds, initial values and upper bounds are checked for consistency (i.e. you cannot enter an initial value outside the bounds or enter a lower bounds greater than the upper bound).

Declaring Connection Types

Connection Types are declared using a multi-tab forms-based editor. Each of the four principal tabs allows you to declare different aspects of the Connection Type:

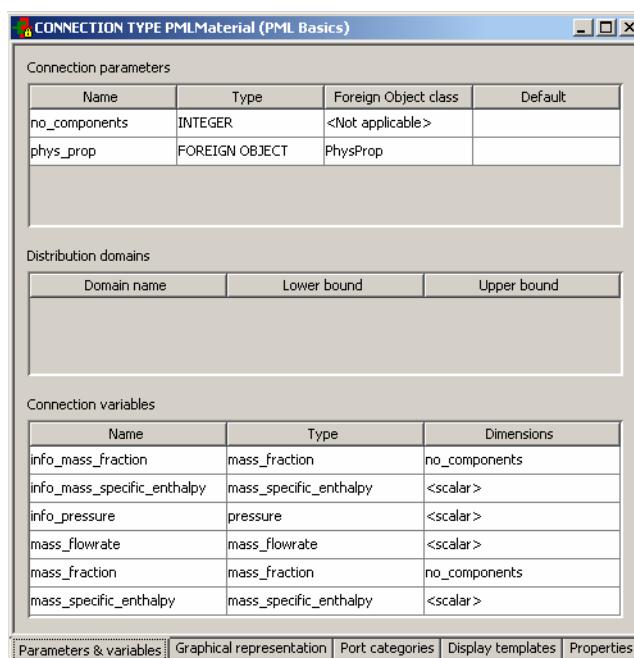
¹It is possible to override the bounds on certain Variables. This is done using in PRESET section of the Process entity.

- Parameters & Variables tab
- Graphical representation tab
- Port categories tab
- Display templates tab

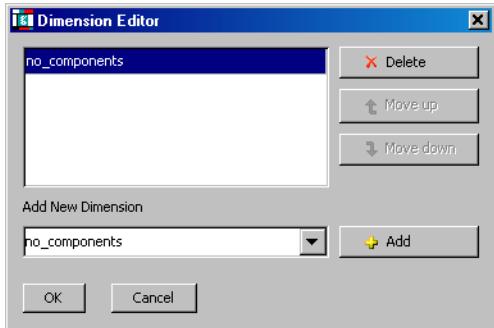
The Parameters and Variables tab

To declare quantities for a Connection Type simply double click on the cells labeled <**new**> and enter the name of the quantity. You can then enter information pertaining to Parameters, Distribution Domains and Variables - these are identical to those that are declared in Models.

Figure 2.2. The PMLMaterial Connection type - the Parameters and Variables Tab.



- For Parameter declarations, a *Type* - Integer, Real or ForeignObject - must be provided.
 - If ForeignObject is selected then a class can also be provided.
 - For Integer and Real Parameters it is also possible to provide a default value.
- For Distribution Domain declarations, lower and upper bounds must be provided.
- For Variable declarations, a Variable Type must be provided; this should be selected from a drop-down list of all Variable Types declared in this Project (or cross-referenced Projects). The Connection Type can include scalar and Array Variables:
 - To define the dimensionality of the Array click on the <**scalar**> cell to access the Dimension Editor.
 - In the Add New Dimension box either select an Integer Parameter that has been declared in this Connection Type or type in a *literal* value (e.g. 7).
 - It is possible to declare multiple dimensioned Variables by Adding more than one Dimension - multiple dimensions can be ordered using the Move Up and Move Down buttons

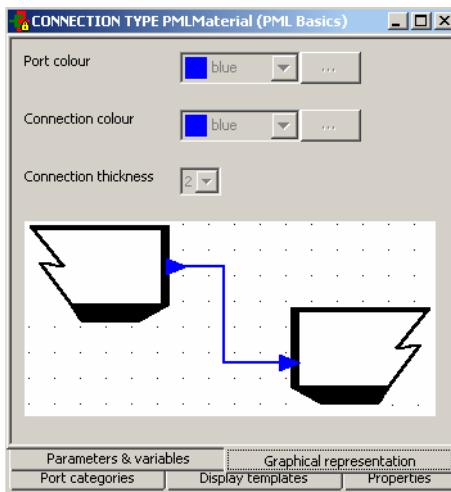


The Graphical representation tab

Connections between different Units in a flowsheet Model are associated with a Connection Type. Such connections are displayed graphically on the flowsheet Model's topology tab - the graphical representation of such connections is determined by its Connection Type.

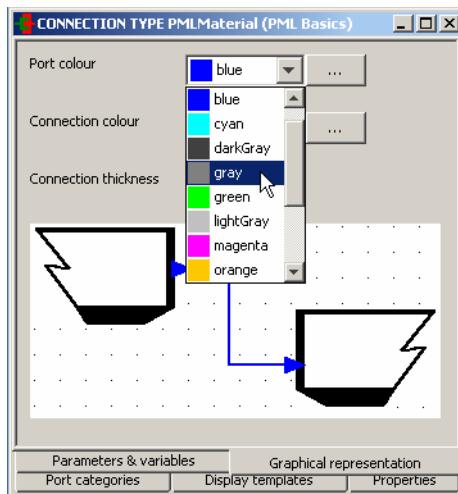
The information provided on the *graphical representation* tab determines the colour of the Ports and of the connectivity line, as well as the line thickness.

Figure 2.3. Connection Type - *Graphical Representation* tab



To change colours of Ports or Connectivity lines, the user has the option of selecting a predefined colour from a drop-down list (as shown below).

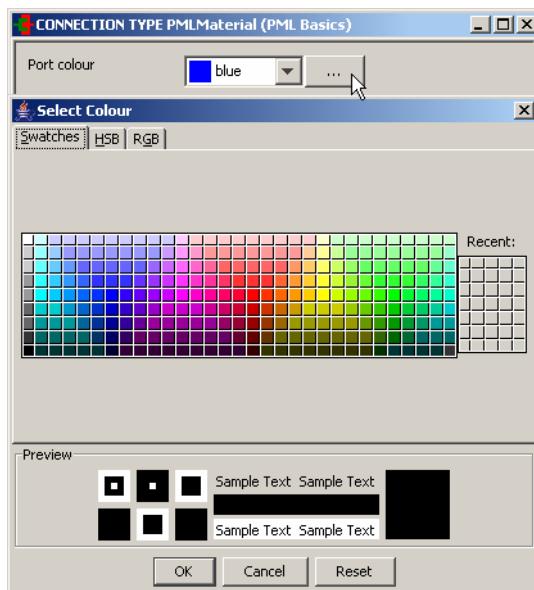
Figure 2.4. Choosing predefined colours for Ports (or Connections).



Alternatively, the user is able to define custom colours by doing the following:

1. Click on the ... button
2. Use either Swatches, HGB or RGB to define the exact colour you want
3. When finished, click OK to select the chosen colour.

Figure 2.5. Defining custom colour for ports or connections.



The Port categories tab and Connectivity rules

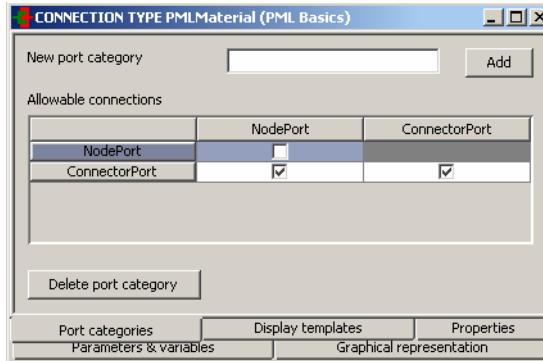
gPROMS enforces a number of rules to ensure that only valid connections can be made when building flowsheet Models, and as such all Ports must be defined as an *Inlet*, an *Outlet* or a *Bi-directional* Port. When defining a Model Port the developer must specify which of these categories the Port belongs to and gPROMS enforces the rules shown in the following table (e.g. it is possible to connect an *Outlet* Port to an *Inlet* Port but not an *outlet* to an *outlet*):

Table 2.1. Enforced connectivity rules

	Inlet	Outlet	Bi-directional
Inlet	Disallowed	Allowed	Allowed
Outlet	Allowed	Disallowed	Allowed
Bi-directional	Allowed	Allowed	Allowed

In addition, for a particular Connection Type, it is possible to define an additional set of rules by defining new user-specified categories. The gPROMS Process Model Library (PML) makes use of this capability: in the PML a Port must be either a *Node* or a *Connector* with *Node-to-Node* connections forbidden (see also: Understanding the PML):

Figure 2.6. The PMLMaterial Connection type in the gPROMS PML - Port categories



To define new connectivity rules; simply enter each of the categories by providing each with a name and clicking Add. Then specify whether a particular connection is valid by *checking* the appropriate box in the *Allowable connections* table: leaving the box *unchecked* means that the connection is not valid.

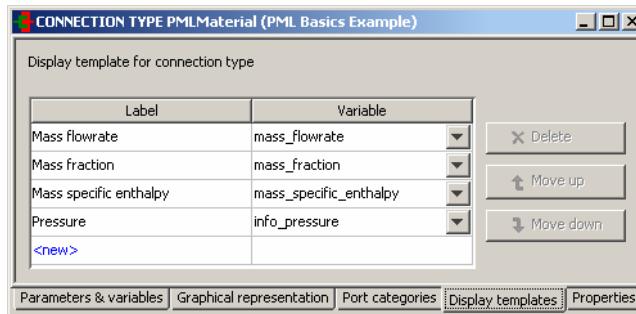
If you wish to delete a particular Port category, then simply click on its name in the *Allowable connections* table and then click on the Delete port category button at the bottom of the window.

The Display templates tab

The *Display templates* tab enables you to define which of the Variables carried by the Connection Type should appear in results *stream tables*.

On this tab you provide a label for each of the Variables that should be displayed in the stream table and the order in which the quantities should appear in the table. Note that only those quantities that appear on the *Display templates* tab will appear in stream tables.

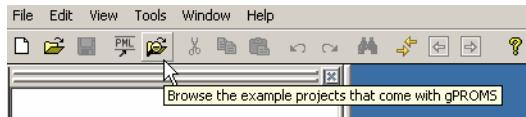
Figure 2.7. Connection Type - Display templates tab



To enter information, simply click on the relevant cells that contain *<new>* and then select a Variable from the drop-down list. Re-order the table as desired using the Move up and Move down buttons.

Chapter 3. Defining Models and Processes

The development of a basic gPROMS process model is explained by reference to the gPROMS Project Buffer Tank.gPJ that can be found in the installation. You can access this by clicking on the Browse Examples button on the gPROMS Toolbar and then navigating to "General capabilities\Other examples\Buffer Tank.gPJ".



An illustrative buffer tank example is used to demonstrate the following:

- Defining Models
 - the gPROMS language to enter Model Equations
 - how to declare the Parameters and Variables that appear in these Equations
- Defining Processes
 - how to set values for Model Parameters
 - how to specify the values of Model Variables to satisfy the degrees of freedom
 - how to provide initial values for the *state* (differential) Variables

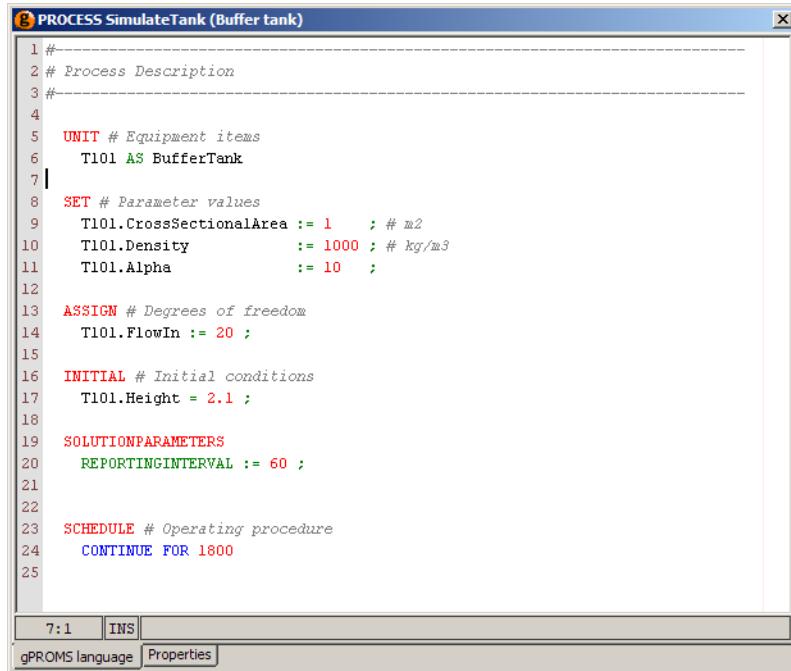
Note: to create your own Model and Process Entities; select New entity....from the Entity menu - choosing Model or Process as the Entity type (see also: Entities).

Figure 3.1. The Buffer Tank Model entity

A screenshot of the gPROMS Model Editor window. The title bar says 'MODEL BufferTank (buffer_tank)'. The main area contains the following code:

```
1  PARAMETER
2      Density          AS REAL
3      CrossSectionalArea AS REAL
4      Alpha            AS REAL
5
6  VARIABLE
7      HoldUp           AS Mass
8      FlowIn, FlowOut   AS MassFlowrate
9      Height            AS Length
10
11 EQUATION
12
13     # Mass balance
14     $HoldUp = FlowIn - FlowOut ;
15
16     # Relation between liquid level and holdup
17     Holdup = CrossSectionalArea * Height * Density ;
18
19     # Relation between pressure drop and flow
20     FlowOut = Alpha * SQRT ( Height ) ;
```

The bottom of the window shows a status bar with '4:32' and buttons for 'INS', 'Interface', 'Topology', 'gPROMS language', and 'Properties'.

Figure 3.2. The Buffer Tank Process entity.


```

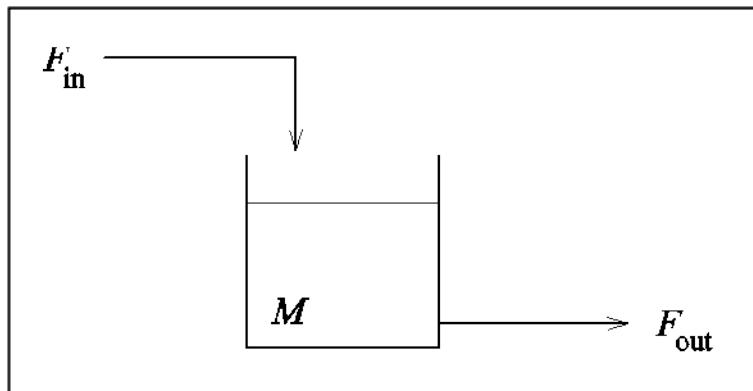
1 #
2 # Process Description
3 #
4
5 UNIT # Equipment items
6 T101 AS BufferTank
7
8 SET # Parameter values
9   T101.CrossSectionalArea := 1      ; # m2
10  T101.Density        := 1000     ; # kg/m3
11  T101.Alpha          := 10       ;
12
13 ASSIGN # Degrees of freedom
14   T101.FlowIn := 20 ;
15
16 INITIAL # Initial conditions
17   T101.Height = 2.1 ;
18
19 SOLUTIONPARAMETERS
20   REPORTINGINTERVAL := 60 ;
21
22
23 SCHEDULE # Operating procedure
24   CONTINUE FOR 1800
25

```

7:1 INS
gPROMS language Properties

An illustrative buffer tank example

Buffer Tank.gPJ describes a simple buffer tank with gravity-driven outflow (see the figure below). It is a good choice for illustrating the main features of the gPROMS language because it comprises only one simple unit operation, for which a *primitive* model can be constructed. Primitive models are mathematical models that are completely specified in terms of explicitly declared variables and equations. They usually correspond to simple unit operations or parts thereof. Primitive models form the building blocks for the construction of higher-level, composite model of complex unit operations or entire process flowsheets.

Figure 3.3. Buffer tank with gravity-driven outflow.

The dynamic mathematical model of the buffer tank process takes the following form:

Equation 3.1. Mass balance

$$\frac{dM}{dt} = F_{in} - F_{out}$$

Equation 3.2. Relation between liquid level and holdup

$$\rho Ah = M$$

Equation 3.3. Characterisation of the output flowrate

$$F_{\text{out}} = \alpha \sqrt{h}$$

Here, M and h are the mass and level of liquid in the tank, and F_{in} and F_{out} are the inlet and outlet flowrates respectively. ρ , A and α denote the density of the liquid material, the cross-sectional area of the tank and the outlet valve constant, respectively. For the purposes of this example, these last three quantities are assumed to be known constants.

Defining a gPROMS Model

In gPROMS, Model Entities are the central part any process model. A working gPROMS Project will contain (or reference) at least one Model:

A Model is defined as a set of quantities and mathematical equations that, when coupled with a set of specifications, describe the behaviour of a given system.

The gPROMS language declaration for a basic Model will typically consist of three parts¹:

- PARAMETER declarations
- VARIABLE declarations
- EQUATION declarations

Figure 3.4. gPROMS Language definition for a Buffer Tank Model.

```

MODEL BufferTank (buffer_tank)
1  PARAMETER
2    Density      AS REAL
3    CrossSectionalArea AS REAL
4    Alpha        AS REAL
5
6  VARIABLE
7    HoldUp       AS Mass
8    FlowIn, FlowOut   AS MassFlowrate
9    Height        AS Length
10
11 EQUATION
12
13  # Mass balance
14  $HoldUp = FlowIn - FlowOut ;
15
16  # Relation between liquid level and holdup
17  Holdup = CrossSectionalArea * Height * Density ;
18
19  # Relation between pressure drop and flow
20  FlowOut = Alpha * SQRT ( Height ) ;
21

```

The PARAMETER section

The Parameter section is used to declare the parameters of a Model. Parameters are time-invariant quantities that will *not*, under any circumstances, be the result of a calculation. Quantities such as physical constants (π , R , etc.), Arrhenius coefficients and stoichiometric coefficients usually fall into this category. In the buffer tank process, ρ , A and α were assumed constant and are thus declared as parameters of the Buffer Tank Model:

PARAMETER

¹A Model may contain more parts. A comprehensive overview can be found in gPROMS Language declaration for Models..

```
Rho          AS REAL
CrossSectionalArea AS REAL
Alpha        AS REAL
```

Each parameter has a unique name (identifier) by which it can be referenced (for example, in expressions). Identifiers in the gPROMS language start with a letter (a–z and A–Z) and may comprise letters, numbers (1–9) and underscores (_). The gPROMS language is *not* case sensitive, i.e. Temp and TEMP are considered to be identical.

Each parameter is also declared to be of a certain type (e.g. INTEGER, LOGICAL or REAL). All three parameters of the Buffer Tank Model are of type REAL.

Parameter declarations may optionally include the assignment of default values. For instance:

```
PARAMETER
  NoComp      AS INTEGER
  NoReactions AS INTEGER DEFAULT 1
```

Finally, note that the categorisation of certain quantities as Parameters is sometimes tenuous. Designating a quantity as a Parameter has the advantage of reducing the total number of Variables in a model. However, this quantity can no longer be treated as an unknown in any future use of the model. Consider, for instance, the quantities that characterise the size and geometry of a vessel. From the point of view of dynamic simulation, these can be viewed as Parameters. However, from the point of view of steady-state design calculations performed with the same model, these quantities may be considered unknowns under certain circumstances. It may, therefore, be better to classify them as Variables.

The VARIABLE section

The VARIABLE section is used to declare the Variables of a Model. All quantities that are calculated in Model Equations must be declared as Model Variables. For instance, in the example process, M , h , F_{in} and F_{out} are variables of the Buffer Tank Model:

```
VARIABLE
  HoldUp       AS Mass
  FlowIn, FlowOut AS MassFlowrate
  Height        AS Length
```

Like Parameters, Variables are always Real continuous numbers. All Variables must be given a type, however, Variable Types are *user-defined* (see also: Declaring Variable Types).

The EQUATION section

The EQUATION section is used to declare the equations that determine the time trajectories of the variables already declared in the VARIABLE section.

The gPROMS language is purely declarative. That is, the order in which the equations are declared is of no importance. Simple equations are equalities between two real expressions (see the figure below). These expressions may comprise:

- Integer or real constants (e.g. 2, 3.14159, etc.).
- Parameters that have been declared in the PARAMETER section (e.g. Rho, Alpha, PI, etc.).
- Variables that have been declared in the VARIABLE section (e.g. HoldUp, Height, FlowOut, etc.). The special symbol \$ preceding a variable name denotes the derivative with respect to time of that variable (e.g. \$HoldUp etc.).

Figure 3.5. Buffer tank Model

```

1  PARAMETER
2    Density          AS REAL
3    CrossSectionalArea AS REAL
4    Alpha            AS REAL
5
6  VARIABLE
7    HoldUp           AS Mass
8    FlowIn, FlowOut   AS MassFlowrate
9    Height           AS Length
10
11 EQUATION
12
13  # Mass balance
14  $HoldUp = FlowIn - FlowOut ;
15
16  # Relation between liquid level and holdup
17  Holdup = CrossSectionalArea * Height * Density ;
18
19  # Relation between pressure drop and flow
20  FlowOut = Alpha * SQRT ( Height ) ;
21

```

The screenshot shows a software window titled "gPROMS MODEL BufferTank (buffer_tank)". The main area contains the gPROMS code for a buffer tank model. The code includes declarations for parameters (Density, CrossSectionalArea, Alpha), variables (HoldUp, FlowIn, FlowOut, Height), and equations (mass balance, relation between liquid level and holdup, relation between pressure drop and flow). The interface at the bottom shows tabs for "Interface", "Topology", "gPROMS language" (which is selected), and "Properties".

Similarly to most programming languages, expressions are formed by combining the above operands with the arithmetic operators + (addition), - (subtraction), * (multiplication), / (division) and ^ (exponentiation), as well as built-in intrinsic functions (e.g. square root: SQRT()). The latter are described in greater detail in Intrinsic Functions in gPROMS.

Intrinsic functions have the highest precedence priority, followed by the ^ operator and then the division and multiplication operators. The addition and subtraction operators have the lowest precedence. Naturally, parentheses may be used to alter these precedence rules as required.

Finally, note that comments can be added to clarify the contents of the Model where needed. As shown in the figure above, gPROMS accepts two types of comments. One type begins with # and extends to the end of the current line. The other type starts with { and ends with } and may span multiple lines. Moreover, comments of this type may be nested within one another.

Defining a gPROMS Process

In the gPROMS language a Model is used to define the physical behaviour of a system and it usually contains PARAMETER, VARIABLE and EQUATION declarations. A model can usually be used to study the behaviour of the system under many different circumstances. Each such specific situation is called a *simulation activity*. The coupling of Models with the particulars of a dynamic simulation activity is done in a Process.

A gPROMS Project may contain multiple PROCESSES, each corresponding to a different simulation activity (e.g. simulation of plant startup, simulation of plant shutdown, etc.). Each such PROCESS must be given a different name and these will be automatically placed in alphabetical order in the gPROMS Project tree. A PROCESS is partitioned into the following key sections:

- The UNIT section
- The SET section
- The ASSIGN section
- The INITIAL section
- The SOLUTIONPARAMETERS section
- The SCHEDULE section

The gPROMS Language definition for the entire PROCESS (named SimulateTank) for a dynamic simulation activity involving the buffer tank process is shown in the figure below.

Figure 3.6. An example Process for the buffer tank.

```

1 #
2 # Process Description
3 #
4
5 UNIT # Equipment items
6   T101 AS BufferTank
7
8 SET # Parameter values
9   T101.CrossSectionalArea := 1      ; # m2
10  T101.Density          := 1000    ; # kg/m3
11  T101.Alpha            := 10      ;
12
13 ASSIGN # Degrees of freedom
14   T101.FlowIn := 20 ;
15
16 INITIAL # Initial conditions
17   T101.Height = 2.1 ;
18
19 SOLUTIONPARAMETERS
20   REPORTINGINTERVAL := 60 ;
21
22
23 SCHEDULE # Operating procedure
24   CONTINUE FOR 1800
25

```

7:1 INS
gPROMS language Properties

The UNIT section

The first item of information required to set up a dynamic simulation activity is the process equipment under investigation. This is declared in the UNIT section of a PROCESS.

Equipment items are declared as instances of Models. For example

```
UNIT
  T101 AS BufferTank
```

creates an instance of MODEL BufferTank, named T101. T101 is described by the variables declared within the BufferTank Model and its time-dependent behaviour is partially determined by the corresponding equations.

The SET section

Before an instance of a Model can actually be used in a simulation, all its parameters must be specified (unless they have been given default values). This is done in the SET section of a PROCESS.² For example,

```
SET
  T101.Rho           := 1000 ; # kg/m3
  T101.CrossSectionalArea := 1      ; # m2
  T101.Alpha          := 10      ;
```

sets the parameters of T101 to appropriate values. Note that:

- in order to refer to parameter Rho of instance T101 of Model BufferTank, we use the *pathname notation* T101.Rho

²The specification of parameter values can also be performed within Models, using a SET section that is completely equivalent to the one described here. However, it is generally advisable that parameters be set at the PROCESS level. This practice maximises the reusability of the underlying Models and minimises the probability of error.

- It is recommended that you use pathname completion to help construct full and valid pathnames correctly; this is available within all entities in gPROMS. Semantic errors, such as referencing a quantity in a lower-level Model that doesn't exist, are only detected when a Model based activity is executed.
- It is also common, particularly for composite Models, to use the WITHIN construct to complete pathnames
- Parameter values are set using the assignment operator (`:=`). In other words, the arithmetic expression appearing on the right hand side is first evaluated; its value is then given to the parameter appearing on the left hand side. This is another general rule of the gPROMS language:

A General Rule of the gPROMS Language

gPROMS always uses the symbol `:=` to *assign* a value or expression appearing on the right hand side to the *single* identifier appearing on the left hand side. gPROMS always uses the symbol `=` to declare the *equality* of the two general expressions appearing on either side of this symbol.

The ASSIGN section

The set of equations resulting from the instantiation of Models declared in the UNIT section is typically under-determined. This simply means that there are more variables than equations. The number of *degrees of freedom* in the simulation activity is given by:

$$\text{Number of degrees of freedom } (N_{DOF}) = \text{Number of variables} - \text{Number of equations.}$$

For the simulation activity to be fully defined, N_{DOF} variables must be specified as either constant values or given functions of time. Variables specified in this way are the input variables (or "inputs") of this simulation activity. The remainder of the variables are the *unknown* variables, the time variation of which will be determined by the solution of the system equations. Clearly, the number of unknowns is equal to the number of available equations - we therefore have a "square" system of equations.

The specification of input variables is provided in the ASSIGN section of the PROCESS³. For instance,

```
ASSIGN  
T101.Fin := 20 ;
```

designates the inlet flowrate as an input and assigns it a constant value of 20. Again, in order to emphasise the assignment form of these specifications, input specifications use the assignment operator (`:=`).

The inlet flowrate may not be constant but may vary with the simulation time, for instance by linearly increasing

```
ASSIGN  
T101.Fin := 20 + 1.2*TIME ;
```

In this example, the built-in function TIME is used to reference the value of the simulation time. Please note that the value of the simulation time depends on the chosen units of measurement.

TIME can be used with any of gPROMS' built-in functions, for instance in order to create a sinusoidal oscillation:

```
ASSIGN  
T101.Fin := 20 + SIN(TIME) ;
```

The INITIAL section

Before dynamic simulation can commence, consistent values for the system variables at $t = 0$ must be determined. To this end, a number of additional specifications are needed. These augment the system of equations that describe

³The specification of degrees of freedom can also be performed within Models, using an ASSIGN section that is completely equivalent to the one described here. However, it is generally advisable that variables be assigned at the PROCESS level. This practice maximises the reusability of the underlying Models and minimises the probability of error.

the behaviour of the system and result in a square system of equations at $t = 0$. The solution of the latter provides the condition of the system at $t = 0$.

Traditionally, the term "initial condition" refers to a set of values for the differential variables at $t = 0$. However, gPROMS follows a more general approach where the initial conditions are regarded as additional equations that hold at $t = 0$ and can take any form. This, of course, allows for the traditional specification of "initial values" for the differential variables or, indeed, for any appropriate subset of system variables; however, it also makes possible the specification of much more general initial conditions as equations of arbitrary complexity.

The **INITIAL** section is used to declare the initial condition information pertaining to a dynamic simulation activity. For instance,

```
INITIAL  
T101.Height = 2.1 ;
```

specifies an initial condition for the buffer tank system by stating that the height of liquid in the tank at $t = 0$ is 2.1m. Note that, in contrast to the **SET** and **ASSIGN** sections, the equality operator (=) is used here to emphasise the fact that initial conditions are general equations.⁴

An initial condition that is frequently employed for the dynamic simulation of process systems is the assumption of steady-state, constraining the time derivatives of the differential variables to zero. In gPROMS, this can be achieved by manually specifying all derivatives to be zero:

```
INITIAL  
T101.$Holdup = 0 ;
```

However, this would be tedious for models with large numbers of differential variables, so the keyword **STEADY_STATE** may be utilised to specify this initial condition, as shown below:

```
INITIAL STEADY_STATE
```

In this latter case, no further specifications are required.

The SOLUTIONPARAMETER section

The user also has the option to control various aspects of model-based activities carried out in gPROMS such as solver settings and output specifications. The **SOLUTIONPARAMETERS** section is used for this purpose. Detailed information regarding this topic will be covered in more detail in Numerical Solver Parameters.

For example,

```
SOLUTIONPARAMETERS  
REPORTINGINTERVAL := 60 ;
```

The **REPORTINGINTERVAL** is the interval at which result values will be collected during the dynamic simulation (note that it does **not** effect the accuracy of the subsequent integration in any way). For this example, an interval of 60 is a reasonable choice. The **REPORTINGINTERVAL** may be over-ridden from the simulation execution dialog.

The user does not need give any settings in this section. In such a case the user will be prompted to enter a **REPORTINGINTERVAL** in a dialog box.

The SCHEDULE section

Information on the external manipulations (e.g. known disturbances) that are to be simulated is provided in the **SCHEDULE** section of the **PROCESS**. We restrict our attention to the simplest possible case, allowing the system to operate without any external disturbance over a specified period of time. This is achieved via the:

⁴The specification of initial conditions can also be performed within Models, using an **INITIAL** section that is completely equivalent to the one described here. However, it is generally advisable that initial conditions be specified at the **PROCESS** level. This practice maximises the reusability of the underlying Models and minimises the probability of error.

CONTINUE FOR *TimePeriod*

construct in the SCHEDULE section of the PROCESS.

gPROMS can be used to simulate much more complex cases, including detailed operating procedures of entire plants: see Defining Schedules and Defining Tasks.

Chapter 4. Arrays

The gPROMS language provides some advanced mechanisms for the declaration of complex equation structures in Models.

In many cases, a number of Parameters, Variables or Equations that appear in a Model are closely related. Examples include:

- the stoichiometric coefficients, ν_{ij} , of a set of components $i=1,\dots,NoComp$ participating in a set of reactions $j=1,\dots,NoReact$;
- the concentrations, C_i , of components $i=1,\dots,NoComp$ in a multi-component system;
- the equations expressing the conservation of components $i=1,\dots,NoComp$ in a multi-component system.

In such cases, we need effective mechanisms for declaring and handling these entities as a group rather than individually. In a manner similar to most high-level programming languages, gPROMS achieves this aim via the use of *arrays*.

We must consider

- Declaring arrays of Parameters, Variables, Selectors and Units
- Rules for referring to array elements and array expressions
- Using arrays in equations

Declaring arrays in Models

Arrays are used in many places during Model construction

- Declaring arrays of Parameters
- Declaring arrays of Variables
- Declaring arrays of Selectors
- Declaring arrays of Units in Composite Models

In all these cases

- Arrays can have any number of dimensions.
- The size of each dimension can be a general integer expression involving a combination of:
 - integer constants;
 - scalar integer Model Parameters;
 - individual elements of arrays of integer Model Parameters;
 - integer arithmetic operators - these include the usual arithmetic operators +, -, *, and ^, as well as the integer division operator DIV and the division remainder operator MOD.
- The index of each dimension ranges from 1 to the size of dimension, with the exception of zero-length Arrays.

Declaring arrays of Parameters in Models

Model Parameters are declared in the Parameter section of gPROMS Models to belong to the basic types INTEGER or REAL. Such Parameters may be scalars or arrays of one, two or more dimensions. Consider, for instance, the Parameter section in a model of a liquid-phase continuous stirred tank reactor (CSTR). This is shown in the gPROMS code below.

Example 4.1. Parameter section of a liquid-phase CSTR Model

```
# MODEL LiquidPhaseCSTR

PARAMETER

    # Number of components
    NoComp AS INTEGER

    # Number of reactions
    NoReact AS INTEGER

    # Component molar densities
    Rho      AS ARRAY(NoComp) OF REAL

    # Stoichiometric coefficient of component i in reaction j
    Nu       AS ARRAY(NoComp,NoReact) OF REAL    DEFAULT 0

    # Order of component i in reaction j
    Order    AS ARRAY(NoComp,NoReact) OF REAL    DEFAULT 0
```

Here, NoComp and NoReact denote the numbers of chemical components and chemical reactions occurring in this system. Each of these is a simple (scalar) INTEGER Parameter. On the other hand, the densities of the pure components form a vector of real quantities declared as an array of length NoComp:

```
Rho AS ARRAY(NoComp) OF REAL
```

For the purposes of this example, the pure component densities are assumed to be constant but different to each other.

Similarly, Nu and Order are two-dimensional arrays of REAL Parameters. The number of elements in the first dimension is NoComp; the number of elements in the second dimension is NoReact. We note that, if a DEFAULT value is specified for an array Parameter, this is taken to refer to *all* elements of that array.

Declaring arrays of Variables in Models

Arrays of Model Variables are declared in a manner very similar to that used for Parameters. For example, the Variable section of the liquid-phase CSTR Model entity is shown in the gPROMS code below.

Example 4.2. Variable section of a liquid-phase CSTR Model

```
# MODEL LiquidPhaseCSTR

PARAMETER
  ...

VARIABLE

# Input and output molar flowrates
Flow_In, Flow_Out AS MolarFlowrate

# Liquid phase volume
V           AS Volume

# Component molar holdups
HoldUp       AS ARRAY(NoComp) OF Moles

# Input and output component mole fractions
X_In, X_Out    AS ARRAY(NoComp) OF MoleFraction

# Component concentrations
C           AS ARRAY(NoComp) OF Concentration

# Reaction rates
Rate        AS ARRAY(NoReact) OF ReactionRate
```

Arrays of Parameters and Variables may have any number of dimensions. The number of elements in each dimension is specified in terms of an integer expression (e.g. HoldUp AS ARRAY(NoComp+1) OF REAL is acceptable). The total number of elements in an array is the product of the number of elements in each dimension.

Declaring arrays of Selectors in Models

As with Variables and Parameters, arrays of Selectors may also be defined (see The Case conditional construct for an introduction to Selectors), as shown in the example below.

Example 4.3. Arrays of Selectors

```
# MODEL LiquidPhaseCSTR

PARAMETER
  NoDiscs AS INTEGER
  ...

VARIABLE
  ...

SELECTOR
  DiscFlag      AS ARRAY(NoDiscs) OF (Intact, Burst) DEFAULT Intact
```

Declaring arrays of Units in Composite Models

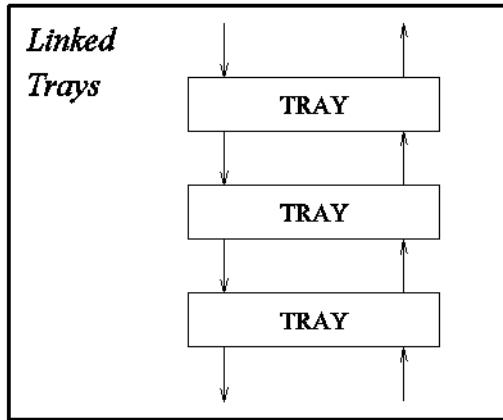
As with Variables and Parameters, arrays of Units may also be defined (see Composite Models). The figure below illustrates a potential use of this feature in the definition of a Model for a series of distillation column trays.

Figure 4.1. Model for a series of linked trays.

```
# MODEL LinkedTrays

PARAMETER
    NoTrays AS INTEGER
    ...
    ...

UNIT
    Stage      AS ARRAY(NoTrays) OF Tray
```



Here, the higher-level Model `LinkedTrays` contains an array, called `Stage`, of instances of Model `Tray`. The Parameters and Variables within these instances can be referenced by combining the pathname and array notations. For instance, an equation within the `LinkedTrays` model may refer to the Variable:

`Stage(1).LiquidHoldup`

Also, an equation may employ the Variable:

`Stage(TopSection.NoTrays DIV 2).T`

referring to the temperature at the middle tray of the top section of the column.

Referring to array elements

The contents of an array may be referenced in several different ways (consider the declarations given below:)

- Entire arrays can be referenced by using their names alone. For instance, `Rho` denotes the entire array of component molar densities.
- Individual elements can be referenced by using the name of the array and an index to the element in question enclosed in brackets. For one-dimensional arrays, this index should be an integer expression. For instance, the second element of array `Rho` is `Rho(2)` while the element of array `HoldUp` before the last is `HoldUp(NoComp-1)`. For multi-dimensional arrays, the index is a list of such expressions, one for each dimension. Thus, `Nu(2,4)` refers to the element on the second row and fourth column of array `Nu`.
- A subset of the elements in one or more dimensions can be referenced through the use of 'slice' notation. For instance, `Holdup(2:4)` refers to the 2nd, 3rd and 4th elements of array `Holdup`. `Nu(2:4,3:5)` refers to the slice of array `HoldUp` included between rows 2 to 4 and columns 3 to 5 (a 3×3 array in itself). Naturally, `Nu(1:NoComp,1:NoReac)` is equivalent to `Nu`. Similarly, `Nu(1:1,3:3)` is equivalent to `Nu(1,3)`.
- An entire dimension of an array can be referenced by leaving a blank. For instance, `Nu(2,)` refers to the entire second row of array `Nu`, while `Nu(,1:3)` refers to columns 1 to 3. Naturally, `Nu(,,)` is equivalent to `Nu`.

```
PARAMETER
# Number of components
NoComp AS INTEGER

# Number of reactions
NoReact AS INTEGER

# Component molar densities
Rho      AS ARRAY(NoComp) OF REAL

# Stoichiometric coefficient of component i in reaction j
Nu       AS ARRAY(NoComp,NoReact) OF REAL    DEFAULT 0

VARIABLE
# Component molar holdups
HoldUp      AS ARRAY(NoComp) OF Moles
```

General rules for array expressions

A powerful concept in gPROMS is that of array expressions. Consider, for example, the algebraic expression:

$x * y + w * z$

If x , y , w and z are scalar Variables, then the above also corresponds to a scalar. However, in gPROMS, the expression $x * y + w * z$ is valid even if x , y and z are arrays provided they have the same dimensionality and size. For example, if we have the declarations:

```
PARAMETER
n, m      AS INTEGER

VARIABLE
x, y, z   AS ARRAY (n,m) OF SomeQuantity
w          AS SomeQuantity
```

then the expression $x * y + w * z$ also represents a two-dimensional array of size $n \times m$, the (i,j) th element of which is equal to $x_{ij}y_{ij} + wz_{ij}$ for $i=1,\dots,n$ and $j=1,\dots,m$.

Although in the above examples, the gPROMS interpretation of the array expression coincided with the standard mathematical one, this is not always the case. For example, the expressions $x * y / z$ and $w / x + z ^ y$ are also valid in gPROMS, representing two-dimensional arrays of size $n \times m$, the (i,j) th elements of which are equal to $x_{ij}y_{ij}/z_{ij}$ and $w/x_{ij} + z_{ij}^{y_{ij}}$ respectively.

In general, consider an expression $x \oplus y$ where x and y are scalar or array expressions, and \oplus is a binary arithmetic operator ($+$, $-$, $*$, $/$, $^$). This is a valid gPROMS expression if and only if it conforms to one of the four cases listed below:

Case	x	y	Dimensionality of $x \oplus y$	Interpretation of $x \oplus y$
1	Scalar	Scalar	Scalar	$x \oplus y$
2	Array	Scalar	Same as x	$x_{ijk\dots} \oplus y$
3	Scalar	Array	Same as y	$x \oplus y_{ijk\dots}$
4	Array	Array	Same as x and y	$x_{ijk\dots} \oplus y_{ijk\dots}$

Clearly, case 4 is valid only if both x and y have exactly the same dimensionality and size.

The above rules can be applied recursively to check the validity and to interpret expressions of arbitrary complexity. At the lowest level, x and y will be (scalar) constants, scalar Parameters or Variables, or arrays of Parameters or Variables, or slices of arrays of Parameters or Variables. For example, it can be verified that the following is a valid two-dimensional expression of size 3×2 :

```
3.23 / x(1:3, 4:5) * z(5:7, 1:2) + w(10:12, 2:3) + 4.13
```

Using arrays in equations

Elements of arrays (both Parameters and Variables) can be used in Equations as if they were individual Parameters or Variables. For example, the equation that defines the concentration of component 2 in the liquid-phase CSTR can be written as follows:

```
HoldUp(2) = C(2) * V ;
```

However, arrays can be used more effectively to declare several equations simultaneously (i.e. for all components). This can be done in two different ways:

- implicitly :gPROMS automatically expands the equation
- explicitly :using the FOR construct

Writing implicit array equations

We have seen how array expressions can be formed by combining arrays of Parameters or Variables, or elements or slices of these. By analogy, gPROMS allows the definition of array equations of the form:

Expression E = Expression F;

that are valid provided they conform to one of the following four cases:

Case	E	F	Dimensionality of E = F	Interpretation of E = F
1	Scalar	Scalar	Scalar	$E = F$
2	Array	Scalar	Same as E	$E_{ijk\dots} = F$
3	Scalar	Array	Same as F	$E = F_{ijk\dots}$
4	Array	Array	Same as E and F	$E_{ijk\dots} = F_{ijk\dots}$

Thus, in view of the following Variable definitions:

```
PARAMETER
  ...
VARIABLE
  # Liquid phase volume
  V           AS Volume

  # Component molar holdups
  HoldUp      AS ARRAY(NoComp) OF Moles

  # Component concentrations
  C           AS ARRAY(NoComp) OF Concentration
  ...
```

the following is a valid equation:

```
HoldUp = C * V ;
```

gPROMS automatically expands such equations into an set of equations. For example, if NoComp = 5, the above will expand to:

```
HoldUp(1) = C(1) * V ;
HoldUp(2) = C(2) * V ;
...
HoldUp(5) = C(5) * V ;
```

Writing explicit array equations using the FOR construct

We have seen how array equations can be written in an implicit manner by exploiting the array expression capability of gPROMS. An alternative is to write array equations explicitly using a FOR construct that is similar to that provided by most high-level programming languages. Thus, consider the equation describing the conservation of component i in a multi-component buffer tank. This can be written mathematically as:

$$\frac{dM_i}{dt} = F^{in}x_i^{in} - F^{out}x_i, \quad i = 1, \dots, NoComp$$

In gPROMS, this can be written in two completely equivalent ways, namely implicitly, in the form:

```
$M = Fin*Xin - Fout*X ;
```

or explicitly, in the form:

```
FOR i := 1 TO NoComp DO
    $M(i) = Fin*Xin(i) - Fout*X(i) ;
END
```

The above are completely equivalent: which one you use depends entirely on your preference. However, situations do exist in which the required equations cannot be described via implicit declaration, and the use of explicit FOR constructs is essential.

The counter of a FOR construct (e.g. i in the above example) is an integer quantity that may be referenced only by equations enclosed within the construct. The range of this counter must be specified in terms of any arithmetic expressions involving integer constants, integer Parameters and/or integer arithmetic operators. Moreover, a step increment may be specified. For instance,

```
FOR i := NoComp+1 TO 2*NoComp STEP 2 DO
    ...
END
```

will start by assign i a values of $NoComp+1$ and then will increment it by 2 until it exceeds $2*NoComp$. If no increment is specified, its value defaults to 1. A FOR construct may enclose an arbitrary number of equations of any type -- including other For constructs. This allows nesting of For constructs to arbitrary depth; in such cases:

- each FOR construct must use a different name for its counter variable;
- any expression that appears within each For construct (including those defining its range and increment) may involve the counters of any enclosing For constructs.

Zero-Length Arrays

For dynamic Arrays (i.e. Arrays whose bounds are set by an expression involving other Parameters), it is possible to set the length of the Array to zero¹. This is useful for two reasons:

- Greater modelling power and flexibility

¹In principle, one could also set the length to zero explicitly, but this would be pointless!

Suppose we wish to create a simulation of a flowsheet containing a reactor and a mixer. The ability to set Arrays to zero length means that we may use the same model for both the reactor and mixer. The *NoReact* Parameter can be set to zero for the mixer instance, causing the model to revert to a mixer. This is because any equations indexed over an Array of zero length are completely omitted from the Model instance, as are any terms indexed over the Array. This means that the equations defining the rates of reaction, reaction constants and the rate terms in the material and energy balance equations are all omitted, resulting in a smaller, more efficient formulation.

- More flexibility when defining flowsheet Topologies

Zero length Arrays mean that Models with dynamic Ports can be used without having to have at least one connection.

Chapter 5. Intrinsic gPROMS functions

Intrinsic gPROMS functions are used in equations to perform mathematical operations that would be difficult or even impossible to declare using normal language operators. The gPROMS language contains two categories of intrinsic functions, namely:

- Vector intrinsic functions - that take a single argument (scalar or array) and return a result of same dimensionality as the input.
- Scalar intrinsic functions - that take multiple arguments (scalar or array) and return a scalar result.

Vector intrinsic functions

All vector intrinsic functions have the following characteristics:

- they take a single argument representing a scalar or array expression;
- they return a result of dimensionality and size identical to those of their argument.

The table below lists all vector functions that are recognised by gPROMS.

Table 5.1. Vector intrinsic functions

Identifier	Function
ACOS	The arccosine (in radians) of the argument
ASIN	The arcsine (in radians) of the argument
ATAN	The arctangent (in radians) of the argument
ABS	The absolute value of the argument
COS	The cosine of the argument (in radians)
COSH	The hyperbolic cosine of the argument
EXP	The exponential of the argument
INT	The largest integer that does not exceed the argument
LOG	The natural logarithm of the argument
LOG10	The logarithm to base 10 of the argument
SGN	The sign of the argument
SIN	The sine of the argument (in radians)
SINH	The hyperbolic sine of the argument
SQRT	The square root of the argument
TAN	The tangent of the argument (in radians)
TANH	The hyperbolic tangent of the argument

The result of each of the above functions is obtained by applying the corresponding operation to each element of the argument. For example, consider the declarations:

```
PARAMETER
  n, m      AS  INTEGER
```

VARIABLE

```
x, y, z    AS ARRAY (n,m) OF SomeQuantity
w           AS           SomeQuantity
```

Then, $x * SQRT(y+w) / SIN(z)$ is a valid expression representing an $n \times m$ array, the $(i,j)^{th}$ element of which is equal to:

$$\frac{x_{ij}\sqrt{y_{ij}+w}}{\sin z_{ij}}$$

for $i=1,..,n$ and $j=1,..,m$.

Scalar intrinsic functions

All scalar intrinsic functions have the following characteristics:

- they take an arbitrary number of arguments, each representing a scalar or array expression;
- they return a scalar result.

The table below lists all scalar functions that are recognised by gPROMS.

Table 5.2. Scalar intrinsic functions

Identifier	Function
SIGMA	The sum of all elements of all arguments
PRODUCT	The product of all elements of all arguments
MIN	The smallest of all elements of all arguments
MAX	The largest of all elements of all arguments

The use of scalar intrinsic functions provides a powerful mechanism for writing complex mathematical expressions in gPROMS. However, some care is necessary in their use with array equations written using automatic expansion. Consider, for instance, a mixing tank receiving a number of multi-component input streams. The conservation equation for component i can be written mathematically as:

$$\frac{dM_i}{dt} = \sum_{k=1}^{NoInput} F_k^{in} x_{k,i}^{in} - F_{out} x_i, \quad i = 1,..,NoComp$$

In gPROMS, this can be written as:

```
FOR i := 1 TO NoComp DO
  $M(i) = SIGMA(Fin*Xin(1:NoInput,i)) - Fout*X(i) ;
END
```

Note that the 'alternative' formulation using automatic expansions:

```
$M = SIGMA(Fin*Xin) - Fout*X ;
```

is actually incorrect since:

- the expression `Fin*Xin` violates the conformance rules for array expressions;
- the expression `SIGMA(Fin*Xin)` is a scalar, not a vector of length `NoComp`.

A complete model for the mixing tank, illustrating many of the important points highlighted above, is given in the gPROMS code below.

Example 5.1. Multi-component mixing tank Model entity

```
# MODEL MixingTank

PARAMETER
  NoComp, NoInput      AS INTEGER
  CrossSectionalArea  AS REAL
  Rho                  AS ARRAY(NoComp) OF REAL
  ValvePosition        AS REAL

VARIABLE
  Fin                 AS ARRAY(NoInput) OF Flowrate
  Xin                AS ARRAY(NoInput,NoComp) OF MassFraction
  Fout               AS Flowrate
  X                  AS ARRAY(NoComp) OF MassFraction
  M                  AS ARRAY(NoComp) OF Mass
  TotalHoldup         AS Mass
  TotalVolume         AS Volume
  Height              AS Length

EQUATION

# Mass balance
FOR i := 1 TO NoComp DO
  $M(i) = SIGMA(Fin*Xin(,i)) - Fout*X(i) ;
END

# Mass fractions
TotalHoldup = SIGMA(M) ;

M = X * TotalHoldup ;

# Calculation of liquid level from holdup
TotalVolume = SIGMA(M/Density) ;

TotalVolume = CrossSectionalArea * Height ;

Fout = ValvePosition * SQRT ( Height ) ;
```

As an additional example, the gPROMS code below illustrates the use of nested FOR constructs to implement the matrix-matrix multiplication operation between matrices A ($n \times m$) and B ($m \times q$), resulting in a matrix C ($n \times q$).

Example 5.2. Matrix multiplication Model entity

```
# MODEL MatrixMultiplication

PARAMETER
  n, m, q      AS INTEGER

VARIABLE
  A      AS ARRAY (n, m) OF SomeQuantity
  B      AS ARRAY (m, q) OF SomeQuantity
  C      AS ARRAY (n, q) OF SomeQuantity

EQUATION
  FOR i := 1 TO n DO
    FOR j := 1 TO q DO
      C(i,j) = SIGMA(A(i,)*B(,j))
    END
  END
```

Chapter 6. Conditional Equations

The physical behaviour of many process operations is described in terms of *discontinuous* equations, the form of which depends on the current variable values and, in certain cases (e.g. involving hysteresis effects), also some aspects of the past history of the system.

gPROMS provides **two** powerful facilities for describing discontinuous equations in Model Entities. As background it helps to understand State-Transition Networks (STNs which form a general basis for modelling discontinuities:

- The CASE construct: this provides a direct description of general STNs in the gPROMS language. For example:

```
# An example of the CASE conditional construct - for flow over a weir.  
SELECTOR  
    WeirFlag AS (Above, Below)  
    ...  
EQUATION  
    ...  
CASE WeirFlag OF  
    WHEN Above : FlowOut = 1.84 * (Rho/MolecularWeight)  
        * WeirLength * ABS(Height-WeirHeight)^1.5 ;  
        SWITCH TO Below IF Height < WeirHeight ;  
    WHEN Below : FlowOut = 0 ;  
        SWITCH TO Above IF Height > WeirHeight ;  
END # Case  
...
```

- The IF construct may be used to described a special form of reversible symmetric STNs that occur very frequently in practical applications. For example:

```
# An example of the IF conditional construct - for flow over a weir.  
IF Height > WeirHeight THEN  
    FlowOut = 1.84 * (Rho/MolecularWeight)  
        * WeirLength * ABS(Height-WeirHeight)^1.5 ;  
ELSE  
    FlowOut = 0 ;  
END # If
```

It should be noted that, in Model entities, we are interested in discontinuities that arise because of the intrinsic behaviour of the system and not as a result of external discrete actions imposed on the system by its environment or its operators (e.g. the opening and closing of manual valves). See: *Defining Schedules*.

Using State-Transition Networks to model discontinuities

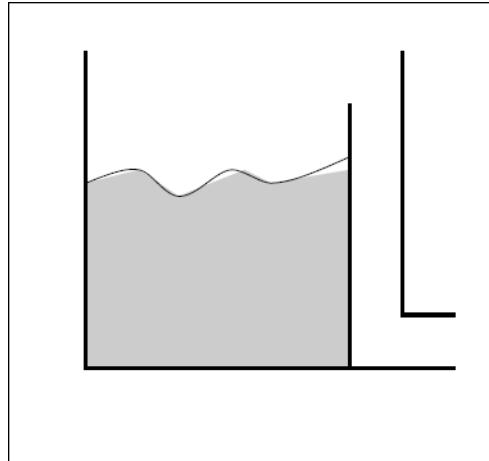
Discontinuities in the description of the physical behaviour of process systems may arise in different ways such as:

- transitions from laminar to turbulent flow;
- reversal of the direction of flow;
- appearance and disappearance of thermodynamic phases;
- equipment failure;

and many others.

State-Transition Networks (STNs) provide a general way of describing discontinuous systems. This concept is best introduced via an example. Consider the vessel depicted in the figure below. When the level of liquid in the vessel, h , is below the height of the weir, h_w , no outflow is observed. When, on the other hand, the liquid level exceeds the weir height, the rate of outflow is assumed to be proportional to $h - h_w$.

Figure 6.1. Vessel with overflow weir



The mathematical model of the transient behaviour of this system can be written as follows:

Mass balance

$$\frac{dM}{dt} = F_{\text{in}} - F_{\text{out}}$$

Calculation of liquid level in the tank

$$M = \rho Ah$$

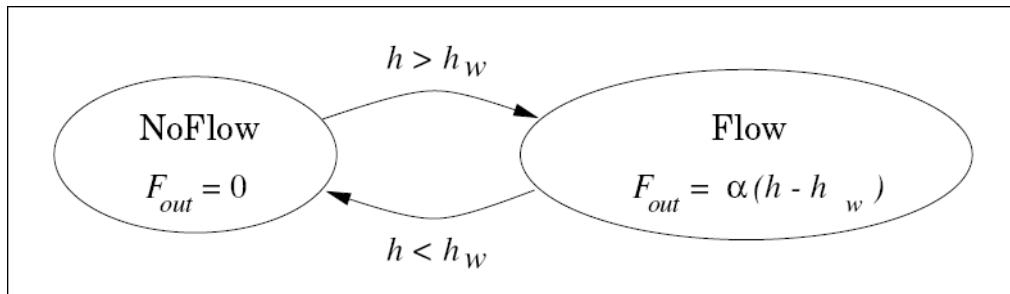
Characterisation of the output flowrate

$$F_{\text{out}} = \begin{cases} 0, & \text{if } h \leq h_w \\ \alpha(h - h_w), & \text{if } h > h_w \end{cases}$$

We note that two different sets of equations are needed to describe the behaviour of this system depending on whether the level of the liquid is above or below the weir. Thus, the system may exist in two distinct *states*, **Flow** and **NoFlow**, that correspond respectively to whether or not liquid flows over the weir. At any particular time, the system is in exactly one of these states. However, *transitions* from one state to the other will occur instantaneously if certain conditions are met. For example, if, while the system is in state **NoFlow**, the height of the liquid exceeds that of the weir, the system will instantaneously jump to state **Flow**. Conversely, if, while the system is in state **Flow**, the height of the liquid drops below that of the weir, the system will instantaneously jump to state **NoFlow**.

The above situation can be represented graphically in terms of an STN as shown in the figure below. The two circles (or ellipses) denote the two possible system states; for convenience, the form of the discontinuous equation (involving the characterisation of the output flowrate) in each of these states is also shown within these circles.

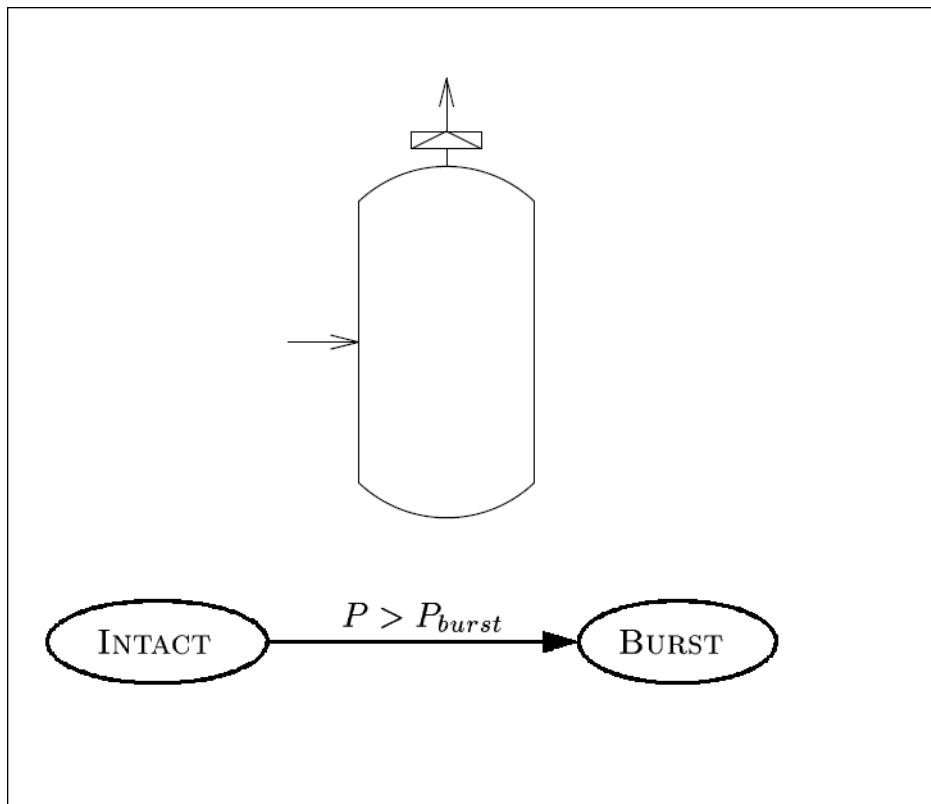
On the other hand, the mass balance and liquid level equations do not appear in this figure as their form is independent of the state the system is in. The transitions between the two states are also shown in figure as arrows connecting the corresponding circles. Again for convenience, each arrow is labelled with the logical condition that triggers the corresponding transition.

Figure 6.2. STN representation of vessel with overflow weir

The STN represents a *reversible, symmetric discontinuity* because:

- the system may jump from either of the two states to the other and,
- the logical condition for one the two transitions is the exact negation of that for the other.

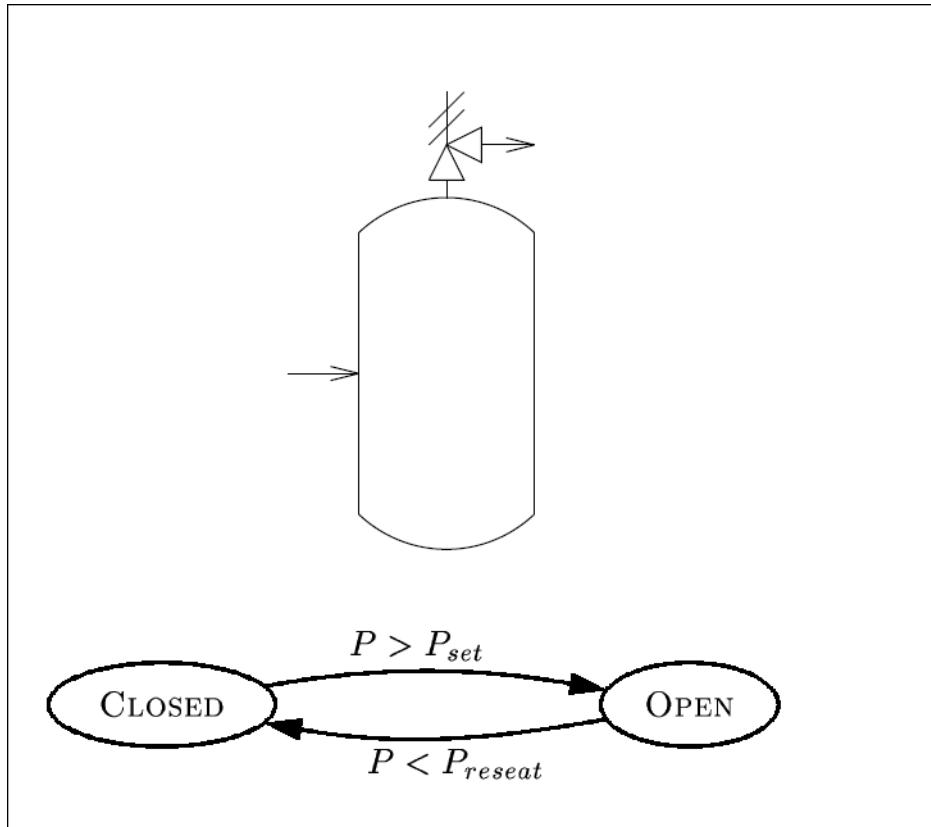
An example of a different type of discontinuity is shown in the figure below. Here, a vessel is fitted with a bursting disc. The disc can either be intact (with no gas flow from the vessel) or burst (with gas venting from the disc to the flare stack). This gives rise to two distinct system states (**Intact** and **Burst**). As in the previous example, some of the equations that describe the system take a different form in each of these states while some others remain unchanged. A transition from **Intact** to **Burst** occurs when the pressure in the vessel rises above the set pressure and the disc shatters. The resulting outflow of gas will then cause an reduction of the pressure which, eventually, may drop below its set value. However, the system cannot return to its **Intact** state once the disc has shattered - unless it is repaired as a result of an external action. Consequently, this is an example of an *irreversible discontinuity*.

Figure 6.3. Vessel with bursting disc

A final example is that of a vessel fitted with a safety relief valve (see figure below). The valve can be either open or closed, which again gives rise to two system states (**Open** and **Closed**). A transition from the **Closed** to the **Open** state occurs when the pressure in the vessel rises above the set pressure, while a transition from the **Open**

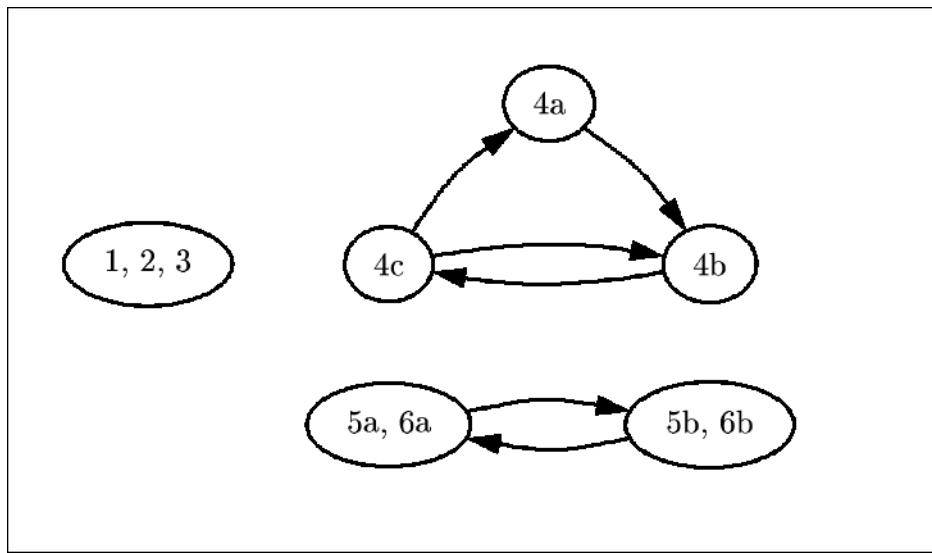
to the **Closed** state occurs when the pressure falls below a (lower) reset pressure. This is a *reversible, asymmetric discontinuity* because, although there are possible transitions in both directions, the two transition conditions are not the exact negation of each other.

Figure 6.4. Vessel with safety relief valve



We note that, in all three examples, only a subset of the model equations are directly related to the discontinuity and change from one state to another. The rest of the equations remain unchanged regardless of the state the system is in. Summarising, a discontinuity in the physical behaviour of a system gives rise to a number of possible system states. Naturally, at any given time, the system can be in exactly one of these states. Some of the equations that determine the behaviour of the system hold irrespective of the system state. However, some others take a different form in each state. Transitions between the different states take place when certain logical conditions are satisfied. A system may exhibit more than one physical discontinuity described by multiple STNs and/or more than two states within the same STN. For instance, a more detailed model of the weir vessel would seek to characterise the nature of the fluid flow in the outlet pipe. This would give rise to three system states, i.e. **Laminar**, **Turbulent** and **Choked**. A complex STN for a hypothetical system is depicted in the figure below. Here, the system exhibits two separate physical discontinuities involving three and two possible states respectively.

- Equations 1, 2 and 3 remain unaffected by the discontinuities and are valid throughout.
- Equation 4 is affected by the first discontinuity and is written as 4a, 4b or 4c, depending on the state of the system.
- Equations 5 and 6 are affected by the second discontinuity and are written as 5a, 5b and 6a, 6b in each of the two states respectively.

Figure 6.5. Hypothetical system model.

The Case conditional construct

The gPROMS example below illustrates the use of the CASE construct in a Model of a vessel with a bursting disc.

Example 6.1. Model entity for a vessel equipped with a bursting disc

```

# MODEL VesselWithDisc

PARAMETER
  R                      AS REAL  DEFAULT 8.314  # J/K.mol
  VesselVolume           AS REAL
  BurstPressure          AS REAL
  AtmPressure            AS REAL
  DiscConstant           AS REAL

VARIABLE
  FlowIn, FlowOut        AS MolarFlowrate
  ReliefFlow              AS MolarFlowrate
  HoldUp                 AS Moles
  T                       AS Temperature
  Pressure                AS Pressure

SELECTOR
  DiscFlag               AS (Intact, Burst) DEFAULT Intact

EQUATION
  # Mass balance
  $HoldUp = FlowIn - FlowOut - ReliefFlow ;

  # Ideal gas law
  Pressure * VesselVolume = Holdup * R * T ;

CASE DiscFlag OF
  WHEN Intact : ReliefFlow = 0 ;
    SWITCH TO Burst IF Pressure > BurstPressure ;
  WHEN Burst   : ReliefFlow = DiscConstant * SQRT(R*T) ;
END # Case

# Energy balance
: : : : : : : : : : : : : : : : : : : : :
```

We note that this Model presents two features of interest:

1. A SELECTOR section is used for the declaration of the system states that arise from the discontinuity:

```
  SELECTOR  
    DiscFlag AS (Intact, Burst) DEFAULT Intact
```

declares an enumerated ("selector") variable, DiscFlag that can take only two values, namely Intact or Burst, with the former being the default value at the start of the simulation (see below). The default specification is optional and may be omitted.

2. The Model equations include the CASE equation:

```

CASE DiscFlag OF
  WHEN Intact : ReliefFlow = 0 ;
                  SWITCH TO Burst IF Pressure > BurstPressure ;
  WHEN Burst   : ReliefFlow = DiscConstant * SQRT(R*T) ;
END # Case

```

that defines

- the equation(s) that hold in each state, and

- the logical condition(s) that trigger transitions between states.

More precisely, the above CASE construct states that:

- When the system is in the `Intact` state, the relief flow is zero. The system remains in this state as long as the pressure in the vessel is lower than the bursting pressure of the disc. When it exceeds that limit, a transition to the `Burst` state is initiated.
- When the system is in the `Burst` state, the relief flow is calculated from a sonic flow relationship. The form of the equation presented here is only for illustration purposes. A more detailed form would take account of various other effects, including the transition from sonic to sub-sonic flow as the pressure in the vessel decreases. As this is an irreversible discontinuity, there is no transition going back to the `Intact` state.

Some general considerations when using the Case construct

In general, a Case equation comprises two or more clauses, one for each possible value of the corresponding Selector variable. Each of the clauses comprises a list of equations, followed by an optional list of Switch statements that define transitions from the current clause to other clauses of the Case equation. The list of equations may include any combination of simple, array and even conditional equations - including not only Case constructs but also If constructs. The latter feature allows nesting of conditional equations to arbitrary depth. It is important, however, to observe the following restrictions:

- The number of equations in each clause of a Case construct must be the same.
- Each Selector variable may be used in *only one* Case construct.

The reason for the first restriction is obvious if one considers that the number of variables in the Model remains unaffected by the occurrence of transitions. Consequently, any change in the number of equations would lead to an over- or under-specified problem. The second restriction is imposed to avoid inconsistencies that might arise from different Case attempting to force the same Selector variable to switch to different values at the same time.

Initial values of Selector variables

Another important consideration concerning the use of Case equations is that, in order for a simulation experiment to commence, the initial (i.e. at time $t=0$) value of the corresponding Selector variable has to be specified. Thus, in our example the user must specify whether or not the disc is initially intact or not. This information cannot be inferred automatically by gPROMS: the mere fact that the initial system pressure is below the bursting value does not necessarily mean that the disc is intact - it may well have burst as a result of earlier operation! If a default value has been specified for the Selector variable in the Model, then this will be used as its initial value for the simulation. More generally, this value can be set or overridden for individual simulation experiments. This is done in the `INITIALSELECTOR` section of the Process (or Model). For instance:

```
UNIT T101 AS VesselWithDisc
...
INITIALSELECTOR
  T101.DiscFlag := T101.Burst ; # Disc is initially burst
INITIAL
  T101.Pressure - T101.BurstPressure = -1E5 ;
...
```

Thus, in this example, we specify the disc as being burst despite the fact that the initial pressure of the system is specified to be 1 bar below the bursting pressure. From the syntactical point of view, it is important to note the use of the full pathname `T101.Burst` to denote the value of the `SELECTOR` variable. A specification of the form:

```
UNIT T101 AS VesselWithDisc
...
SELECTOR
```

```
T101.DiscFlag := Burst ; # Disc is initially burst
```

would be meaningless as the identifier `Burst` is not known directly to the Process section - it is defined only within the context of MODEL `VesselWithDisc` of which T101 is an instance.

The If conditional construct

Case constructs provide a general way in which STNs of arbitrary complexity can be described in the gPROMS language. However, reversible and symmetric discontinuities are by far the most commonly encountered discontinuities in industrial processing systems. Although such discontinuities can be declared using Case constructs, gPROMS provides the alternative IF conditional construct specifically as a convenient shorthand for the declaration of this common type of discontinuity.

Example 6.2. Model entity for a vessel equipped with an overflow weir

```
# MODEL VesselWithWeir

PARAMETER
  Rho          AS REAL
  MolecularWeight AS REAL
  CrossSectionalArea AS REAL
  WeirHeight    AS REAL
  WeirLength    AS REAL

VARIABLE
  HoldUp       AS Mass
  FlowIn, FlowOut   AS MassFlowrate
  Height        AS Length

EQUATION
  # Mass balance
  $HoldUp = FlowIn - FlowOut ;

  # Calculation of liquid level from holdup
  Holdup = CrossSectionalArea * Height * Rho ;

  IF Height > WeirHeight THEN
    # Francis formula for flow over a weir
    FlowOut = 1.84 * (Rho/MolecularWeight)
              * WeirLength * ABS(Height-WeirHeight)^1.5 ;
  ELSE
    FlowOut = 0 ;
  END # If
```

The gPROMS example above demonstrates the use of an IF equation in the declaration of a Model for a vessel fitted with an overflow weir.

```
IF Height > WeirHeight THEN
  # Francis formula for flow over a weir
  FlowOut = 1.84 * (Rho/MolecularWeight)
            * WeirLength * ABS(Height-WeirHeight)^1.5 ;
ELSE
  FlowOut = 0 ;
END # If
```

A logical condition (in this case, `Liquid_Level > Weir_Height`) is used to choose between two clauses, each comprising a list of equations. If the logical condition is satisfied, the equations declared in the first clause are

included in the system model, otherwise the equations of the second clause are included. As with Case equations, the number of equations in each clause must be the same. As If equations are a special case of Case equations, there is always a Case equation that achieves the same result. For instance, the IF equation for the overflow weir is equivalent to the following CASE equation:

```
SELECTOR
  WeirFlag AS (Above, Below)
  ...
EQUATION
  ...
CASE WeirFlag OF
  WHEN Above : FlowOut = 1.84 * (Rho/MolecularWeight)
    * WeirLength * ABS(Height-WeirHeight)^1.5 ;
    SWITCH TO Below IF Height < WeirHeight ;
  WHEN Below : FlowOut = 0 ;
    SWITCH TO Above IF Height > WeirHeight ;
END # Case
...
```

A subtle difference between If and Case equations is that, in If equations, the initially active state of the system cannot be specified explicitly by the user. Instead, it is determined automatically by the initialisation calculation, which ensures that the consistent initial values obtained satisfy both the logical condition *and* the equations in this state. However, the solution of non-linear systems involving such conditional equations is far from trivial. Moreover, it is possible that a valid solutions exists in either clause of an If equation; in such cases, the solution found will depend on the initial guesses and the numerical method employed during the initialisation procedure. In view of these factors, it may sometimes be preferable to use a Case equation instead, especially if the initial state of the system is known *a priori*.

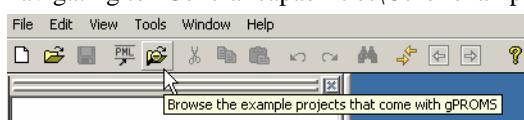
Chapter 7. Distributed Models

A significant number of unit operations in chemical or biochemical processes take place in distributed systems in which properties vary with respect to one or more spatial dimensions as well as time. For instance, a tubular reactor is described in terms of parameters and variables that, in addition to time, depend on the axial and radial position within the reactor (e.g. $T(z,r,t)$ etc). Other common examples of distributed unit operations include packed bed absorption, adsorption and distillation columns and chromatographic columns. In other unit operations, material properties are characterised by probability density functions instead of single scalar values. Examples include crystallisation units and polymerisation reactors, in which the size of the crystals and the length of the polymer chains respectively are described in terms of distribution functions. The form of the latter may also vary with both time and spatial position. In fact, most complex processes involve a combination of distributed and lumped unit operations. The equations that determine the behaviour of such unit operations are typically systems of integral, partial differential, ordinary differential and algebraic equations (IPDAEs).

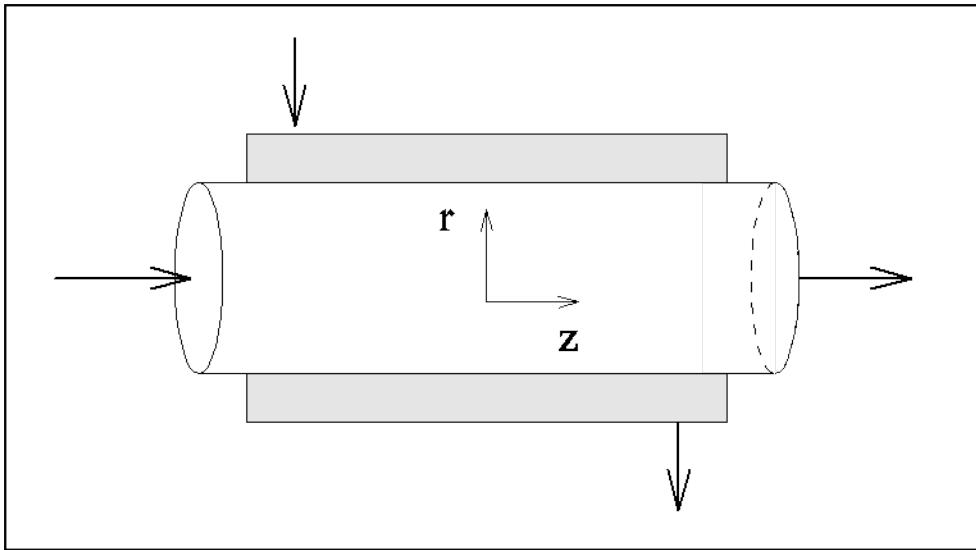
To develop a process model that considers distributed quantities we need to consider

- The definition of distributed Model entities
 - Declaring Distribution domains
 - Declaring Distributed Variables
 - Defining Distributed Equations
 - Introducing Partial Differential Equations
 - Introducing Integral Expressions
 - Explicit and implicit Distributed Equations
 - Providing Boundary conditions
- Requirements for specifying discretisation methods and non-uniform grids in Process entities.

Distributed modelling is explained by reference to the gPROMS Project tubular.gPJ that can be found in the installation. You can access this by clicking on the Browse Examples button on the gPROMS Toolbar and then navigating to "General capabilities\Other examples\tubular.gPJ".



The tubular model is illustrated in the figure below; which shows a tubular reactor used to carry out a liquid-phase exothermic chemical reaction. The intensive properties of the fluid in the tube vary with both axial and radial position as well as with time. The reactor is surrounded by a well-mixed cooling jacket. Thus, the intensive properties of the cooling medium are assumed to be uniform throughout the jacket but may still vary with time.

Figure 7.1. Tubular flow reactor

Declaring Distribution Domains

The temperature in the reactor varies with time, axial and radial position ($T(z,r,t)$). Although all Variables that are declared within a Model are automatically assumed to be functions of time, variations over other *distribution domains* (in this case the axial and radial domains, z and r respectively) have to be specified explicitly. Distribution domains are declared in the DISTRIBUTION_DOMAIN section of a Model. The gPROMS code below shows how two such domains called Axial and Radial are declared in a Model of a tubular reactor. The extents of both domains are specified in terms of two Model Parameters, namely ReactorLength and ReactorRadius, respectively.

Example 7.1. Parameter and DISTRIBUTION_DOMAIN sections for a Model of a tubular reactor

```
# MODEL TubularReactor

PARAMETER

    # Number of components
    NoComp          AS INTEGER

    # Geometrical parameters
    ReactorRadius,
    ReactorLength  AS REAL

    # Transport properties

    # Axial and radial mass diffusivities
    Dz, Dr          AS REAL

    # Axial and radial thermal conductivities
    Kz, Kr          AS REAL

    # Reaction

    # Stoichiometric coefficients
    Nu              AS ARRAY(NoComp) OF INTEGER

    ...

DISTRIBUTION_DOMAIN
    Axial   AS [ 0 : ReactorLength ]
    Radial  AS [ 0 : ReactorRadius ]

    ...
```

In general, the lower and upper bounds of the range of each Distribution Domain can be specified in terms of real expressions involving real constants and/or real parameters. Thus, the following are also valid Distribution Domain declarations:

```
# Normalised axial and radial domains
DISTRIBUTION_DOMAIN
    z AS [ 0 : 1 ]
    r AS [ 0 : 1 ]

# Axial domain encompassing the second half of the reactor
DISTRIBUTION_DOMAIN
    HalfAxial      AS [ ReactorLength/2 : ReactorLength ]
```

Declaring Distributed Variables

A Model may involve Variables with different degrees of distribution. For instance, in the tubular reactor example, the temperature of the fluid and the concentrations of the various chemical components within the tube are indeed functions of both the radial and axial positions. However, the wall temperature is a function only of axial position, while the temperature in the cooling jacket does not vary with spatial position at all. Note that all of these variables are also functions of time, as is always the case with Variables in gPROMS.

Example 7.2. Variable section for a Model of a tubular reactor

```
# MODEL TubularReactor

PARAMETER
  ...

DISTRIBUTION_DOMAIN
  ...

VARIABLE
  # Reactor temperature
  T AS DISTRIBUTION(Axial, Radial) OF Temperature

  # Concentrations
  C AS DISTRIBUTION(NoComp, Axial, Radial) OF Concentration

  # Feed composition
  Cin AS ARRAY(NoComp) OF Concentration

  # Cooling jacket temperature
  Tc AS Temperature

  ...

```

- Variable T, which represents the temperature in the reactor, is declared as a DISTRIBUTION over the two continuous domains, Axial and Radial.
- Variable C, representing the concentrations of the various components in the reactor, is clearly an array of variables distributed over both the radial and axial domains. In gPROMS, an array of distributions is represented by adding one or more extra domains to a Distribution. These domains are *discrete* in nature and they do not need to be declared explicitly in the DISTRIBUTION_DOMAIN section - a simple integer expression in the VARIABLE declaration suffices.
- For example, the concentration variable C ranges from 1 to NoComp, the number of components in the system), as well as over the two *continuous domains*, Axial and Radial.
- Variable Cin, representing the concentrations of the various components in the feed, is distributed over the discrete domain of components only. Although this could be written as:

```
Cin AS DISTRIBUTION(NoComp) OF Concentration
```

here we prefer to use the Array concept as it is more natural.

- Variable Tc, representing the temperature in the cooling jacket, is solely a function of time.

In essence, then, Distribution is a generalisation of the Array concept that allows a Variable to vary over both continuous and discrete domains. Conversely, an Array is a special case of a Distribution that is used to declare Variables that are distributed over discrete domains only. Although Distributions can also be used for that purpose, the Array construct is retained for compatibility with other programming languages. Note that it is not permitted to declare a Variable that is distributed over two domains of the same type. For instance, a temperature field over a square domain **cannot** be declared as:

```
T AS DISTRIBUTION(XDomain, XDomain) OF Temperature
```

The reason for this restriction is that a more complex syntax would then be required in order to distinguish between partial derivatives of the Variable T with respect to the first and the second independent Variables. This does not actually lead to any real restriction in functionality: Variable T could easily be declared as:

```
T AS DISTRIBUTION(XDomain, YDomain) OF Temperature
```

where XDomain and YDomain are declared to be identical:

```
DISTRIBUTION_DOMAIN  
  XDomain, YDomain AS [ 0.0 : Length ]
```

This also has the advantage of allowing different discretisation methods to be applied to each of the two domains.

Defining Distributed Equations

As with lumped models, Distributed Variables in Models are related through sets of equations that are declared in the Equation section. For example, consider the following declarations within a Model of a tubular reactor:

```
# MODEL TubularReactor  
  
PARAMETER  
  
  # Geometrical parameters  
  ReactorRadius,  
  ReactorLength  AS REAL  
  
  # Heat transfer parameters  
  U, S           AS REAL  
  
  ...  
  
DISTRIBUTION_DOMAIN  
  Axial  AS  [ 0 : ReactorLength ]  
  Radial AS  [ 0 : ReactorRadius ]  
  
VARIABLES  
  Vz, Vr AS DISTRIBUTION (Axial, Radial) OF Velocity  
  T       AS DISTRIBUTION (Axial, Radial) OF Temperature  
  Twall  AS DISTRIBUTION (Axial)          OF Temperature  
  Tc      AS                      Temperature
```

In this case, $Vz * T$ is a valid expression that is distributed over the entire Axial and Radial domains. Similarly,

```
U * S * ( T(,ReactorRadius) - Tc )
```

is also a valid expression distributed over the entire Axial domain. In some cases, it may be desired to define an expression over *part* of a particular domain. This can be achieved by using *slices* of distributions, very similar to the slice concept for arrays. For example, the expression:

```
Vz(0:ReactorLength/2, ) * T(0:ReactorLength/2, )
```

is distributed over the first half of the Axial domain and the entire Radial domain. The mathematical modelling of distributed systems often requires a rather subtle distinction between the entire domain *including* its boundaries, and the domain *excluding* all or part of its boundaries. In standard mathematical terminology, these two kinds of domain are referred to as 'closed' and 'open' respectively. One major reason for introducing this distinction is that some of the equations (e.g. conservation laws) may hold only in the interior of a domain while being replaced by appropriate boundary conditions on the domain boundaries. To allow the modellers to make the above distinction, gPROMS employs the notation shown in the table below.

Table 7.1. Closed and open domain notation

Mathematical notation	Interpretation	gPROMS notation
[a,b]	$z \in [a, b] \Leftrightarrow a \leq z \leq b$	a : b

Mathematical notation	Interpretation	gPROMS notation
(a,b]	$z \in (a, b] \Leftrightarrow a < z \leq b$	$a + : b$
[a,b)	$z \in [a, b) \Leftrightarrow a \leq z < b$	$a : b -$
(a,b)	$z \in (a, b) \Leftrightarrow a < z < b$	$a + : b -$

Thus, the Variable slice $Vz(0 | + : ReactorLength, 0 | + : ReactorRadius | -)$ denotes the values $Vz(z, r)$ for the values of z and r satisfying $0 < z \leq ReactorLength$ and $0 < r < ReactorRadius$. We conclude by formally defining the validity of expressions involving distributed Variables. Consider an expression $x ? y$ where x and y are scalar or distributed expressions, and $?$ is a binary arithmetic operator ($+, -, *, /, ^$). Then this is a valid gPROMS expression if and only if it conforms to one of the four cases listed below:

Case	x	y	Dimensionality of $x ? y$	Interpretation of $x ? y$
1.	Scalar	Scalar	Scalar	$x ? y$
2.	Array	Scalar	Same as x	$x_{\{...\}} ? y$
3.	Scalar	Distribution	Same as y	$x ? y_{\{...\}}$
4.	Distribution	Distribution	Same as x and y	$x_{\{...\}} ? y_{\{...\}}$

Clearly, case 4 is valid only if both x and y are distributed over exactly the same domains, also taking account of whether each of these is open or closed. For example, the following is a valid expression:

$Vz(0 | + : ReactorLength, ReactorRadius | -) * Twall(0 | + : ReactorLength)$

that is distributed over the Axial domain which is open on (i.e does not include) the left boundary ($z=0$) but closed on (i.e includes) the right boundary ($z=ReactorLength$). On the other hand, the expression:

$Vz(0 | + : ReactorLength, ReactorRadius) * T(0 : ReactorLength, ReactorRadius)$

is **invalid** because the first operand Vz is distributed over a domain that is open on the left and closed on the right, while the second operand T is distributed over a domain that is closed on both ends.

Introducing Partial Differential Equations

Partial differentiation of a distributed Variable or expression with respect to a domain over which it is distributed is achieved with the PARTIAL operator. Its syntax is of the form:

`PARTIAL (Expression, DistributionDomain)`

where *Expression* is a general expression and *DistributionDomain* is one of the distribution domains in the system. Normally, at least one of the Variables involved in the differentiated expression will be distributed over the specified domain, otherwise the result of the differentiation will be zero. Partial operators may also be nested. The result of a Partial operator is generally a distributed expression that has exactly the same degree of distribution as the *Expression* being differentiated.

In the gPROMS language it is possible to write expressions involving both

- First order partial derivatives
- Higher order partial derivatives

First order partial derivatives

Considering the example presented in Distributed Equations, the following are examples of valid first order partial derivative expressions:

$\frac{\partial T}{\partial z}$, $z \in [0, L], r \in [0, R]$	PARTIAL(T,Axial)
$\frac{\partial(V_z T)}{\partial r}$, $z \in (0, L], r = R$	PARTIAL(Vz(0 +:L, ReactorRadius) * T(0 +:L, ReactorRadius), Radial)
$\frac{\partial}{\partial r} \left(k_r \frac{\partial T}{\partial r} \right)$, $z = 0, r \in (0, R)$	PARTIAL(Kr(0, 0 +:ReactorRadius -) * PARTIAL(T(0, 0 +:ReactorRadius -), Radial), Radial)

Note that the partial differentiation operator with respect to time is denoted by symbol $\$$ rather than the operator PARTIAL. Thus:

$\frac{\partial T}{\partial t}$	$\$T$
---------------------------------	-------

There are two reasons for this:

- The use of $\$$ is consistent with the time derivative operator in lumped systems.
- The numerical solution methods in gPROMS treat the time domain quite differently to the explicitly declared distribution domains.

Higher-order partial derivatives

PARTIAL operators may be nested to express higher order derivatives as follows:

```
PARTIAL( Expression, PARTIAL( Expression, DistributionDomain ), DistributionDomain )
```

Alternatively, the following abbreviated form may be used:

```
PARTIAL ( Expression, DistributionDomain, DistributionDomain )
```

Here differentiation first takes place with respect to the first domain, then with respect to the second etc. For example:

$$\frac{\partial^2 T}{\partial z^2}, \quad z \in (0, L), r \in (0, R)$$

```
PARTIAL(T(0|+:ReactorLength|-, 0|+:ReactorRadius|-, Axial, Axial))
```

Conservative discretisation formulae for partial derivatives

There are two main approaches to discretise a partial derivative of an expression (for a given numerical method):

1. Apply the chain rule to reduce the term to a series of derivatives of a single variable and apply the discretisation scheme to each simple derivative
2. Apply the discretisation scheme directly to the complex derivative

A very common example of this is the convection term in conservation equations. The product of some conserved quantity, c , is multiplied by a bulk velocity v and the partial derivative with respect to position, x , is required. If the first approach above is applied, as illustrated below, then the numerical solution may contain errors resulting in the quantity c not being conserved.

$$\frac{\partial(vc)}{\partial x} = v \frac{\partial c}{\partial x} + c \frac{\partial v}{\partial x} \approx v_k \frac{c_k - c_{k-1}}{\delta x} + c_k \frac{v_k - v_{k-1}}{\delta x}$$

For this reason, gPROMS always applies the second "conservative" formulation to complex derivatives, as shown below for the simple convection term.

$$\frac{\partial(vc)}{\partial x} \approx \frac{v_k c_k - v_{k-1} c_{k-1}}{\delta x}$$

For this reason, therefore, conserved quantities are always conserved in the numerical solutions that gPROMS provides.

Introducing Integral Expressions

Integrals occur frequently in equations arising in a number of branches of physics and engineering. In process engineering applications, they often occur in population balance models describing, for instance, crystal size distributions, activity distributions of recycled catalyst particles, and the age and size distribution of microbiological cultures. They also appear when average values of distributed Variables need be calculated. Integration of a distributed Variable with respect to a domain is achieved with the `INTEGRAL` operator. Its syntax is of the form:

```
INTEGRAL ( IntegralRange ; Expression )
```

where *Expression* is a general expression involving Variables that are distributed over one or more distribution domains and *IntegralRange* represents the range of integration. The result of a Integral operator is generally an expression that is distributed over one less domain than the *Expression* being integrated.

In the gPROMS language it is possible to evaluate

- Single integrals
- Multiple integrals

Single integrals

The following are examples of single integrals:

$\int_0^1 z^2 dx$	<code>INTEGRAL(z := 0:1 ; z^2)</code>
$\int_0^L (T(z, r) - T_c) dz \quad r \in (0, R)$	<code>INTEGRAL(z := 0:ReactorLength ; T(z, 0 +:ReactorRadius -) - Tc)</code>

Note that an integration variable (e.g. *z* in the above examples) is introduced to define the range of integration. The integrand is generally an expression that may involve the Model Variables and/or the integration variable. The numerical method used to evaluate the integral depends on whether or not a distributed Model Variable appears in the integrand and the numerical methods specified (see Specifying Discretisation Methods).

Also note that, in the first example above, the result of the Integral is just a scalar quantity. On the other hand, the second example results in an expression that is distributed over the open domain $(0, R)$.

Multiple integrals

Multiple integrals can be defined via a shorthand notation. For example, the mean temperature in the entire tubular reactor is given by:

$$\bar{T} = \frac{2}{LR^2} \int_0^L \int_0^R rT(z, r) dr dz$$

which, in gPROMS, can be written as:

```
2 / (ReactorLength*ReactorRadius^2) *
INTEGRAL(z := 0:ReactorLength , r := 0:ReactorRadius ; r*Temp(z,r))
```

Relationship between the Integral and Sigma Operators

The Distribution concept can be considered as a generalisation of an Array, so the Integral operator can also be used for the integration of a given expression over discrete domains that define Array sizes. Thus, Integral can itself be viewed as a generalisation of the Sigma intrinsic function for carrying out discrete domain summations. For instance, the molar fractions of the reactants at the tubular reactor entrance are defined as:

$$x_i = \frac{c_i}{\sum_k c_k}$$

This equation can be represented in terms of either the SIGMA function or the INTEGRAL function, as shown below:

```
# Using SIGMA function
X(,0) = C(,0) / SIGMA(C(,0)) ;

# Using INTEGRAL operator
X(,0) = C(,0) / INTEGRAL(i := 1:NoComp ; C(i,0)) ;
```

However, the Integral operator is more general than the Sigma function; whereas Sigma always results in a scalar by summing *all* dimensions of its argument, Integral can have a more narrowly specified summation domain. For instance, consider a two-dimensional array Variable A(5,10). Then

```
SIGMA ( A(2:4, ) )
```

is the scalar $\sum_{i=2}^4 \sum_{j=1}^{10} A_{ij}$, whereas

```
INTEGRAL (i := 2:4 ; A(i, ) )
```

is a vector of length 10, the *j*th element of which is $\sum_{i=2}^4 A_{ij}$.

Explicit and Implicit Distributed Equations

As in the case of array equations, there are two different ways of writing distributed equations in gPROMS: in an *implicit* manner or an *explicit* manner.

Implicit specification

The first exploits the concept of distributed expressions to define equations in an *implicit* manner. For example, the following equation sets the temperature throughout the interior of the reactor to a uniform value of 298K:

```
T(0 | +:ReactorLength | - , 0 | +:ReactorRadius | - ) = 298 ;
```

This compact form of the equation will be automatically expanded by gPROMS.

Explicit specification

An alternative way of writing the same equation is in an *explicit* form by making use of For constructs:

```
FOR z := 0 | + TO ReactorLength | - DO
  FOR r := 0 | + TO ReactorRadius | - DO
    T(z,r) := 298 ;
```

```
    END  
  END
```

The two forms are completely equivalent, from the points of view of both the definition of the equation and its numerical solution. Thus, which one you use depends on preference. However, the definition of some distributed equations require the extra flexibility afforded by the use of the FOR construct. One such case involves equations which involve the independent Variables directly. Another case arises with equations involving SIGMA and/or INTEGRAL operators that need to be applied only to *some* of the domains of their arguments. For example, consider the chemical species conservation equations within the tubular reactor. These are of the form:

$$\frac{\partial C_i}{\partial t} = -v \frac{\partial C_i}{\partial z} + D_z \frac{\partial^2 C_i}{\partial z^2} + \frac{D_r}{r} \frac{\partial}{\partial r} \left(r \frac{\partial C_i}{\partial r} \right) + \sum_{j=1}^{NR} \nu_{ij} r_j, \quad i = 1..NC, \quad z \in (0, L), \quad r \in (0, R)$$

These can be written in gPROMS as follows:

```
FOR i := 1 TO NoComp DO  
  FOR z := 0 |+ TO ReactorLength | - DO  
    FOR r := 0 |+ TO ReactorRadius | - DO  
      $Concentration(i,z,r) =  
        - Velocity * PARTIAL(C(i,z,r),Axial)  
        + Dz * PARTIAL(C(i,z,r),Axial,Axial)  
        + (Dr/r) * PARTIAL(r * PARTIAL(C(i,z,r),Radial),Radial)  
        + SIGMA(Nu(i,) * r(,z,r)) ;  
    END  
  END  
END
```

Note how the range of application of each FOR construct is defined so as to ensure that the equation is enforced only at the interior of the domain of interest. As a second example consider the energy conservation equation for the cooling jacket. This leads to a lumped equation that is related to the reactor energy balance through an integral term describing the heat flux over the entire length of the reactor:

$$\rho_c C_{p,c} V_c \frac{dT_c}{dt} = f_c C_{p,c} (T_{c,in} - T_c) + U S \int_0^L (T(z, R) - T_c) dz$$

This can be written in gPROMS as follows:

```
Rhoc * Cpc * Vc * $Tc = Fc * Cpc * ( TcIn - Tc )  
  + U * S * INTEGRAL( z := 0:ReactorLength ; T(z,ReactorRadius)-Tc ) ;
```

Providing Boundary Conditions

In contrast to initial conditions, which may differ from one simulation experiment to the next, boundary conditions are part of the description of the physical system behaviour itself. In gPROMS, they are therefore specified within Models. Boundary conditions can be viewed simply as additional equations relating the Model Variables; consequently, they may be included in the Equation section, together with all other model equations. However, for the sake of clarity, the user is encouraged to include the boundary conditions in a separate section, under the keyword Boundary. For instance, the boundary condition for heat transfer at the tubular reactor wall,

$$-k_r \frac{\partial T}{\partial r} \Big|_{r=R} = U_h (T - T_{wall}), \quad z \in (0, L)$$

can be written as follows:

```
BOUNDARY
```

```
...
```

```
# Heat transfer relation at tube wall
FOR z := 0 |+ TO ReactorLength|- DO
    - Kr * PARTIAL(T(z,ReactorRadius),Radial) =
        Uh * ( T(z,ReactorRadius) - Twall(z) ) ;
END

...
EQUATION
```

In any case, gPROMS currently treats the BOUNDARY and EQUATION sections in exactly the same way for the purposes of numerical solution.

Specifying Discretisation Methods

The solution of systems of IPDAEs is generally a difficult problem. Changing the value of a parameter or one of the boundary conditions may lead to completely different behaviour from that originally anticipated. Furthermore, although some numerical methods can accurately solve a given system, other numerical methods may be totally unable to do so.

The systems of IPDAEs defined within gPROMS Models are solved using the method-of-lines family of numerical methods. This involves discretisation of the distributed equations with respect to all spatial domains, which reduces the problem to the solution of a set of DAEs.

A number of different techniques fall within the method-of-lines family of methods, depending on the discretisation scheme used for discretising the spatial domains. Ideally, this discretisation scheme should be selected automatically — or, indeed, a single discretisation method that can deal efficiently with all forms of equations and boundary conditions would be desirable. However, this is not technically feasible at the moment and therefore gPROMS relies on the user to specify the preferred discretisation method. Three specifications are necessary to completely determine most discretisation methods:

- *Type of spatial discretisation method.* The proper choice of the discretisation method is often the critical decision for solving a system of IPDAEs. As we mentioned earlier, because no method is reliable for all problems, the incorrect choice of method may lead to physically unrealistic solutions, or even fail to obtain any results.
- *Order of approximation.* The order of approximation for partial derivatives and integrals in finite difference methods, and the degree of polynomials used in finite element methods has a great influence on the accuracy of the solution. This is especially true if coarse grids or only a small number of elements are used.
- *Number of discretisation intervals/elements.* The number of discretisation intervals in finite difference methods and the number of elements in finite element methods are also of great significance in determining the solution trajectory. A coarse grid or a small number of elements for a steep gradient problem may result in an unacceptably inaccurate solution. On the other hand, too fine a grid or too many elements will increase the required computational efforts drastically, leading to an inefficient solution procedure.

The gPROMS language allows users to specify all three characteristics. DISTRIBUTION_DOMAINs are treated as Parameters and can be Set to the desired discretisation method, order and granularity of approximation. The table below lists the currently available numerical methods, their corresponding keywords in the language and the currently supported orders of approximation for each.

Table 7.2. Numerical methods for distributed systems in gPROMS

Numerical method	Keyword	Order(s)
Centered finite difference method	CFDM	2, 4, 6
Backward finite difference method	BFDM	1, 2
Forward finite difference method	FFDM	1, 2

Numerical method	Keyword	Order(s)
Orthogonal collocation on finite elements method	OCFEM	2, 3, 4

As was mentioned earlier, the numerical methods applied to integrals depend on the nature of the integrand. If the integrand is an expression involving only the integration variable, then the integration method is fixed (since there is no way to specify the method). These *implicit* integrals are all evaluated using 5th order Gaussian Quadrature. If the integrand involves one or more distributed Model Variables, then the method of the integration is *explicitly* specified (because all distributed Variables must be defined over a Distribution Domain, which must be set a value as described in the table above). The following procedure below is applied to any integrals of this nature.

1. First, if the integral is defined over more than one domain, it is decomposed into a nested set of 1-D integrations. The innermost integrals are evaluated first, which provide terms in the integrands at the next level, which now become ordinary 1-D integrals themselves. This procedure is repeated until the outermost integral (i.e. the one with the highest dimension) has been evaluated.
2. Each of the 1-D integrals that must be evaluated in step 1 are first decomposed into a sum of integrals over a set of subintervals. This is based on the range of the Distribution Domain and number of intervals specified in its numerical method. This gives a number of interval boundaries, x_i . An integral of the form

$$\int_a^b \phi dx$$

then becomes

$$\int_a^{x_i} \phi dx + \int_{x_i}^{x_{i+1}} \phi dx + \cdots + \int_{x_{i+m-1}}^{x_i+m} \phi dx + \int_{x_i+m}^b \phi dx.$$

So, if the integral is specified over the interval [a,b] within a Distribution Domain defined to be over the interval [0,L] with a numerical method using N intervals, the number of subintervals used for the integration will be roughly $(b-a)N/L$.

3. Each of the subintegrals in step 2 is integrated using a polynomial approximation consistent with the numerical method specified for the Distribution Domain.

Overall, the numerical methods for evaluating integrals do not in general correspond to any well-known methods. In some cases, the methods may reduce to trapezoidal or Simpson's rules; but not always. However, and most importantly, the method that is applied is always consistent with the numerical method used to approximate the partial derivatives over the same Distribution Domain.

The numerical methods applied to the various integrals that may be encountered in gPROMS Models are summarised in the table below.

Table 7.3. Numerical methods for integrals in gPROMS

Type of integral	Numerical method used	Number of intervals
Implicit	5th order, six point Gaussian Quadrature	—
Explicit	approximation is consistent with numerical method used to approximate partial derivatives	depends on the Distribution Domain and the integration interval

Clearly, the numerical methods used in evaluating integrals have a direct effect on the accuracy of the solution. There are some situations where the Gaussian Quadrature used in evaluating implicit integrals results in significant errors. One example is the power function x^n . When $n < 1$, the results of the numerical integration can be quite poor. Of course, when the integral can be solved analytically, it is always better to include the analytical expression rather than the integral, as in this case. However, should numerical integration be required, greater accuracy can sometimes be achieved by defining a distributed Variable (over a newly specified domain), equating

it to the integrand and then integrating the Variable. Then, the number of elements can be specified such that the accuracy of the integral is as required. An example of this is shown below.

```
DISTRIBUTION_DOMAIN
  MyIntegrationDomain AS [1:100]

VARIABLE
  Integrant AS DISTRIBUTION(MyIntegrationDomain) OF NoType
  Implicit   AS NoType
  Explicit   AS NoType

SET
  MyIntegrationDomain := [ BFDM, 1, 200 ] ;

EQUATION
  FOR x := 1 TO 100 DO
    Integrant(x) = 1/x ;
  END
  Implicit = INTEGRAL( x := 1:100; 1/x ) ;
  Explicit = INTEGRAL( x := 1:100; Integrant(x) ) ;
```

Here, the same integration is performed using the two methods. The implicit method will be quite inaccurate, whereas the explicit one will be much better (depending on the order and number of elements specified for MyIntegrationDomain).

Example 7.3. Setting the discretisation methods, orders and granularities

```
# PROCESS StartUpSimulation

UNIT
  R101 IS TubularReactor
  ...

SET
  R101.Axial  := [ CFDM, 2, 150] ;
  R101.Radial := [ OCFEM, 3,    4] ;
  ...
```

An excerpt from a Process entity involving an instance R101 of a 2D tubular reactor Model. The Axial domain within this instance is to be discretised using centered finite differences of second order over a uniform grid of 150 intervals. On the other hand, the Radial domain is to be handled using third order orthogonal collocation over four finite elements. Note that the specification of discretisation methods is done separately for each distribution domain in each instance of the corresponding Model, thus allowing maximal flexibility in this respect.

Similarly to other Parameters, although it is possible to specify numerical solution method information within the Models themselves, in the interests of model reusability and generality, is often better to associate these with the specific instances of Models that are included in Processes.

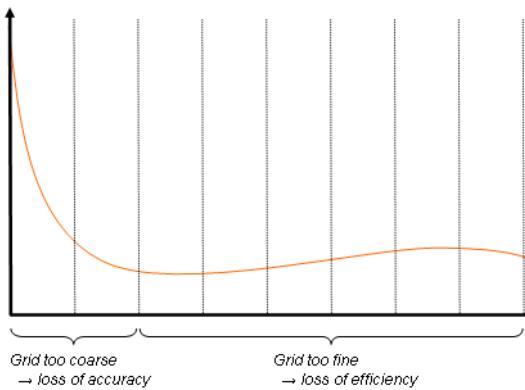
Non-uniform grids

The discretisation methods described so far have all been based on a uniform grid. For finite-difference methods, all elements are the same size: the length of the Distribution_Domain divided by the number of elements. The same is true of Orthogonal Collocation on Finite Elements (although *within* each element, the collocation points are placed according to the order of the method and *may* be non-uniform, though always symmetrically placed).

For many problems, uniform grids are unsuitable because there may be regions where there are large gradients and other regions where the gradients are small. Applying a uniform grid to the whole domain would therefore

result in a loss of accuracy where the gradients are too high, because the grid would be too coarse, and would be inefficient in the low-gradient regions, where the grid would be too fine. This is illustrated in the figure below.

Figure 7.2. Example of a problem requiring non-uniform grids



There are two main approaches to this problem. If the behaviour of the system is roughly known *a priori*, then a non-uniform grid may be specified to account for the spacial variation of the gradients. If the behaviour it not know sufficiently well, then adaptive non-uniform grids must be employed. Here, the solution procedure places the grid points in order to minimise the error.

gPROMS supports the use of a number of user-specified non-uniform grids. A non-uniform grid can be specified through two mechanisms:

1. Manually specifying the grid points
2. Specifying a grid transformation

Examples demonstrating the use of the concepts can be found in the gPROMS Project `nonuniformgrids.gPJ` in the examples sub-directory. It allows to compare the results of differently sized equidistant grids against each other and also against non-uniform grids. In particular it can be seen that the same precision can be achieved with a lower number of discretisation points using a non-uniform grid when compared against an equidistant grid.

Manually specifying grid points

The first approach to specifying a non-uniform grid is for the user to specify the location of all the grid nodes. This is done in the SET section when Setting the Distribution Domain Parameter. Rather than specifying the number of elements, simply enter the normalised positions of each of the internal grid nodes. The outer two nodes are fixed at 0 and 1 automatically, representing the lower and upper bounds of the domain, respectively. Below is an example specification for a second-order centred finite-difference scheme with 10 non-uniform elements.

```
DISTRIBUTION_DOMAIN
Axial AS [0 : ReactorLength]

SET
Axial := [CFDM, 2, (0.356, 0.524, 0.635,
                     0.719, 0.785, 0.841,
                     0.888, 0.930, 0.967)] ;
```

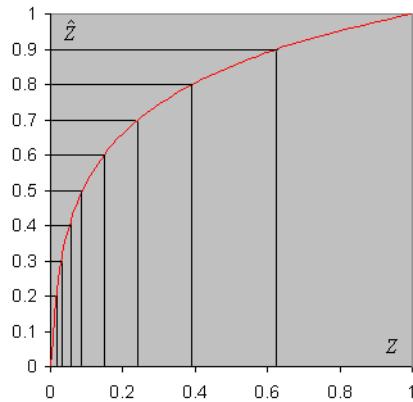
Specifying a grid transformation

An easier (but less general) way to specify the grid nodes is by use of a tranformation. If the problem is expected to exhibit large gradients at the start of the domain, which reduce towards the end of the domain, a logarithmic transformation can be used to place more nodes near the lower bound of the domain. This can be represented by the following equation, the effect of which is illustrated in the figure below.

$$\hat{z} = \frac{\ln(\alpha z + 1)}{\ln(\alpha + 1)},$$

where \hat{z} is the transformed coordinate and z the original coordinate. Below it can be seen that a uniform grid in the transformed domain leads to the desired non-uniform grid in the original domain.

Figure 7.3. A logarithmic transformation



Conversely, should one desire more grid points at the end of the domain, an exponential transformation may be used. The form of the transformation is:

$$\hat{z} = \frac{\exp(\alpha z) - 1}{\exp(\alpha) - 1},$$

To specify a transformed domain, enter the type of transformation with its parameter (α) in parentheses to the specification of the Distribution Domain. For the logarithmic transformation, with $\alpha = 4$, this would be specified as follows.

```
DISTRIBUTION_DOMAIN
Axial AS [0 : ReactorLength]

SET
Axial := [CFDM, 2, 10, TRANSFORM(LOG, 4.0)] ;
```

Other numerical methods are specified in exactly the same way. A list of the available transformations, their keywords and arguments is given below.

Table 7.4. Domain transformations available in gPROMS

Domain transformation	Keyword	Parameter(s)
Logarithmic	TRANSFORM(LOG, α)	α larger than or equal to zero
Exponential	TRANSFORM(EXP, α)	α can take any real value

Please note that for the exponential transformation a negative value will be the inverse transformation of the corresponding positive value.

Chapter 8. Composite Models

A composite Model is one that contains one or more other Model entities as a sub-Model. Composite Models can either be constructed graphically on the topology tab of a flowsheet model or using the gPROMS language; or even some combination of these two approaches.

In the case of graphical model construction, Connections between sub-Models can only be made to Model Ports (*see*: Constructing flowsheet Models). Whereas in the gPROMS language, Connections can be made via Model Ports and also by writing equations that directly access the Model Variables and Parameters. It should be note that graphical connections between Model Ports are automatically represented in the gPROMS language tab and vice-versa.

- Motivation for Model decomposition: the benefits of building reusable Model components.
- How to build composite Models in gPROMS
 - Declaring instances of lower-level Models in the UNIT Section
 - Topology connections in the gPROMS Language
- The use WITHIN construct for simplifying notation when referring to quantities within sub-Models,
- Making specifications for composite Models
 - Model specifications
 - Setting Parameter values in composite Models

Motivation for Model Decomposition

Certain complex unit operations may involve many tens of thousands of Variables and equations. Although in principle all of these could be written in a single Model entity, in practice such an undertaking would be extremely tedious and error-prone. The gPROMS language provides tools for managing such complexity.

The key principle involved is called *hierarchical sub-Model decomposition*, whereby the Model for a complex unit operation is constructed progressively in a number of hierarchical levels. This is much easier than constructing a very large primitive Model (see also: Defining Models and Processes) for the unit operation because at each level in the hierarchy you can concentrate on only a small fraction of the modelling task. As a result, the Models are easier to construct and less likely to contain errors.

Moreover, this strategy promotes Model reusability and efficient Model development practices, since suitably Parameterised sub-Models can be used several times, but only be constructed and tested *once*. The gPROMS language encourages hierarchical sub-Model decomposition by offering mechanisms that support:

- the declaration of high-level Models that contain instances of lower-level Models
- the connection of the above instances using Equations and topology connections.

Instances of lower-level Models: Units

In gPROMS, an instance of a Model is called a Unit. Consequently, if we wish to insert one or more instances of one or more Models within another (higher-level) Model, we have to introduce a Unit section within the latter.

Consider, for instance, the declaration of a distillation column Model that is outlined in the figure below.

Figure 8.1. Distillation Column Model

```
# MODEL DistillationColumn

PARAMETER
    # Number of trays
    NoTrays          AS INTEGER

    # Feed tray position
    FeedPosition      AS INTEGER

UNIT
    Condenser         AS TotalCondenser
    Reboiler          AS PartialReboiler
    TopSection        AS LinkedTrays
    BottomSection     AS LinkedTrays
    Feed              AS FeedTray

VARIABLE
    ColumnEnergyRequirement AS Energy_Flowrate

EQUATION
    #Definition of column energy requirement
    Reboiler.HeatingLoad - Condenser.CoolingLoad = ColumnEnergyRequirement
```

The PARAMETER and VARIABLE sections of this composite Model are very similar to those of simple (primitive) Models – see Defining Models. However, the UNIT section, above specifies that the Model also comprises a number of instances of other Models, namely:

- Condenser. This is an instance of Model TotalCondenser.
- Reboiler. This is an instance of Model PartialReboiler.
- TopSection, BottomSection. These are both instances of Model LinkedTrays.
- Feed. This is an instance of Model FeedTray.

Each of the lower-level Models may either be primitive or include a UNIT section themselves. For instance, TotalCondenser, PartialReboiler and FeedTray are likely to be primitive Models. In contrast, LinkedTrays is most probably a composite Model. In any case, there is no limitation with respect to the number of levels in this hierarchical decomposition.

Finally, the EQUATION section introduces an Equation that determines the net energy requirement for the entire column:

```
Reboiler.HeatingLoad - Condenser.CoolingLoad = ColumnEnergyRequirement ;
```

The equation involves three Variables. One of these (ColumnEnergyRequirement) belongs directly to the DistillationColumn Model having been declared explicitly in its Variable section. The other two Variables (Reboiler.HeatingLoad and Condenser.CoolingLoad) belong to the Units Reboiler and Condenser , respectively. Of course, for this to be correct, Models PartialReboiler and TotalCondenser must contain Variables Reboiler.HeatingLoad and Condenser.CoolingLoad respectively.

The above equation illustrates a *general* property of higher-level Models. This is their ability to refer to entities (e.g. Parameters and Variables) that are declared within the Units that they contain - as well, of course, as their own entities. Furthermore, as we have seen, this reference is done using a *pathname* construct. The latter can be arbitrarily long. For example, suppose that the TotalCondenser Model is not primitive but comprises instances of several lower-level Models; then the following may be a valid pathname:

```
Condenser.RefluxDrum.LevelController.Gain
```

referring to the gain of the controller used to control the liquid level in the reflux drum of the condenser.

Finally note that the DistillationColumn Model does not yet express how the flows of material and energy between the sub-units are equated; this could be done directly with Equations. For example:

...

EQUATION

```
#Definition of column energy requirement
Reboiler.HeatingLoad - Condenser.CoolingLoad = ColumnEnergyRequirement

# Connectivity for reboiler/Bottom Section
Reboiler.Vapour_out = BottomSection.Vapour_in;
Reboiler.y_vapour_out = BottomSection.y_vapour_in;
Reboiler.T_vapour_out = BottomSection.T_vapour_in;
```

...

Of course, Equations need to be provided for all the connections between all of the Units.

However, in practice it is usually more convenient to connect Units using topology connections to Model Ports (assuming that they have been defined of course) – see Topology connectivity using the gPROMS Language.

Topology connectivity using the gPROMS Language

Connections made between a Model's Ports (see: Defining Ports), whether created graphically (*see*: Constructing flowsheet Models) on the composite Model's topology tab or directly in the gPROMS language, should be placed in the TOPOLOGY section; the general syntax for this is shown below

TOPOLOGY

```
UnitName.PortName      = UnitName.PortName          # for scalar PORTS
UnitName.PortName(PortNumber) = UnitName.PortName      # for array PORTS
UnitName.PortName(PortNumber) = UnitName.PortName(PortNumber) # for array PORTS
UnitName.PortName      = UnitName.PortName(PortNumber) # for array PORTS
```

EQUATION

... Model equations ...

The following should be noted:

- Graphical connections are automatically represented in the *gPROMS language* tab and likewise any connections added directly in the gPROMS language will be shown on the composite Model's *topology* tab (following a syntax check). Similarly connections deleted from either location will be synchronised.
- The TOPOLOGY section comes *just* before the EQUATION section in a gPROMS Model entity.
- When connecting Units via Ports the user must ensure that the Connection Types are the same and that all Connectivity rules are satisfied.
- When a Connection is made all Parameters, Distributions and Variables in the Ports are equated.

Arrays of Units

Recalling the DistillationColumn Model used to introduce lower-level Model instances, one of its sub-Models is a Model of a column section, called LinkedTrays:

```
# MODEL DistillationColumn

PARAMETER
  ...
UNIT
  Condenser      AS TotalCondenser
  Reboiler        AS PartialReboiler
  TopSection      AS LinkedTrays
  BottomSection   AS LinkedTrays
  Feed           AS FeedTray
  ...
  ...
```

As its name implies, `LinkedTrays` could contain a number of instances of a `Tray Model`. Clearly it would be convenient to define an `Array` of `Tray Model` instances, and this can be done as follows.

```
# Model LinkedTrays

PARAMETER
  NoTrays AS INTEGER
  ...
UNIT
  Trays    AS ARRAY(NoTrays) OF Tray
  ...
  ...
```

See also Declaring arrays of Units in Models.

Referring to arrays of Units is done in a similar manner to Parameters and Variables (see Referring to array elements). For example, one would refer to the liquid mole fraction of component 2 in the 5th tray of the top section of the column using the following path name:

```
Column.TopSection.Trays(5).x(2)
```

Variable pathnames and WITHIN

As the number of intermediate hierarchical levels increases, so does the length of the pathnames required to reference Parameters and Variables at or close to the bottom of the hierarchy. Pathnames of the form:

```
SeparationSection.Column(2).TopSection.Stage(1).T
```

are quite common when dealing with complex processes.

It is recommended that you use pathname completion to help construct full and valid pathnames correctly; this is available within all entities in gPROMS. Semantic errors, such as referencing a quantity in a lower-level Model that doesn't exist, are only detected when a Model based activity is executed.

Nevertheless, writing equations with long pathnames can become tedious and make code difficult to read, especially if a large part of the pathname is common to many of the Parameters or Variables referenced by an equation. The `WITHIN` construct helps relieve some of this burden.

A `WITHIN` construct encloses a list of equations and defines a *prefix* to be used for all Parameters and Variables referenced by the enclosed equations. Suppose, for instance, that Model `Tray` has a Variable `Q` that determines the heat loss from the tray to the environment. However, it contains no equation that actually determines this heat loss. Consider now using this `tray Model` within the top and bottom sections of a column. We wish to specify a simple heat transfer equation for determining the heat loss in the top section; however, the bottom section is well insulated. One way we can achieve this is as follows:

```
MODEL DistillationColumn

PARAMETER
    TAmbient AS REAL
    UA        AS REAL
    NoTrays   AS INTEGER

UNIT
    TopSection, BottomSection AS LinkedTrays

EQUATION
    WITHIN TopSection DO
        FOR k := 1 TO NoTrays DO
            WITHIN Stage(k) DO
                Q = UA * (T - TAmbient) ;
            END # Within Stage(k)
        END # For k
    END # Within TopSection

    WITHIN BottomSection DO
        FOR k := 1 TO NoTrays DO
            WITHIN Stage(k) DO
                Q = 0 ;
            END # Within Stage (k)
        END # For k
    END # Within BottomSection
```

In trying to interpret the equation:

```
Q = UA * (T - TAmbient) ;
```

gPROMS will need to identify (*resolve*) the symbols Q, UA, T and TAmbient. It starts doing this by searching the Model corresponding to the UNIT mentioned in the innermost WITHIN statement. In this case, this is Model Tray which does, indeed, contain Variables Q and T. However, symbols UA and TAmbient still remain unresolved. Therefore, gPROMS considers the next enclosing WITHIN statement; this indicates that it should search Model LinkedTrays (of which TopSection is an instance). However, this Model does not contain the missing identifiers. So gPROMS now has to consider Model DistillationColumn itself – which does indeed allow it to resolve UA and TAmbient.

It is interesting to note that both the DistillationColumn and the LinkedTrays Models contain the Parameter NoTrays. However, this does not result in any ambiguity in resolving this Parameter when it appears in each of the two FOR constructs: gPROMS always tries to resolve symbols by searching the innermost WITHIN first. Thus, NoTrays in:

```
WITHIN TopSection DO
    FOR k := 1 TO NoTrays DO
        ...
    END
END # within TopSection
```

clearly refers to TopSection.NoTrays and *not* to Parameter NoTrays in DistillationColumn.

Expressions involving arrays of Units

Occasionally, it will be necessary to write expressions involving of arrays of units and/or slices of arrays of units (i.e. a subset of the elements of an array – see Referring to array elements). The rules governing expressions involving arrays of units are similar to those governing array expressions involving only Variables. However, there are some additional complications with arrays of units, so one should be familiar with the General rules for array expressions and Using arrays in equations before continuing.

There are two situations to consider when writing expressions of arrays of units. The simplest case is when slices are specified for all dimensions of all arrays; the other is when at least one dimension of an array is unspecified (e.g. $A(2:3,)$).

In the examples to come, the following conventions are used.

- Variable names always begin with the letter V; all other entities are Units.
- Whole arrays are always indicated using parentheses and their dimensionality is indicated using commas to delimit the indices. For example, a two-dimensional array will be written as $V(,)$ rather than $V()$ or V , which are equally valid in gPROMS but could be confused with a one-dimensional array and a scalar respectively.

The first, and simplest, case to consider is when all dimensions of all arrays are specified (either by giving a specific element or a slice of elements). The expression below is an example of such an expression.

$UA(1:2) . UB . P(1:3) . V1 + UC . UD(1:2) . P(1:3) . V2 = 3 ;$

This case is quite simple. It is clear that this expression should be expanded to give:

$UA(1) . UB . P(1) . V1 + UC . UD(1) . P(1) . V2 = 3 ;$
 $UA(1) . UB . P(2) . V1 + UC . UD(1) . P(2) . V2 = 3 ;$
 $UA(1) . UB . P(3) . V1 + UC . UD(1) . P(3) . V2 = 3 ;$

$UA(1) . UB . P(1) . V1 + UC . UD(1) . P(1) . V2 = 3 ;$
 $UA(2) . UB . P(2) . V1 + UC . UD(2) . P(2) . V2 = 3 ;$
 $UA(2) . UB . P(3) . V1 + UC . UD(2) . P(3) . V2 = 3 ;$

The rules governing expressions like these are the same as those for ordinary arrays. Each of the terms on the left-hand side of the expression can be thought of as 2×3 arrays. The presence and location of any scalar elements do not affect this behaviour: UB and UC are in different places in the paths but neither their location nor their existence changes the dimensionality of the two terms. So the whole expression can be considered dimensionally equivalent to:

$VA(1:2, 1:3) + VB(1:2, 1:3) = 3 ;$

and this is a legal array expression, because VA and VB have exactly the same dimensions.

Even the dimensionality of the variables is unimportant to the validity of expressions of this type. The next example demonstrates this.

$UA(3:3, 1:2) . UB . P(1:4) . V1 + UC . P(1, 5:6) . V2(1:4) = 3$

Now the dimensions of UA and UC.P are identical (1×2) and the dimensions of UB.P are identical to UC.P.V2, so each term is equivalent to a $1 \times 2 \times 4$ array and the expression is equivalent to:

$VA(3:3, 1:2, 1:4) + VB(1, 5:6, 1:4) = 3$

So when all indices of all arrays are specified completely, the rules are identical to ordinary arrays: each term must be a scalar or of the same dimensionality.

When it is necessary to refer to whole arrays, the situation becomes a little more complicated. Consider the first example again, but now writing the expression for the whole range of array elements:

$UA() . UB . P() . V1 + UC . UD() . P() . V2 = 3 ;$

At first glance, this might look the same. Certainly, the number of elements in $UA()$ must be the same as the number of elements in $UC . UD()$. However, the dimensionality of $P()$ is harder to define in a simple way: the problem is that $P()$ may have different number of elements for each element of $UA() . UB$ or $UC . UD()$. A more relevant example of this is given below.

$COLUMN_A(,) . TRAY() . V = COLUMN_B(,) . TRAY() . V ;$

Here, we have two 2-dimensional arrays of distillation-column units, perhaps forming a separation network. There is no guarantee that each column will have the same number of trays: in fact it is extremely unlikely. So it is not possible to consider this expression, or the one before, as a simple array expression. What must be done instead is to consider the dimensions in each term of the expression more carefully.

First, it is clear that `COLUMN_A(,)` and `COLUMN_B(,)` must have the same dimensionality. Next, for each element of `COLUMN_A(,)` and `COLUMN_B(,)`, the number of trays must also be equal, so that the following condition is met:

The dimensionality of `COLUMN_A(i, j).TRAY()` must be equal to the dimensionality of `COLUMN_B(i, j).TRAY()` for all i and j .

This must be true for the whole path of each term in the expression (unless the term is scalar). We can now define a *dimension tree* for each term, which describes completely the dimensionality of the term.

The dimension trees for both terms in the example:

`UA(3:3,1:2).UB.P(1:4).V1 + UC.P(1,5:6).V2(1:4) = 3`

are:

- (1,2)
 - 4
 - 4

If we were to write the expression as:

`UA(,).UB.P().V1 + UC.P(,).V2() = 3`

with `UA(,)` and `UC.P(,)` both being 1x2 arrays; `UA(1, 1).UB.P` having 3 elements; `UA(1, 2).UB.P` having 4 elements; `UC.P(1, 1).V2` having 4 elements and `UC.P(1, 2).V2` having 3 elements, then the dimension trees would be:

- (1,2) [`UA(,)`]
 - 3
 - 4

and:

- (1,2) [`UC.P(,)`]
 - 4
 - 3

As these two trees are not identical, the two terms will not be compatible and the expression will be illegal.

The general rule for expressions involving arrays of units is therefore an extension of the rule for array Variables. If we have an expression of the form:

Expression E = Expression F;

it will be valid provided it conforms to one of the following four cases:

Case	E	F	Dimension tree of E = F
1	Scalar	Scalar	Scalar

Case	<i>E</i>	<i>F</i>	Dimension tree of <i>E</i> = <i>F</i>
2	Dimension tree	Scalar	Same as <i>E</i>
3	Scalar	Dimension tree	Same as <i>F</i>
4	Dimension tree	Dimension tree	Same as <i>E and F</i>

In case 4, the dimension trees of *E* and *F* must be identical. Either expression may comprise binary operations of the form $x \oplus y$, for which the following rules must also apply:

Case	<i>x</i>	<i>y</i>	Dimension tree of <i>x</i> \oplus <i>y</i>
1	Scalar	Scalar	Scalar
2	Dimension tree	Scalar	Same as <i>x</i>
3	Scalar	Dimension tree	Same as <i>y</i>
4	Dimension tree	Dimension tree	Same as <i>x and y</i>

Again, in case 4, the dimension trees of *x* and *y* must be identical.

Model specifications

It is usually recommended that the values of all unknown Model quantities are provided in Process entities (*See also: Defining Process Entities*), where:

- Parameter values are fixed in the SET section
- Variables are specified in the ASSIGN section
- Initial conditions are provided in the INITIAL section
- The initial values of Selectors are provided in the INITIALSELECTOR section

However, the same sections exist in Model entities. So it is equally possible to provide a specification directly in the Model that declares the quantity to be specified or any composite Model that includes the Model. *See also: gPROMS language for Models.*

Care should be taken to remember that making a specification in a Model can greatly reduce the generality of such a Model. In general a quantity may be given a value *at most once* and it is not possible to overwrite a specification given at a lower level. However, giving a Parameter the exactly same value more than once does not cause an error.

Consider, for instance, the following situation:

- Model X declares a Parameter S to be of type REAL.
- Model Y contains a unit XX which is an instance of X.
- Model Z contains a unit YY which is an instance of Y.
- Process P contains a unit ZZ which is an instance of Z.

Then, the value of Parameter S can be explicitly set in of the following ways:

1. In X:

```
SET
S := 1.5 ;
```

2. In Y:

```
SET
```

```
XX.S := 1.5 ;
```

3. In Z:

```
SET  
YY.XX.S := 1.5 ;
```

4. In P:

```
SET  
ZZ.YY.XX.S := 1.5 ;
```

If a Parameter is explicitly SET in a Model, it will have that value in *all* instances of that Model. For example, if we use option 2 above, XX.S will have a value of 1.5 in all subsequent instances of Model Y anywhere in the problem. It is usually advisable that Parameters be explicitly set at the Process level. This practice maximises the reusability of the underlying Models and minimises the probability of error.

Setting Parameter values in Composite Models

Before any Model based activity is executed in gPROMS the values of all Parameters (even if not used) must be resolved. A Parameter's value must have been determined in one of the following ways:

- Explicit Parameter specification: to Set a Parameter to either to a literal value or to another Parameter value (or even some expression involving the two)
- From topology connections : for Connection Type Parameters only
- From implicit *Parameter Propagation in Composite Models: top down propagation from higher level Models to lower level models*
- From a Default specification: only if the Parameter is not given a value directly by any of the three previous approaches

Any Parameter that does not have a value following the above four steps will result in an error that causes the Model based activity to fail. Giving a Parameter the exactly same value more than once does not cause an error; however, clearly, giving a Parameter different values is an error.

Setting Connection Type Parameters

The Parameters included in Connection Types can be set explicitly like regular Model Parameters. However, their values are usually obtained from topology connections and Port Sets:

- **Topology connections:** when a connection between two Ports is made the equivalent Parameters in these Ports are equated.
- **Port sets:** These are configured when the Ports for any component Model entity are configured (also see: Defining Model Ports). For all Ports belonging to the same *set* (i.e. those in the same Port set): the equivalent Connection Type Parameters are equated. This mechanism is often used by component Model developers to equate the Parameters in an *Outlet* Port to those in an *Inlet* Port.

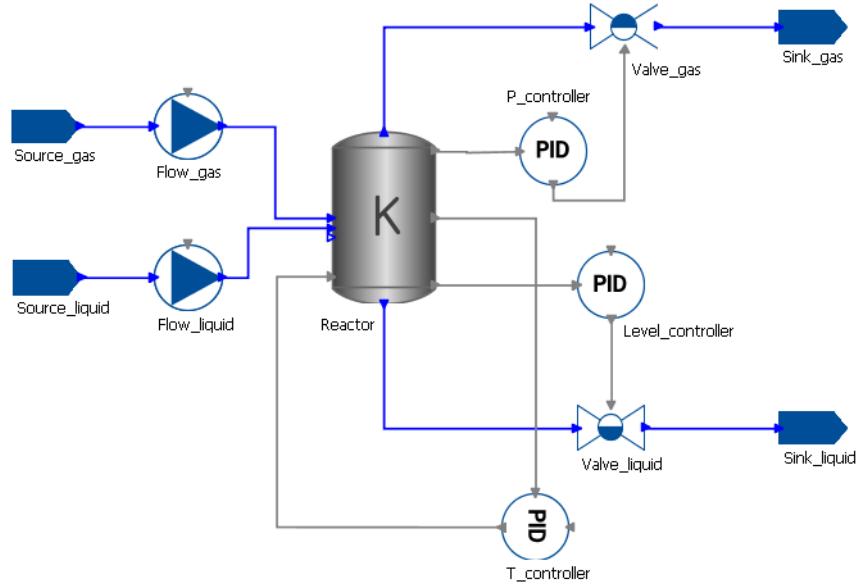
These two mechanisms (if Port sets are implemented) mean that information corresponding to the properties carried by the Connection are automatically propagated along the stream path. In the gPROMS Process Model Library this is used so that the Parameter corresponding to physical properties only needs to be set in the Source Model.

It is of course possible within the component Model to access the Port Parameters and use them directly in Model Equations declarations, or indeed, to Set Model Parameters equal to the Parameters declared by the Port definition.

Example of Parameter Propagation with Port Sets

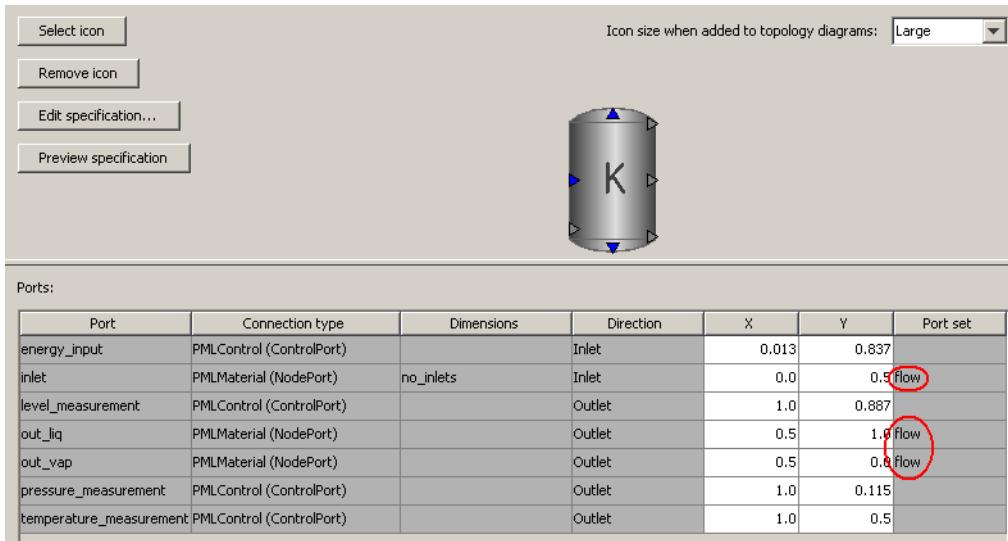
As an example of the use of Port Sets, consider the PML Flowsheet shown below.

Figure 8.2. Reactor Flowsheet



Each of the connector Models in this Flowsheet (pumps, reactor and valves) have common Port Sets linking their inputs to their outputs. This is shown for the reactor Model below.

Figure 8.3. Reactor Port Sets



This means that once the properties of the `Source_gas` Model instance are specified, they automatically propagate along the direction of flow: i.e. to `Flow_gas`, `Reactor`, `Valve_gas`, `Sink_gas`, `Valve_liquid` and `Sink_liquid`. More specifically, because the properties of `Source_gas` define the inlet properties of `Flow_gas` and the inlet of `Flow_gas` shares the same Port Set as its outlet ("flow"), the properties are propagated along. Similarly, the inlet of the `Reactor` is linked to both of its outlets by the same Port Set.

Note, however, that the Parameters are not propagated backwards, so `Source_liquid` must be specified as well. Of course, some of its properties cannot be specified independently and care must be taken to make sure that there are no conflicts. If, for example, one were to specify a different set of components for `Source_liquid`, gPROMS would

report a conflict between the two sets of specifications propagated to the inlet of Reactor. Below are shown two examples of inconsistent component specifications.

Figure 8.4. Inconsistent Parameters propagated through Port Sets: inconsistent components specified

```
1 error(s) occurred constructing the system
When performing Identity Elimination:
  FOR j := 1 TO no_inlets DO
    FOR i IN Components DO
      Error in MODEL Reactor_drum_kinetic at line 148 (506):
        inlet(j).mass_fraction(i) = in_mass_fraction(j, i) ;
        Name "HYDROGEN" not found in enumerated domain. Valid values are:
        ["NITROGEN"(1), "PHENOL"(2), "BENZENE"(3), "CYCLOHEXANE"(4), "WATER"(5), "N_HEXADECANE"(6)]
  Performing Foreign Object termination: "IPPF0::mass:<HYDROGEN,PHENOL,BENZENE,CYCLOHEXANE,WATER,N_HEXADECANE>""
  Foreign Object termination completed successfully.
  Performing Foreign Object termination: "IPPF0::mass:<NITROGEN,PHENOL,BENZENE,CYCLOHEXANE,WATER,N_HEXADECANE>""
  Foreign Object termination completed successfully.
```

Figure 8.5. Inconsistent Parameters propagated through Port Sets: extra component specified

```
1 error(s) occurred constructing the system
Creating EQUATION in Plant.Reactor:
  FOR j := 1 TO no_inlets DO
    Error in MODEL Reactor_drum_kinetic at line 130 (488):
      inlet(j).info_mass_fraction = mass_fraction ;
      Incompatible dimensionalities: LHS: (7), RHS: (6)
  Performing Foreign Object termination: "IPPF0::mass:<HYDROGEN,PHENOL,BENZENE,CYCLOHEXANE,WATER,N_HEXADECANE>""
  Foreign Object termination completed successfully.
  Performing Foreign Object termination: "IPPF0::mass:<NITROGEN,HYDROGEN,PHENOL,BENZENE,CYCLOHEXANE,WATER,N_HEXADECANE>""
  Foreign Object termination completed successfully.
```

Implicit Parameter Propagation

As well as the propagation of Connection Type Parameters along stream paths the values of Model Parameters can propagate from higher- to lower-level Models.

For example, a Parameter that corresponds to the number of components (e.g. NoComp) may well be present in the higher-level Model of a distillation column *and* in all of its constituent Model instances. Ideally, we would like to be able to set the value of this Parameter at the highest level only and rely on an automatic mechanism to propagate it through the hierarchy towards the lower levels. This not only saves effort in specifying the Model but also reduces the possibility of errors arising due to inconsistent specifications, especially during Model development (e.g. specifying NoComp=5 in some parts of the column and NoComp=4 in others).

If a Parameter appearing in an instance of a Model is not SET explicitly, gPROMS will automatically search hierarchically the higher-level Models containing it for a Parameter of *the same name and type* which has been given an explicit value. If this is found, the Parameter in the lower-level Model will adopt the value assigned to the Parameter with the same name in the higher-level Model.

Another way of looking at this is that an explicit SET specification for a Parameter in a higher-level Model X propagates downwards and covers all Parameters of the same name and type in any lower-level Models, instances of which are contained in X. This establishes an *automatic Parameter propagation* mechanism.

For instance, consider the hierarchy of Models X, Y and Z (which all contain a declaration of a Parameter NoComp) : such that

- Model X .
- Model Y contains a unit XX which is an instance of X.
- Model Z contains a unit YY which is an instance of Y.
- Process P contains a unit ZZ which is an instance of Z.

We then have various possibilities:

1. Set Parameter in P:

```
SET  
ZZ.NoComp := 5 ;
```

Although nothing is said explicitly about Parameters ZZ.YY.NoComp and ZZ.YY.XX.NoComp, the automatic Parameter propagation will ensure that these also take the value of 5.

2. Set Parameter in P:

```
SET  
ZZ.NoComp := 5 ;
```

but also in Y:

```
SET  
NoComp := 3 ;
```

This is equivalent to:

```
ZZ.NoComp      := 5 ;  
ZZ.YY.NoComp   := 3 ;  
ZZ.YY.XX.NoComp := 3 ;
```

Note that the value of the Parameter in YY is set explicitly and automatically propagates downwards, setting the value of the Parameter in XX. Therefore, when gPROMS automatically propagates the assignment in P, it cannot override the existing value.

We also recall that the specification of discretisation methods for distribution domains is treated exactly as that for Parameters - hence, it also undergoes automatic propagation. For instance, if:

```
SET  
ZZ.Axial := [OCFEM, 3, 10] ;
```

appears in a Process, all Model instances within ZZ which declare an Axial domain will use the same discretisation method - unless, of course, their Axial specification is explicitly SET to a different value.

Chapter 9. Ordered Sets

You should be familiar with the use of Arrays before proceeding further.

gPROMS allows the use of Ordered Sets as array indices, in addition to simple integer indices. These substantially increase the descriptive power of the modeling language because they allow the user to use strings to reference array elements rather than integers. For example: instead of mole fractions being defined as $x(1)$, $x(2)$ and $x(3)$; $x('H2')$, $x('CH4')$ and even $x('Ethane')$ can be used instead. The importance for ease and correctness of model building should be evident. Ordered Sets can be used for

- Parameters
- Variables
- Units

Each of these entities can be defined as Arrays or Distributions over Ordered Sets.

Developing models involving Ordered Sets requires the following:

- Declaring Ordered Sets
- Declaring Arrays of Parameters, Variables and Units using Ordered Sets
- Ordered Set operations and referencing rules

A set of examples and the gPROMS Project `orderedsets.gPJ` illustrate more complex use of Ordered_Sets.

Declaring Ordered Sets

The Ordered Set is a type of Parameter and is therefore declared in the PARAMETER section of your gPROMS Model.

They are declared as follows:

```
PARAMETER
  Gases, Liquids, Species AS ORDERED_SET
```

As with other Parameters, the values are defined in the set section. In the case of Ordered Sets, it is the set elements that must be defined.

```
SET
  Gases   := [ 'H2', 'CH4', 'Ethane' ] ;
  Liquids := [ 'Octane', 'Decane' ]      ;
  Species := Gases + Liquids           ;
```

Note that the `+` operator is the set union operator in this case. More information on operators may be found here.

Each element of the Ordered Set is a user-defined string. Strings are delimited by single quotes (as shown above) or by double quotes ("") and can contain any character apart from the same character used to delimit the string. Also, each element of the Ordered Set must be unique: if any duplicate elements are defined, these are ignored by gPROMS. The following example specification produces an Ordered Set containing just three elements: "1", "2" and "3", in that order.

```
SET
  Numbers := [ '1', '2', '3', '2' ] ;
```

Some examples of legal and illegal element specifications are shown below:

```
SET
Legal    := [ "1", '2"', "3'" ] ; # all legal
Illegal  := [ '1'' , "2"" ] ; # all illegal
#           \      \____ this element is delimited by " so the string
#           \           may include any character apart from "
#           \____ this one is delimited by ' so it cannot contain '
```

Ordered Sets are also compatible with physical-property interfaces. In this next example, the elements of the Ordered Set are specified by a physical-property Foreign Object.

```
PARAMETER
Species AS ORDERED_SET
PhysProp AS FOREIGN_OBJECT "PhysProp"
NoComp   AS INTEGER

SET
NoComp  := PhysProp.NumberOfComponents ;
Species  := PhysProp.Components ;
```

Declaring Arrays of Parameters, Variables and Units

Each of these types of entity are declared in a very similar way to Arrays over integer domains. So for Parameters the declaration is:

```
PARAMETER
FormulaWeight AS ARRAY(Species) OF REAL
```

As with Arrays generally, multiple dimensions are possible. For example, if an Ordered Set Reactions had also been defined, then the parameter Nu, representing stoichiometric coefficients could be declared by:

```
PARAMETER
Nu AS ARRAY(Species, Reactions) OF INTEGER
```

For Variables, the declaration is:

```
VARIABLE
X AS ARRAY(Species) OF MassFraction
```

Referencing of Parameters and Variables defined in this way (i.e. to specify them in a SET or ASSIGN statement or to refer to them in Equations) is discussed here.

Similarly, Arrays of Units (Model instances) are declared by:

```
UNIT
Reactors AS ARRAY(ReactorNames) OF LiquidPhaseCSTR
```

And the properties of each element of the Unit may be specified by:

```
SET
  WITHIN Reactors('LowTempReactor') DO
    ...
  END
# Etc.
```

Finally, it is also possible to declare Selector variables as Arrays of Ordered Sets. The syntax follows the above rules and those for declaring Arrays of Selector variables over integer domains: enter the name of the Ordered Set rather than an integer bound for the Array size.

Ordered Set Operations and Referencing Rules

The following features may be used when developing a Model containing Ordered Sets:

- Set Operations
- Referencing Rules
- Built-in Functions
- Intrinsic Functions

Set Operations

The allowed set operations are:

- Union, defined by +

example:

```
Species := Gases + Liquids ;
```

- Intersection, defined by *

example:

```
Intermediates := Gases * Liquids ;
```

- Set difference, defined by -

example:

```
NonCondensibles := Gases - Liquids ;
```

For Union and Intersection, there are variants that take an arbitrary number of arguments:

- UNION()

examples:

```
AllComponents := UNION(InputConnections().Components);
```

(InputConnections() is an array of nInputs Connections, each carrying an Ordered Set parameter Components.)

Slices can be used as well:

```
Components := UNION(InputConnections(2:nInputs-1).Components);
```

- INTERSECTION()

example:

```
CommonComponents := INTERSECTION( InputConnections().Components );
```

Note that because the sets are ordered, the operations are non-commutative, i.e. Gases + Liquids <> Liquids + Gases (the order of the species will be different in the two cases).

Also, standard arithmetic operator precedence applies to Ordered Set operations: that is, intersections are performed before unions and differences. The order in which these operations are performed may, however, be modified using parentheses.

Ordered Set Referencing Rules

In Parameter specifications, Equations and Assign statements, one may refer to individual elements, slices or the whole Array, as in the case of integer domains. Of course, rather than using integers to refer to individual elements or define slices, the names of the elements in the Ordered Sets are used. The two examples below illustrate the specification of a single element of a Parameter and an Assignment of a slice of a Variable.

```
SET
  FormulaWeight('H2') := 2 ;

ASSIGN
  Flowrate('CH4':'C4H10') := 0.0 ;
```

In the second example above, the flowrates of all the Array elements in the Ordered Set from 'CH4' to 'C4H10' will be set to 0.

In this next example, a material balance Equation is written (implicitly) for all Species:

```
$M = Fin*Xin - Fout*X ;
```

where M, Xin and X are Arrays over the domain 'Species'.

As with Integer domains, FOR loops can be used instead of implicit declarations of Array Equations:

```
FOR i IN Species DO
  $M(i) = Fin*Xin(i) - Fout*X(i) ;
END
```

Multiple domains are handled quite easily. The example below is a material balance for all Species with generation terms summed over the Reactions domain:

```
$M = Fin*Xin - Fout*Xout + SIGMA( (Nu(,Reactions)*Rate(Reactions)) ) ;
```

(For clarity, this may also have been declared explicitly.)

More sophisticated expressions involving set operations and slices are also possible; some examples are given here.

Built-in Functions

The summation operator, SIGMA, is defined over the Ordered Set, e.g.

```
SIGMA(x(Species)) = 1 ;
```

The integral operator, INTEGRAL, is also defined over an Ordered Set, e.g.:

```
INTEGRAL(s OVER QuadPoints ; x(s)*y(s)) = 100.0 ;
```

where QuadPoints is the Ordered Set.

Slices and set operations within built-in functions are also allowed, e.g.:

```
SIGMA(x('H2O'):'Ethane'))  
INTEGRAL(s OVER S1*S2 ; x(s)*y(s))
```

where S1 and S2 are Ordered Sets.

Ordered Set Intrinsic Functions

A number of intrinsic functions are defined for Ordered Set Parameters.

The first element of an Ordered Set is returned as a string by:

```
OrderedSetParam.First
```

The last element of an Ordered Set is returned as a string by:

```
OrderedSetParam.Last
```

The Cardinality (i.e. the size) of an Ordered Set is returned as an integer by:

```
OrderedSetParam.Card
```

The ith Element of an Ordered Set is returned as a string by:

```
OrderedSetParam.Element(i)
```

(where i = 1 is the first element).

One area where this might be useful is in defining material balance equations for all but one of the species in the model. One possibility is as follows.

```
EQUATION  
FOR i IN Species - Species.Last  
    $M(i) = Fin*Xin(i) - Fout*X(i) ;  
END  
SIGMA(X(Species)) = 1 ;
```

The index of a specific element is returned as an integer by:

```
OrderedSetParam.Index(ElementName)
```

A boolean value indicating whether or not an Ordered Set contains a specific element is returned by:

```
OrderedSetParam.Contains(ElementName)
```

A subset over a certain range is returned by:

```
OrderedSetParam.Subset(m,n) - a subset from index m to n inclusive  
OrderedSetParam.Subset(m) - a subset from index m to the last element inclusive
```

The index can be given as a string argument as well as integers.

Examples of the Use of Ordered Sets

Here, we have a database of molecular weights from which we will copy some into a smaller list of components:

```
PARAMETER  
ReagentSpecies, ProcessSpecies, AllSpecies AS ORDERED_SET
```

```
VARIABLE
```

```
MW AS ARRAY(AllSpecies) OF MolWt
MWsub AS ARRAY(ReagentSpecies) OF MolWt

SET
  ReagentSpecies := [ 'HNO3', 'H2O', 'NaOH', 'tbp/ok' ] ;
  ProcessSpecies := [ 'HNO3', 'H2O', 'Uranium' ] ;
  AllSpecies := ReagentSpecies + ProcessSpecies ;

EQUATION
  MW('HNO3') = 1 + 14 + 3*16 ;
  MW('H2O') = 2*1 + 16 ;
  MW('NaOH') = 23 + 16 + 1 ;
  MW('tbp/ok') = 10*12 + 22 ; # approx
  MW('Uranium') = 238 ;

  FOR i IN ReagentSpecies DO
    MWsub(i) = MW(i) ;
  END
```

(Note that it would not be legal to shorten the names of the Ordered Sets to Reagent, Process and All because Process is a reserved word in gPROMS.)

Equations can be written that use streams with identical species lists:

```
VARIABLE
  MassIn AS ARRAY(ProcessSpecies) OF MassFlow
  MassOut AS ARRAY(ProcessSpecies) OF MassFlow
  Losses AS ARRAY(ProcessSpecies) OF MassFlow

SET
  ProcessSpecies := [ 'HNO3', 'H2O', 'Uranium' ] ;

EQUATION
  FOR i IN ProcessSpecies DO
    MassOut(i) = MassIn(i) - Losses(i) ;
  END
```

The equation can also be written as

```
MassOut = MassIn - Losses;
```

Care needs to be taken when combining streams with different species lists:

```
VARIABLE
  MassInR AS ARRAY(ReagentSpecies) OF MassFlow
  MassInP AS ARRAY(ProcessSpecies) OF MassFlow
  MassOut AS ARRAY(AllSpecies) OF MassFlow

SET
  ReagentSpecies := [ 'HNO3', 'H2O', 'NaOH', 'tbp/ok' ] ;
  ProcessSpecies := [ 'HNO3', 'H2O', 'Uranium' ] ;
  AllSpecies := ReagentSpecies + ProcessSpecies ;

EQUATION
  #...for the species common to all streams
  FOR i IN ReagentSpecies*ProcessSpecies DO
```

```
    MassOut(i) = MassInR(i) + MassInP(i);
END
#...for the species only in the Reagent stream
FOR i IN ReagentSpecies - ProcessSpecies DO
    MassOut(i) = MassInR(i);
END
#...for the species only in the Process stream
FOR i IN ProcessSpecies - ReagentSpecies DO
    MassOut(i) = MassInP(i);
END
```

A mixer might mix streams with different species into a single output. This therefore combines three species lists that may be disjoint sets. Care needs to be taken in writing the material-balance equations:

```
VARIABLE
MassInR      AS ARRAY(Reagents) OF MassFlow
MassInI      AS ARRAY(Inerts) OF MassFlow
MassInS      AS ARRAY(Solids) OF MassFlow
MassOut     AS ARRAY(AllSpecies) OF MassFlow

SET
ReagentSpecies := [ 'HNO3', 'H2O' ] ;
Inerts       := [ 'tbp/ok' ] ;
Solids       := [ 'Uranium' ] ;
AllSpecies   := Reagents + Inerts + Solids ;

EQUATION
FOR i IN Reagents DO
    MassOut(i) = MassInR(i) ;
END
FOR i IN Inerts DO
    MassOut(i) = MassInI(i) ;
END
FOR i IN Solids DO
    MassOut(i) = MassInS(i) ;
END
```

Combining three species lists with common entries

```
VARIABLE
MassInR      AS ARRAY(ProcessSpecies) OF MassFlow
MassInI      AS ARRAY(Inerts) OF MassFlow
MassInS      AS ARRAY(Solids) OF MassFlow
MassOut     AS ARRAY(AllSpecies) OF MassFlow

SET
ProcessSpecies := [ 'HNO3', 'H2O', 'Uranium', 'tbp/ok' ] ;
Inerts       := [ 'tbp/ok', 'Unknown' ] ;
Solids       := [ 'Uranium', 'Unknown' ] ;
AllSpecies   := ProcessSpecies + Inerts + Solids ;

EQUATION
#..for the components common to all streams
FOR i IN ProcessSpecies*Inerts*Solids DO
    MassOut(i) = MassInP(i) + MassInI(i) + MassInS(i) ;
```

```
END
#.for the components in Process and Inert streams only
FOR i IN ProcessSpecies*Inerts - ProcessSpecies*Inerts*Solids DO
    MassOut(i) = MassInP(i) + MassInI(i) ;
END
#.for the components in Process and Solids streams only
FOR i IN ProcessSpecies*Solids - ProcessSpecies*Inerts*Solids DO
    MassOut(i) = MassInP(i) + MassInS(i) ;
END
#.for the components in the Solids and Inert streams only
FOR i IN Solids*Inerts - ProcessSpecies*Inerts*Solids DO
    MassOut(i) = MassInS(i) + MassInI(i) ;
END
#... and so on
```

Summation over a subset of an Ordered_Set

```
VARIABLE
MassIn          AS ARRAY(ReagentSpecies) OF MassFlow
TotalProcessFlow AS                         MassFlow

SET
ReagentSpecies   := [ 'HNO3' , 'NaOH' , 'tbp/ok' , 'H2O' ] ;
ProcessSpecies   := [ 'HNO3' , 'H2O' ]                 ;

EQUATION
TotalProcessFlow = SIGMA(MassIn(ProcessSpecies)) ;
```

As with other Arrays, we can have multiple dimensions. For example, a solid liquid separation process described by a recovery factor (RF) might be modelled as:

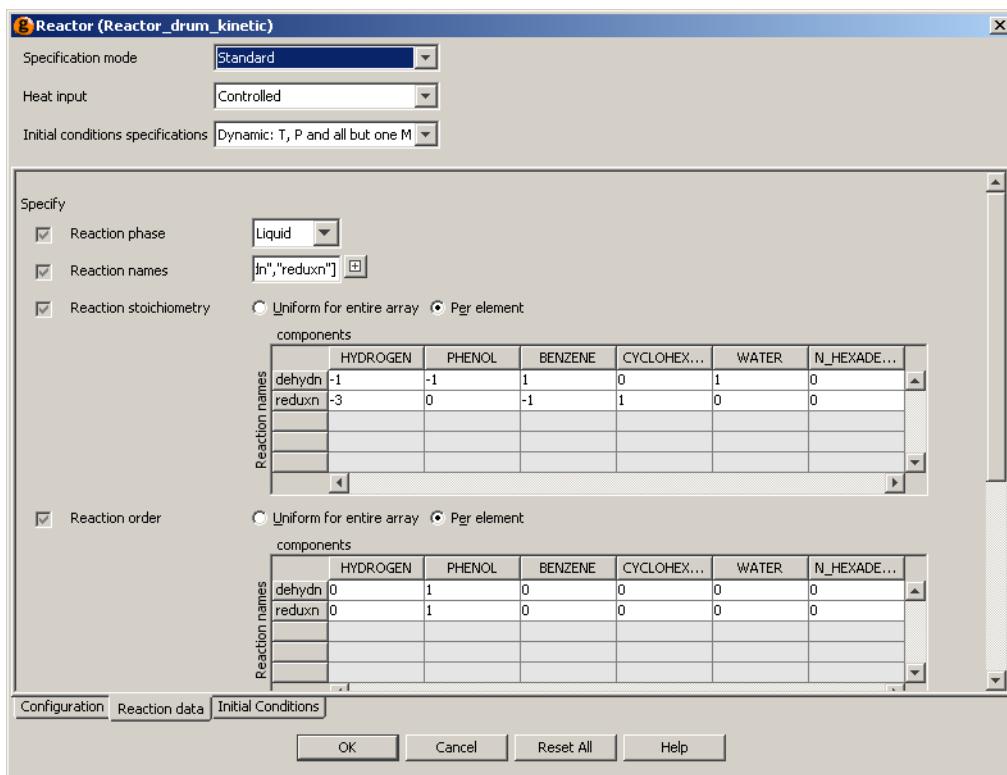
```
VARIABLE
InFlow      AS ARRAY(Species, Phase) OF MassFlow
OutFlow     AS ARRAY(Species, Phase) OF MassFlow
RF          AS ARRAY(Species, Phase) OF MassFlow

SET
Species   := [ 'Cs134' , 'Cs137' , 'Sr90' ] ;
Phase     := [ 'Liquid' , 'Solid' ]           ;

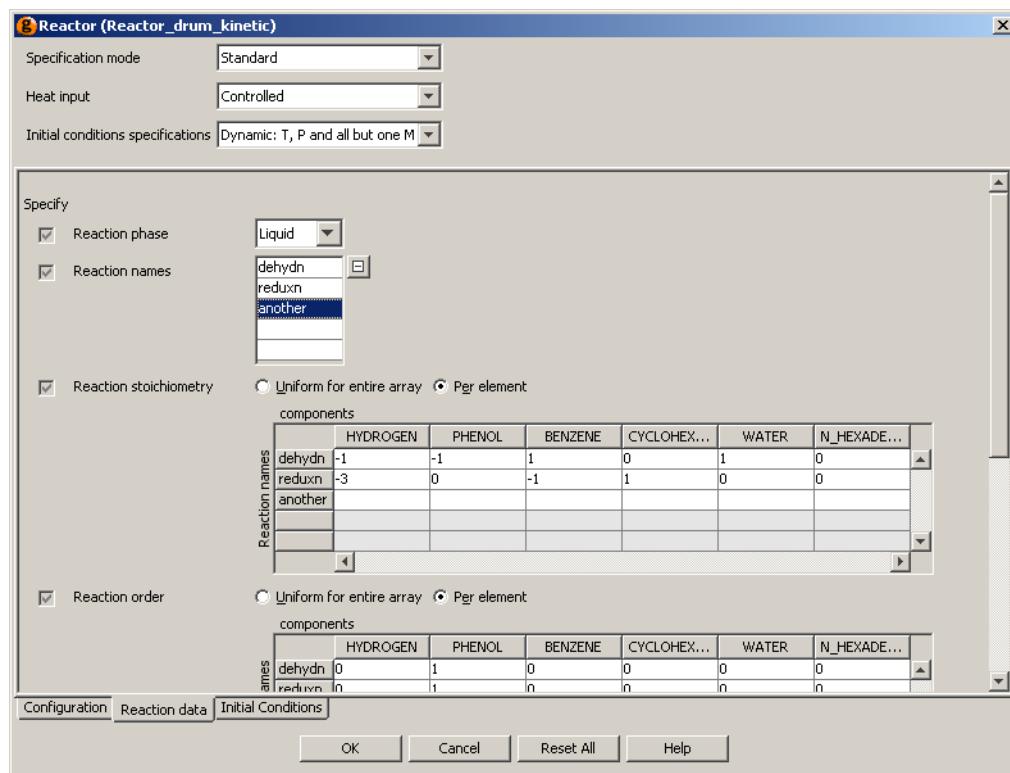
EQUATION
FOR i IN Species DO
    OutFlow(i,'Liquid') = InFlow(i,'Liquid')*(1 - RF(i,'Liquid'))
                           + InFlow(i,'Solid')*RF(i,'Solid') ;
    OutFlow(i,'Solid') = InFlow(i,'Solid')*(1 - RF(i,'Solid'))
                           + InFlow(i,'Liquid')*RF(i,'Liquid') ;
END
```

Ordered Sets in Model Specification Dialogs

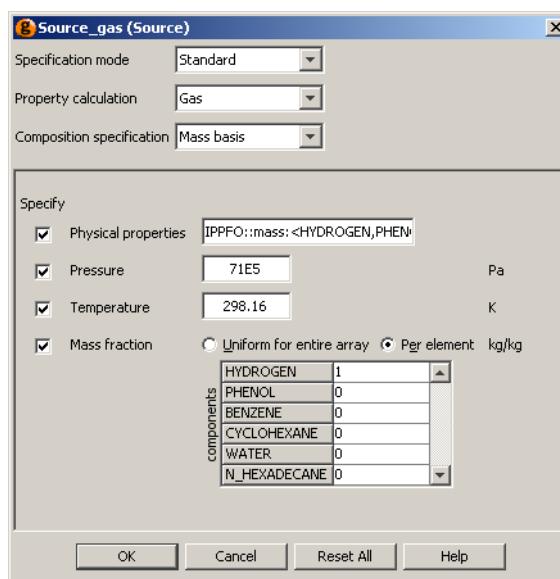
Ordered Sets can be specified in Model specification dialogs just as any other Parameter. The elements of the Ordered Set can be entered by the user and these will then affect the input tables of any Parameters or Variables that depend on the Ordered Set. In the example below, we have model of a reactor with an Ordered Set of reactions and stoichiometric parameters that are indexed over the set of reactions and components.

Figure 9.1. Reaction Data Tables Labelled with Elements from Ordered Sets

The elements of the Ordered Set of reactions (labelled Reaction names) can be specified using gPROMS language, as shown above, or by editing each element individually in a matrix. In order to do this, left click on the button next to the text box. In the image below, another reaction has been entered in this fashion. Notice that the tables for the stoichiometric parameters are automatically updated once the new reaction has been entered (or an existing one deleted — simply by editing the entry and deleting it).

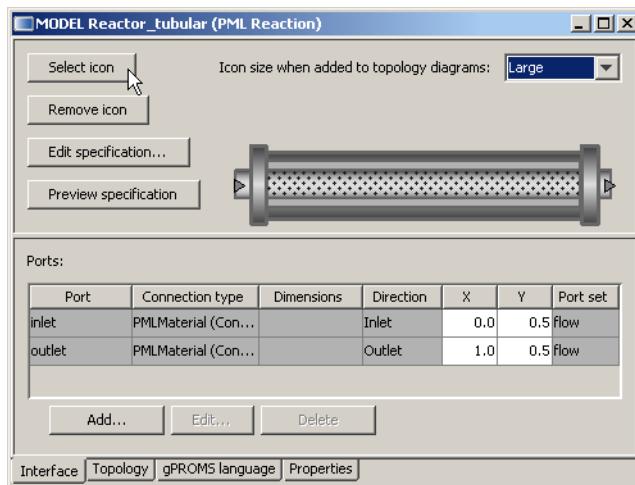
Figure 9.2. Entering a New Reaction: the Data Tables are Automatically Updated

It is also apparent from the above figures, that the components are also represented by an Ordered Set. This can be specified in exactly the same way, but in this example, it is given by a physical property Foreign Object. Just as when changing, adding or removing an element of the reactions Ordered Set, the data-entry tables for any Parameters or Variables that are indexed over the set of components will automatically change. The figure below shows the format for entering component data using the Ideal Physical Property Foreign Object (see the Physical Properties Guide): the Ordered Set of components is automatically updated by the physical-property Foreign Object whenever the specification is changed, and this then updates the table of mass fractions below and the reaction-data tables in the figure above.

Figure 9.3. Ordered Set being defined by a Physical Property Foreign Object

Chapter 10. Defining a Public Model Interface

Providing a Model with a Public Interface allows it to be used quickly and easily on the *topology* tab of flowsheet Models.



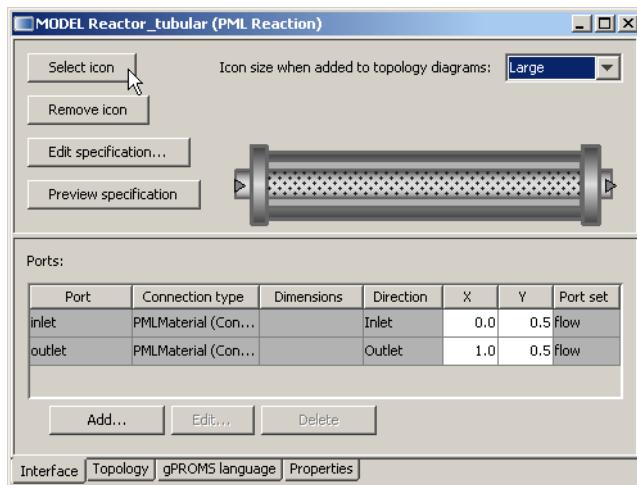
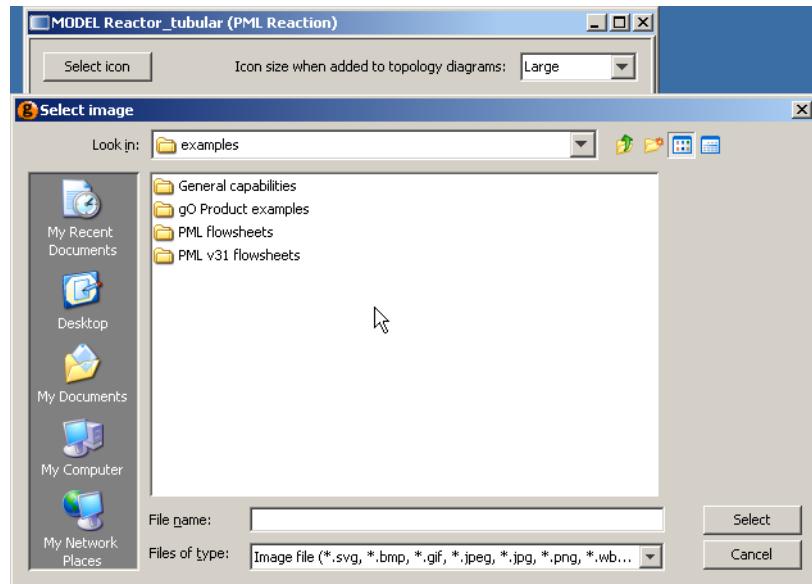
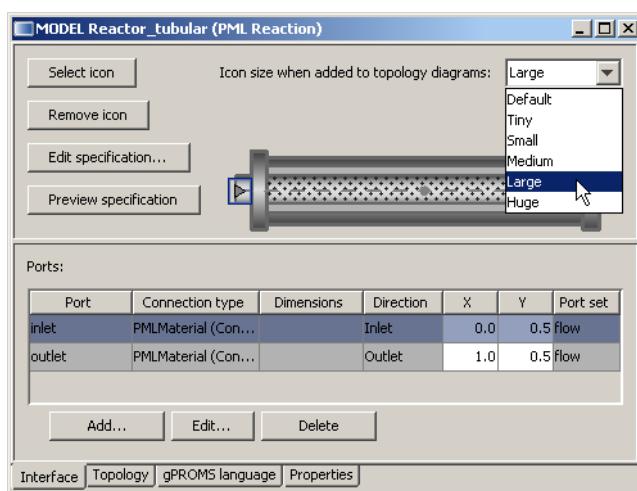
The Model Interface has four key facets:

- A Model icon which determines how the Model is displayed on the *topology* tab of flowsheet Models.
- Model Ports to allow connections to other component Models.
- A Specifications dialog to enable easy specification of Model inputs and initial conditions.
- A Model report to present key results in a clear format following a *Simulation* activity.

Defining a Model icon

The Model icon determines how an instance of the Model is displayed on the *topology* tab of a flowsheet Model. It is possible to associate any icon of your choice with a particular Model. To do so, you need to do the following:

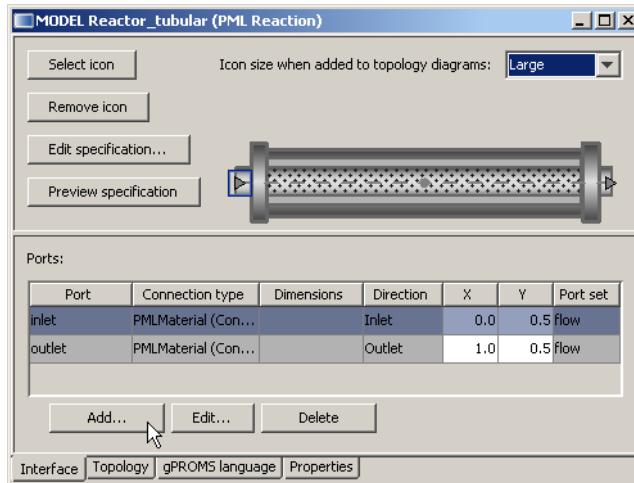
- On the *interface* tab the Model entity click on the Select icon button (see figure (a) below). This will open a dialog box that allows you to browse and select your desired image.
- Use the browser to select your image file and press the OK button (see figure (b) below).
 - ModelBuilder supports the following image formats: .svg, .gif, .jpg (or .jpeg) and .png.
- You have the option of selecting a default size for the icon size (see figure (c) below).

Figure 10.1. Defining an icon - (a) the Select icon button on the interface tab**Figure 10.2. Defining an icon - (b) selecting the desired image file****Figure 10.3. Defining an icon - (c) choosing the default icon size**

Defining Model Ports

Topology connections to and from a Unit are made from its Ports. These are configured from the Port table in the lower pane of the *Interface* tab:

Figure 10.4. The Port table



The Port table shows the following information:

- Port *name*: the name by which the Port will be referenced in the gPROMS language.
- Connection Type: the Connection Type which the Port is associated with (see also: Declaring new Connection Types). Only topology connections of this *type* can be connected to this Port.
- Dimensions: the dimensionality of the Port — both *scalar* and *Array* Ports are supported.
 - Array Ports of *Fixed size(s)* and of *Dynamic size* are supported. For dynamically-sized Ports, the size of the Array is specified by the number of connections made to that Port. If no connections are made, the size of the Array will be set to zero, the benefits of which are discussed here.
- Direction: The Port direction — *Inlet*, *Outlet* or *Bi-directional*. gPROMS enforces the following rules

	Inlet	Outlet	Bi-directional
Inlet	Disallowed	Allowed	Allowed
Outlet	Allowed	Disallowed	Allowed
Bi-directional	Allowed	Allowed	Allowed

- X & Y co-ordinates: the location of the Port on the Model's icon.
- Port set: The *set* to which the Port belongs.
 - For all Ports belonging to the same *set* (i.e. those in the same Port set): the equivalent Connection Type Parameters will be equated. For example; in a device with two flow paths such as a heat exchanger, with a hot stream and a cold stream, the hot *inlet* and *outlet* Ports would be in a hot *set* and the cold *inlet* and *outlet* Ports would be in a cold *set*. (see also: Setting Connection Type Parameters).
 - Ports in the same *set* are indicated graphically on the Model's icon by a dotted connectivity line; indicating (material or information) flow paths.

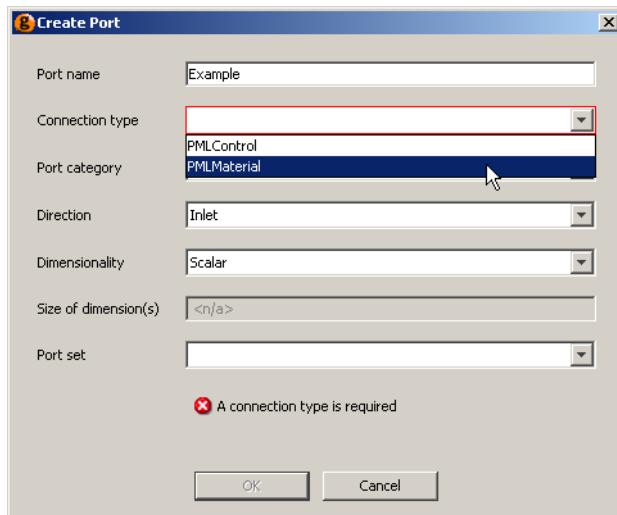
From the interface tab, click on the Add button to Create a new Port.

When you declare a Port in a Model, it is associated with a Connection Type. All the quantities declared by the Connection Type (Variables, Parameters and Distribution Domains) are automatically included in the Model that declares the Port. So an equivalent number of Equations should be provided in the Model entity to make use of the additional Variables. This is done in the gPROMS language declaration for the Model.

Create a new Port

Click on the Add button to define a new Port, or click the Edit button to modify an existing Port. This will activate a *Create Port* (or *Edit Port*) dialog box:

Figure 10.5. Creating a new Port



- Port name: enter the name of the Port
- Connection type: choose the Connection Type from a drop down menu or manually enter the name.
- Port category: if the Connection Type enforces connectivity rules a Port category must be provided; select this from the drop-down menu.
 - The category of a Port determines which other Ports a connection may be made to (see also: The Port categories tab and Connectivity rules).
- Direction: choose an Inlet, Outlet or a Bi-directional Port.
- Dimensionality: you can select a *Scalar* Port, an Array Port of *Fixed size(s)* or an Array Port of *Dynamic size*.
 - If you select *Scalar*, then no further specification is required.
 - If an Array Port of Fixed size(s) is selected, then under Size of dimension(s) enter the size(s) as either a literal value (e.g. 7) or using an Integer Parameter whose value is provided elsewhere.
 - If an Array Port of Dynamic size is selected, then select an Integer Parameter from the Model declarations. This Parameter will be set automatically to a value equal to the number of connections made to the Port.
 - If there are no connections made to the port, the Parameter will be set to zero. This will result in an Array of zero length, the benefits of which are discussed here.
- Port set: you can add a name for a new *set* or select a name of an existing *set* (see also: Port set and Setting Connection Type Parameters).

The locations of Ports on the Model icon are specified directly on the *Interface* tab. The location of a Port is stored in terms of an X co-ordinate and a Y co-ordinate [0 to 1], with (0,0) being in the top left corner of the icon. To determine the location of the Port:

- Either (i) move the Port to the appropriate place on the icon by dragging it using the mouse;
- or (ii) enter a co-ordinate: to do this simply click on the relevant cell and type in the number.

Ports and the gPROMS Language

All Ports defined using the Interface tab, are reflected on the Model's *gPROMS Language* tab with the following syntax:

PART

```
PortName AS ConnectionType  
PortName AS ARRAY (Size <,>) OF ConnectionType.
```

Port sets are also reflected on the Model's *gPROMS Language* tab with the following syntax (though in read-only text):

PARTSET

```
[PortName, ..., PortName] {PortSetName} ;
```

An example of Ports and Port sets for the *Reactor_tubular* Model from the gPROMS Process Model Library is shown below

```
PART  
    in      AS PMLMaterial  
    out     AS PMLMaterial
```

```
PARTSET  
# Start Port Sets  
    [in, out] {flow} ;  
# End Port Sets
```

All the quantities declared for this Connection Type (Variables, Parameters and Distribution Domains) are automatically included in the Model. As with the development of composite Models, these are referenced using a *pathname* construct:

Therefore, to equate the Connection Type Parameters carried by the inlet Port to equivalent Model Parameters; one could write:

```
SET  
no_components := in.no_components,  
phys_prop      := in.phys_prop;  
.....
```

Similarly, the Connection Type Variables are used directly in Model Equations (you may note from this that the *Reactor_tubular* Model is a distributed Model):

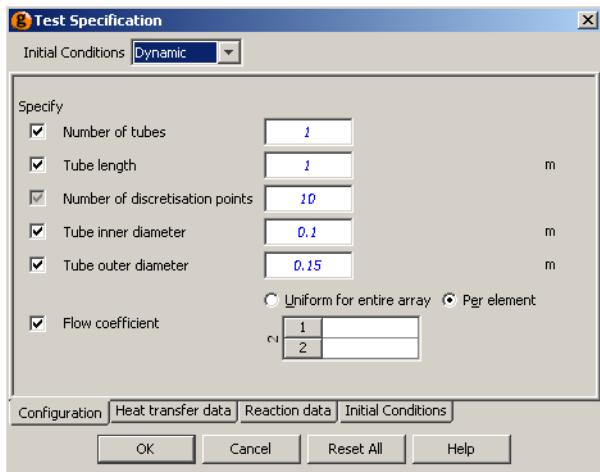
```
EQUATION  
# Using Port Variables in a Model as Boundary conditions for a distributed model  
mass_flowrate(0)          = in.mass_flowrate/number_of_tubes ;  
mass_fraction(,0)          = in.mass_fraction = in.info_mass_fraction ;  
mass_specific_enthalpy(0)  = in.mass_specific_enthalpy = in.info_mass_specific_enthalpy ;  
pressure(0)                = in.info_pressure ;  
  
mass_flowrate(1)          = out.mass_flowrate/number_of_tubes ;  
mass_fraction(,1)          = out.mass_fraction ;
```

```
mass_specific_enthalpy(1) = out.mass_specific_enthalpy ;
```

.....

Defining a Specification dialog and Model Reports

A Model is defined both by its Equations **and** the specifications that must be provided to satisfy its degrees of freedom. In gPROMS, the required set of specifications and the initial conditions for a Model can be stored with that Model. These are then accessed via its Specification dialog, as shown below.



The Specification dialog makes it easy to share the Model with other users and makes it faster and easier to reuse the Model:

- Specification dialogs are accessed from a flowsheet Model's *topology* tab. (see also: Constructing flowsheet Models).
- Specification dialogs allow:
 - Parameters to be Set values,
 - Variables to be Assigned values,
 - Selectors to be given initial values,
 - and Initial conditions to be defined.
- The specifications made using Specification dialogs in a flowsheet Model are displayed as read-only text in the Process entity that includes the flowsheet Model.
- In the associated Process entity the user has the option to include unit dialog specifications or not. This option is accessed
 - *either* from the Entity menu when the Process entity is selected
 - *or* from the short-cut menu accessed by right-clicking on the appropriate Process entity.

When removing dialog specifications; the existing specifications can be left for manual modification or removed completely.

Specification dialogs are configured from a Model's *interface* tab by clicking the Edit specification ... button. This will also give you the opportunity to define a Model report. Model reports are used to present key results in a clear format following a *Simulation* activity (see also: Viewing Model reports).

After clicking the Edit specification ... button you are guided through the following five steps:

- Public Model Attributes
- Define tabs in Dialog
- Configure Specification Dialog
- Define Model Help
- Configure report

To move between the steps use the Next and Previous buttons; when the Specification is complete click the Finish button. At any point it is possible to Preview the specification dialog and the Model reports using the Preview specification and Preview report buttons:

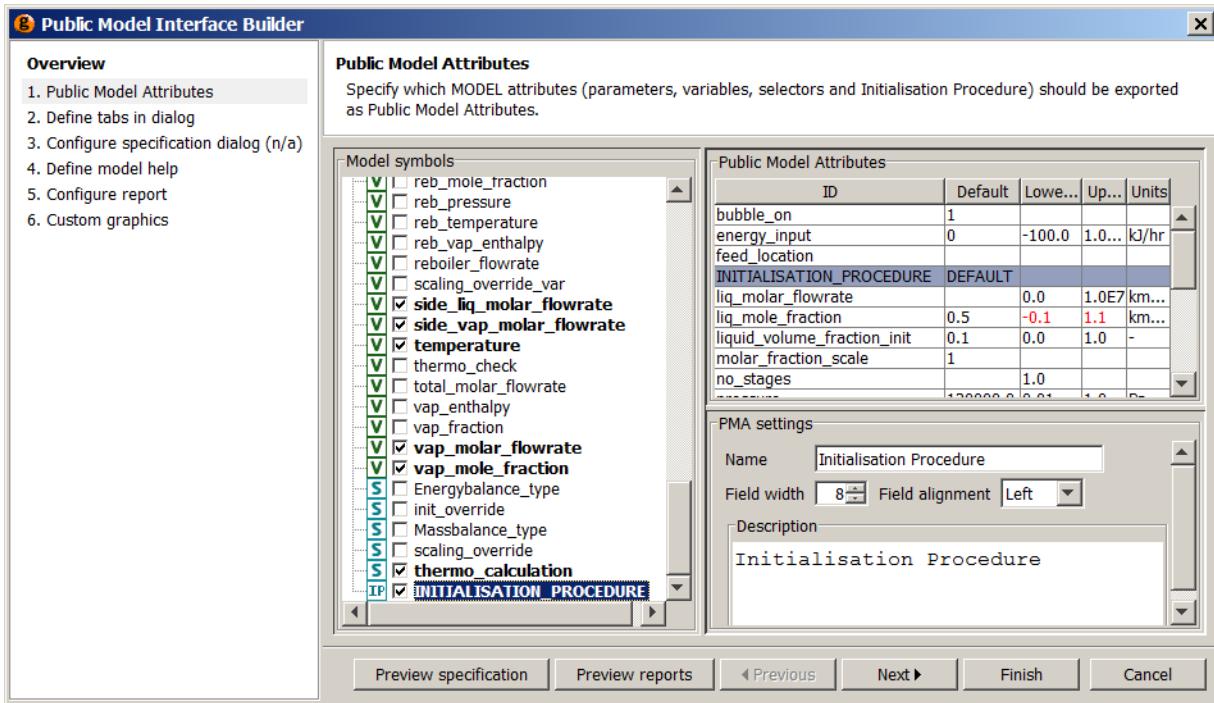
Defining Public Model Attributes

Step 1

The first step is to specify from the full set of Parameters, Variables and Selectors declared by the Model (*the Model symbols*) a **sub-set** which shall be exported as *Public Model Attributes* (PMA). These are essentially those that will *either* appear on a Specification dialog *or* appear on a Model report.

When compared against other Model symbols, Public Model Attributes have the following additional information

- Name: A display name for the PMA not necessarily the same as its ID (i.e. how it is referred to in the gPROMS language)
- Default : The default value for the PMA when it appears on the Specification dialog
- Lower and Upper bounds: These are used to guide the Model user to provide sensible values for the specification
 - It is still possible for a user to provide a value outside these bounds but the value enter will be highlighted with a warning message
 - For Variables it is anticipated that these bounds would be much tighter than those provided by its Variable Type which are usually relatively loose.
- Units: The engineering units are displayed wherever the PMA appears on the Model's Specification dialog and report
- Field width and Field alignment: The size and alignment of the space provided to give the PMAs value.
- Description: In the description, additional information about the PMA can be given; this is displayed to the Model user as a *tool-tip* when the mouse hovers over the PMA on the Specifications dialog.

Figure 10.6. Public Model Attributes page

To define the Public Model Attributes:

- Select the Public Model Attributes from the *Model symbols* pane. Do this by clicking on the *check box* to select the desired Model attribute; all the *checked* symbols will appear in the Public Model Attributes table.
- The default value, the lower bound, the upper bound and the units for the PMA are entered directly in the PMA table.
 - Note that the bounds and units are only meaningful if the attribute is a Parameter or a Variable. The bounds for PMA Variables are initially taken from their Variable Types but it is highly recommended that these are refined to bounds that prevent the Model being used in operating regions for which it is not valid.
- The PMA's name, description and the width of its value field and the alignment for this field are specified in a separate pane and are accessed by selecting the PMA in the PMA table.

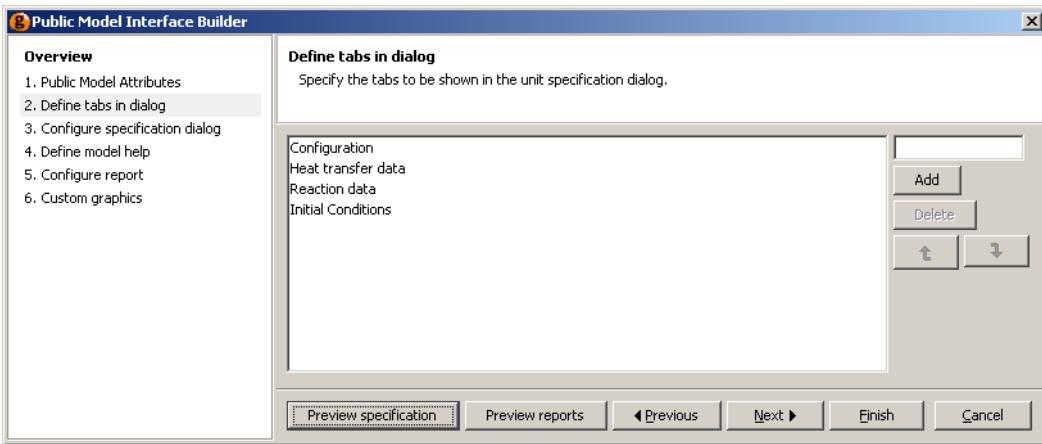
As can be seen in the image above, Initialisation Procedures can be included in a Public Model Interface. A name and description can be given for the Initialisation Procedure and the default value must be set to DEFAULT. At present, the Model user will only have the option of selecting whether or not Initialisation Procedures are used; if they are to be used, they must be the default Initialisation Procedure. Non-default Initialisation Procedures must be specified using the gPROMS language tab of the Process.

Specifications dialog tabs

Step 2

The Specification dialog can have any number of tabs (including zero); these can be given appropriate names.

Tabs are typically used to group similar PMAs together and, equally, to separate dissimilar quantities. For example, it is common to put Variable Assignments on one tab, *Configuration*, and Initial condition specifications on another, *Initial conditions*.

Figure 10.7. Defining the tabs for the Specification dialog

To define a tab:

- Type the tab name in the field on the right-hand-side and click Add
- If multiple tabs are present these can be ordered using the up and down arrow buttons

Configure specification dialog

Step 3

Model specifications are given in terms of the Public Model Attributes (PMAs); these are accessed by the Model user from the Specification dialog. Following the identification of the PMAs in *Step 1*, the following additional information must be provided to configure the behaviour of the dialog:

- which of the PMAs should appear on the dialog
- on which dialog tab the PMAs should appear
- the type of specification required for the PMA
 - Obligatory - the Model user must provide this specification
 - Optional (on) - the Model user can provide this specification; the default is that the specification should be given
 - Optional (off) - the Model user can provide this specification; the default is that the specification is not given

Furthermore, whilst Parameter PMA specifications will automatically appear in the SET section and Selector PMA specifications will automatically appear in the INITIALSELECTOR section, we must specify whether a Variable PMA corresponds to an Initial condition equation (INITIAL section), a Model input (ASSIGN section) or even a Preset value (PRESET section).

Initial conditions

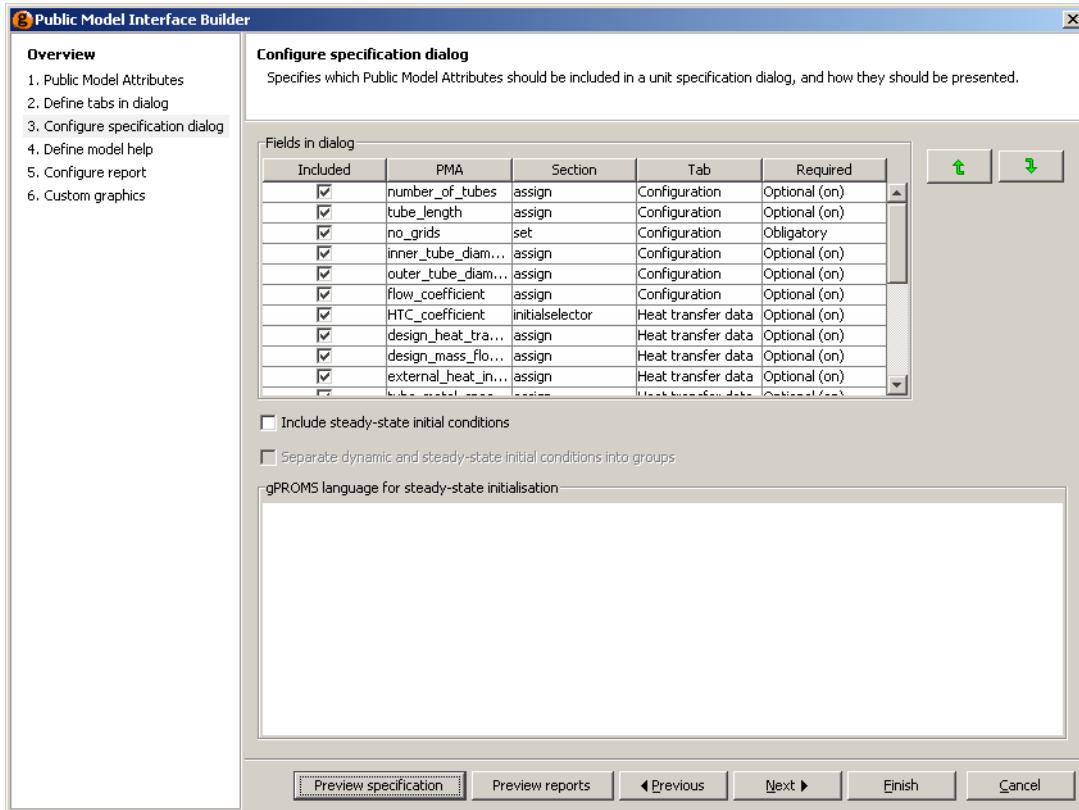
Two types of initial condition specification are possible using a Specification dialog:

- Dynamic: these are of the form:
`PMA_Variable = value;`
- Steady-state: the equations for steady-state Initial conditions must be provided by the Model developer

Both specifications types can be enabled for a Specifications dialog and, if so, these should be separated into different specification groups. If the steady-state group is selected then the Model user need not give any further

specification regarding the Initial conditions. On the other hand, if the dynamic group is selected then the Initial values of the PMA Variables must be provided in the Specification dialog

Figure 10.8. Configuring the specification dialog



To specify which of the Public Model Attributes (PMAs) should be included in the Specification dialog and the appearance of the Specification dialog:

- Select the PMAs that you wish to include in the Specifications dialog by *checking* the box next to the PMA¹.
- If you have selected a PMA Variable: choose the section of the Process entity that the PMA will appear in when given a value: ASSIGN, INITIAL or PRESET.
- If multiple tabs have been selected:- specify which tab of the Specification dialog the PMA should appear on
- Choose the type of specification required for the PMA - *Obligatory*; *Optional (on)* or *Optional (off)*.
- If steady-state initial conditions are required -
 - *check* the Include steady-state initial conditions box
 - if dynamic initial conditions have also been provided (i.e. PMA Variables with INITIAL as the section) then also *check* the Separate dynamic and steady-state initial conditions into groups box
- If the Include steady-state initial conditions box is *checked*: the gPROMS language for the steady-state initial conditions for this Model must be entered in the space provided. For example, the steady-state initial conditions for a distributed tubular reactor (where volume_specific_internal_energy and mass_conc are the state Variables) can be written:

```
FOR z := 0 |+ TO 1 DO
```

¹You may have chosen some PMAs because they are useful output variables.

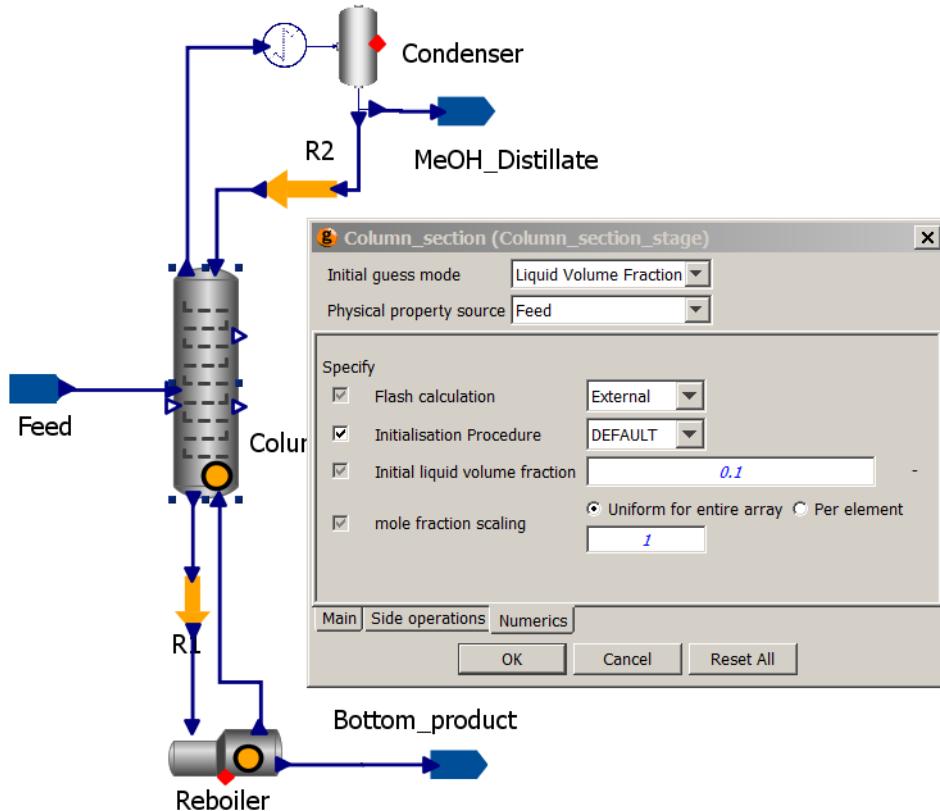
```

$volume_specific_internal_energy(z) = 0;
FOR i := 1 TO no_components DO
    $mass_conc(i,z) = 0;
END # For
END # For

```

For Initialisation Procedures, the type of specification must be set to *Optional (on)*. An example of Initialisation Procedure specification in a Model specification dialog is shown below. (To activate the Model specification dialog, double click on the Unit.)

Figure 10.9. Model Specification Dialog including Initialisation Procedure

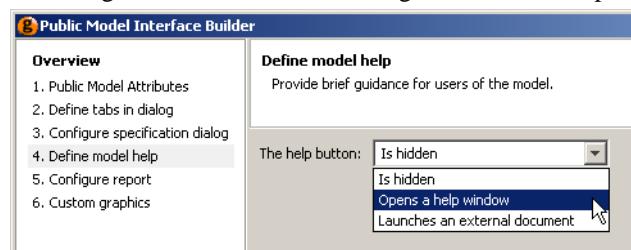


The Model user is able to check or uncheck the Initialisation Procedure in order to enable or disable it. However, the combobox to the right contains only DEFAULT and cannot be changed, since the choice of Initialisation Procedure cannot be made in a Model specification dialog at present.

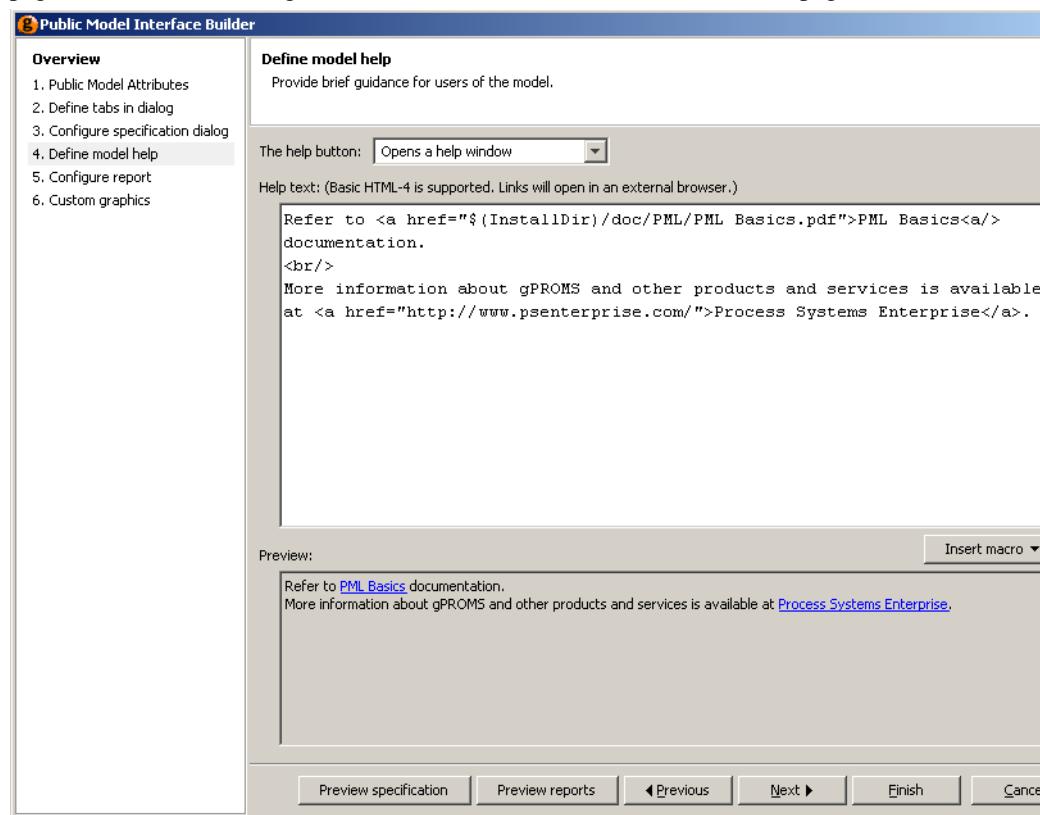
Defining Model help

Step 4

A Help button can be added to the public Model interface. Help can be provided in two different ways or disabled according to the selection made using the listbox in step 4 of the Public Model Interface Builder dialog:



When Opens a help window is selected, the dialog changes to include a text box and a preview pane. The help page must be defined using XHTML and can include links to external web pages and documents, as shown below.



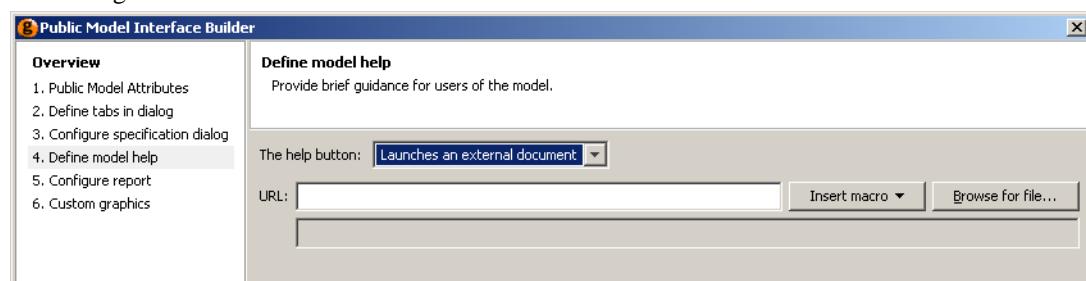
The preview pane is updated in real time, as the XHTML is edited above. Any links in the help page are active in the preview pane and can be followed by left clicking on them. Links to external web sites will open a new browser window or tab (depending on your browser settings); links to files will launch the appropriate reader.

When providing links to documents, the Insert macro button provides a quick way to refer to common directories:



When typing in the path to an external document, selecting one of the options from the list box above will result in the macro being inserted into the text. See the previous screen shot for an example.

The simplest way to provide Model help is to link directly to an external document. This is done by selecting Launches an external document from the Help button: list box. The Public Model Interface Builder dialog will then change to:

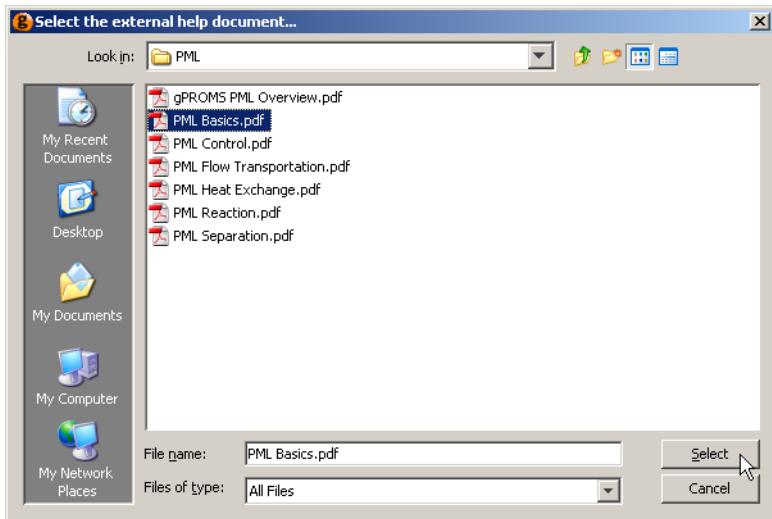


There are two ways to specify the location of the external document:

- Type the location into the URL: text box

- The Insert macro button can be used as before
- Locate the document using the Browse for file... button

When using the file browser, navigate to the desired document and press Select:



If the document is contained in the same directory as the project file (or is contained in one of its sub directories), then another dialog will appear. This allows you to choose whether to specify the location of the document as an absolute path or a relative one.



If documentation is always kept in the same location, then select an absolute path: this way, the project file can be moved to a different location without breaking the link. This would be useful if, for example, a Model developer released a project file to a number of different users but wanted to keep one copy of the documentation in a single public directory. If the documentation is to be kept in the same folder as the project file (or one of its subfolders), then select a relative path so that the project folder can be moved to a different location without breaking the link.

Defining custom reports

Stage 5

Model reports are used to present key results in a clear format following a *Simulation* activity (see also: Viewing Model reports).

There are three ways to configure the reports for a Model. These are:

- None — no report for the Model will be generated.
- Basic — a basic tabular report for the Model will be generated automatically using a simple configuration tool.
- Advanced — the user can fully specify the format of the report, including tables and plots, using xml. This method gives the most control over the reports but is the most complicated to use.

To select the method for specifying reports, left click on the drop-down menu and select the desired option. Selecting Basic enables a GUI in the bottom pane of the window, where you can select the Variables that should be included in the report. Selecting Advanced enables a text editor in the bottom pane, where you may enter xml

to define the report. There may already be some xml present if you have already defined a report using the Basic method.

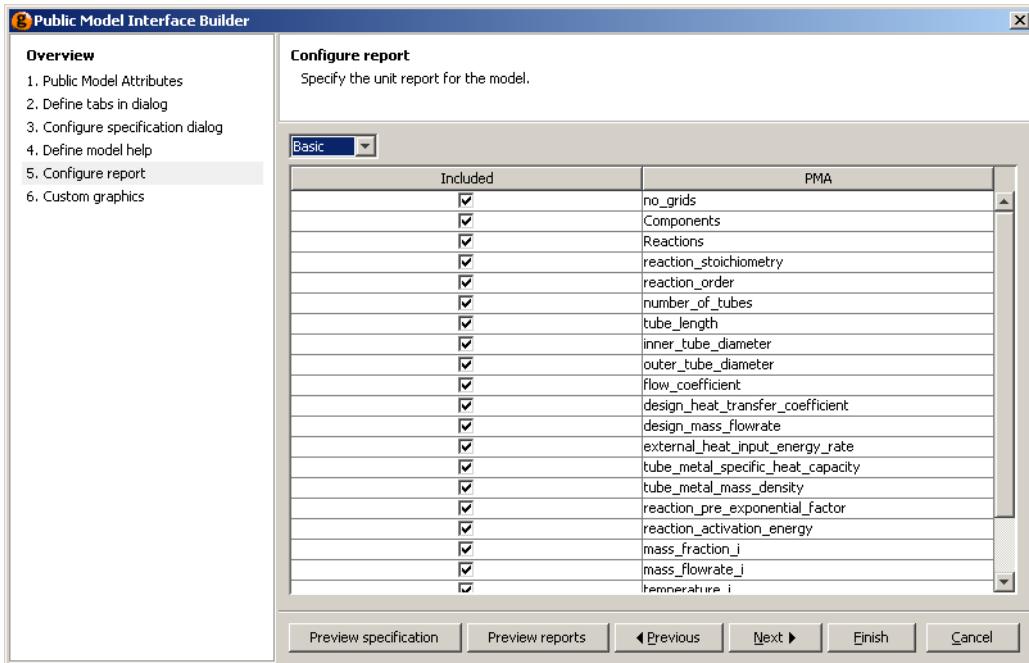
Once you have finished, press the Finish button at the bottom of the window.

Basic Report Configuration

The basic tool for configuring model reports enables you to select variables for inclusion in the report in tabular form only. Check the boxes of all the variables you wish to appear in the report and then click Finish to complete the configuration.

If you want to include any plots in the report, then you must select Advanced from the drop-down menu.

Figure 10.10. Example Model Report configuration



Advanced Report Configuration

Advanced report configuration is achieved using xml. In addition to standard HTML tags, so that headings, images² and hyperlinks to external documents and URLs may be included to enhance the report, there are three custom tags that define five types of Model report. These are:

- Simple Tags — to present basic model attributes.
- Tables — to present tabulated data.
- 2D Plots — to present Variable data graphically as a function of one of the independent domains.
- x-y Plots — to plot values of one Variable as a function of another Variable. (This is a special case of the 2D Plot, so read about 2D Plots first.)
- 3D Plots — to display a surface plot of one Variable as a function of 2 independent domains.
- Contour Plots — to display a contour plot of one Variable as a function of 2 independent domains.

²The following image formats are supported in Model reports: .gif, jpg (and .jpeg) and .png. They can be inserted into model reports using the standard tag, e.g.:

```
 .
```

As with the Basic configuration utility, once you have finished editing the xml, simply press the Finish button at the bottom of the window.

Note that a
 tag is required between any of the entities above in order to ensure they are correctly displayed vertically on the page. To place entities side-by-side, use a table:

```
<table>
  <tr>
    <td><Plot3D ...></td>
    <td><Plot3D ...></td>
  </tr>
</table>
```

Simple Tags

The following simple tags may be used when developing Model Reports.

- <PMA_UNIT> displays the unit name.
- <PMA_NAME id=" . . ."> displays the PMA name of the PMA specified by the `id` attribute.
- <PMA_UOM id=" . . ."> displays the units of measurement for the PMA specified by the `id` attribute.
- <PMA_VALUE id=" . . ."> displays the value(s) of the PMA specified by the `id` attribute.

Tables

Tables can be included in a Model report using two xml tags. The first, <PMA_TABLE>, creates the table; the second, <Attribute/>, specifies a variable for inclusion in the table. There may be multiple <Attribute/> tags within a <PMA_TABLE> tag to form a table containing as many variables as desired. An example is given below.

```
<PMA_TABLE>
  <Attribute id="a_Variable"/>
</PMA_TABLE>
```

The xml above creates a table within the report that displays the values associated with the Variable called `a_Variable`. If the Variable specified in the `id` attribute is distributed over any number of domains, then all of the values will be tabulated automatically.

To include more than one variable, simply add further <Attribute/> tags within the <PMA_TABLE> construct.

The number format for each variable can be set by specifying the `numberFormat` attribute of the <Attribute/> tag:

```
<PMA_TABLE>
  <Attribute id="a_Variable" numberFormat="% . pS" />
</PMA_TABLE>
```

where `p` (the precision) is an integer from 0 to 9 and `S` (the specifier) is one of "G", "f" and "E", respectively representing the General, Fixed and Scientific number formats. If the general format is chosen, then `p` is restricted to integers from 1 to 6 and represents the number of significant figures; the fixed number format allows integers from 0 to 9, which represent the number of decimal places; the scientific format allows between 0 and 5 decimal places. Some examples are given below.

```
<PMA_TABLE>
  <Attribute id="Variable1" numberFormat=". 4G" /> <!--General with 4 s.f.-->
  <Attribute id="Variable2" numberFormat=". 6f" /> <!--Fixed with 6 d.p.-->
  <Attribute id="Variable3" numberFormat=". 3G" /> <!--Scientific with 3 d.p.-->
```

```
</PMA_TABLE>
```

The `<PMA_TABLE>` tag may also contain a `numberFormat` Attribute. This specifies the number format for any `<Attribute>` tags that do not contain a `numberFormat` Attribute. This is a more compact and convenient method for setting the same number format for several Variables. If there is no `numberFormat` Attribute specified for the `<PMA_TABLE>` tag and there are `<Attribute>` tags that do not contain a `numberFormat` Attribute, then the number format for these `<Attribute>` tags is taken from the specification in the ModelBuilder preferences, in the Results section of the Activity execution preferences.

Note that all of the tags and attributes described above are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

The full list of available number formats is given in the table below.

Format name	Format string
General, 1 s.f.	"% .1G"
General, 2 s.f.	"% .2G"
General, 3 s.f.	"% .3G"
General, 4 s.f.	"% .4G"
General, 5 s.f.	"% .5G"
General, 6 s.f.	"% .6G"
Fixed, 0 d.p.	"% .0f"
Fixed, 1 d.p.	"% .1f"
Fixed, 2 d.p.	"% .2f"
Fixed, 3 d.p.	"% .3f"
Fixed, 4 d.p.	"% .4f"
Fixed, 5 d.p.	"% .5f"
Fixed, 6 d.p.	"% .6f"
Fixed, 7 d.p.	"% .7f"
Fixed, 8 d.p.	"% .8f"
Fixed, 9 d.p.	"% .9f"
Scientific, 0 d.p.	"% .0E"
Scientific, 1 d.p.	"% .1E"
Scientific, 2 d.p.	"% .2E"
Scientific, 3 d.p.	"% .3E"
Scientific, 4 d.p.	"% .4E"
Scientific, 5 d.p.	"% .5E"

2D Plots

2D Plots are created using the `<Plot2D>` tag and lines specified with the `<Line/>` tag. The basic format is:

```
<Plot2D version="1">
  <Line idY=" "/>
</Plot2D>
```

The `version` attribute of the `<Plot2D>` tag is mandatory and must be equal to 1.

Each `<Line />` tag specifies which Variable is to be plotted against which independent domain, using the `idY` attribute. The format of the attribute is a string comprising the name of the Variable to be plotted and a specification

indicating which domain should be free and plotted on the abscissa and the values of any domains that need to be fixed³. This is best illustrated with an example.

```
<Plot2D version="1">
  <Line idY="A(TIME=#)" />
</Plot2D>
```

Here we have just one line specified for this 2D Plot (which will be 600 pixels wide and 400 pixels high).

The `idY` attribute of the `<Line />` tag specifies that the Variable A should be plotted with time as the independent variable on the abscissa. Here, we see two features of the specification format: the first domain is always time and is indicated by the string "`TIME=`", followed by either a number or the `#` symbol. The `#` symbol indicates that the domain should be free and will be plotted on the abscissa. Since there are no other domain specifications, A must be defined either as a scalar or as a vector. If A is defined as a scalar, then the `<Line />` tag simply produces one line in the 2D Plot. However, if A is defined as a vector (i.e. distributed over just one domain, either discrete or continuous), then the `<Line />` tag produces one line for every element of the domain.

To clarify the above, if the Variable A is defined in the Model by:

```
VARIABLE
  A          AS NoType
```

Then only one line will be plotted in the graph. However, A may also be defined by:

```
VARIABLE
  A          AS ARRAY(NoComp) OF NoType
```

or

```
VARIABLE
  A          AS ARRAY(Components) OF NoType
```

or

```
VARIABLE
  A          AS DISTRIBUTION(X_Domain) OF NoType
```

where `NoComp` is an integer, `Components` is an Ordered Set and `X_Domain` is a `DistributionDomain`. In any of these cases, a series of lines will be plotted in the graph, one for each element of A.

If, in this second case, you want to plot only a single line, corresponding to a fixed value of the domain over which A is defined, then this can be achieved by (for example):

```
<Plot2D version="1">
  <Line idY="A(TIME=#,1)" />
</Plot2D>
```

Another alternative is to plot the variable against the domain for some fixed value of time. This is done with the following commands.

```
<Plot2D version="1">
  <Line idY="A(TIME=0,#)" />
</Plot2D>
```

The same rules apply to Variables defined over more than one domain, as shown in this next example.

```
<Plot2D version="1">
  <Line idY="A(TIME=#)" />
```

³Of course, there can only be one free domain in a 2D Plot and all other domains need to be fixed.

```
<Line idY="B(TIME=#,1)" />
<Line idY="C(TIME=5,2,#)" />
<Line idY="C(TIME=#,1,0)" />
</Plot2D>
```

Here, we have 4 `<Line/>` tags, which will produce 4 lines in the graph, assuming the following variable definitions.

VARIABLE

A	AS	NoType
B	AS ARRAY(NoComp)	OF NoType
C	AS DISTRIBUTION(NoComp, X_Domain)	OF NoType

So, the first `<Line/>` tag produces a plot of A against time; the second gives B(1) versus time; the third gives the second component of C plotted against the x domain at time t = 5; and finally the last `<Line/>` specifies the first component of C to be plotted agains time with the x domain fixed at 0.

Notice that the abscissa of the graph may be used to represent more than one independent domain. Although this practice is allowed, it may result in confusing graphs, so it would be best to produce two separate graphs: one with time on the abscissa and the other with the x domain.

Note that all of the tags and attributes described above are *case sensitve*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

x-y Plots

x-y plots are essentially a special case of the 2D Plot. The difference is simply that a 2D Plot displays the values of one or more Variables against one of the independent domains; whereas an x-y plot displays the values of one Variable against another Variable. (As with 2D plots, you could display more than one relationship per graph, but this might be rather confusing.)

An x-y plot is easily defined by using an appropriate `<Line/>` tag in a normal `<Plot2D>` construct. This is best illustrated with an example. Consider the following Variable definitions.

VARIABLE

```
VapourMoleFraction AS DISTRIBUTION(NoComp, X_Domain) OF MoleFraction
LiquidMoleFraction AS DISTRIBUTION(NoComp, X_Domain) OF MoleFraction
```

In a normal 2D plot, we could plot either (or both) of these variables as functions of time, the x domain or indeed the number of components; but it may be useful to be able to plot the vapour mole fraction as a function of the liquid mole fraction, to produce an equilibrium diagram. This is achieved with the following xml commands.

```
<Plot2D version="1">
  <Line idY="VapourMoleFraction(TIME=#,1,0)" idX="LiquidMoleFraction(TIME=#,1,0)" />
</Plot2D>
```

This essentially produces a plot of vapour mole fraction against liquid mole fraction of component 1 at x = 0, parameterised by time. One could equally parameterise using the x domain:

```
<Plot2D version="1">
  <Line idY="VapourMoleFraction(TIME=0,1,#)" idX="LiquidMoleFraction(TIME=0,1,#)" />
</Plot2D>
```

One may parameterise using any of the independent domains, with the only restriction being that the *same domain must be free* in both of the `id` attributes in each `<Line/>` tag. Of course, having to fix all of the other independent domains can be a bit restrictive, but one can include more points in the x-y plot by including more `<Line/>` tags, for example:

```
<Plot2D version="1">
```

```
<Line idY="VapourMoleFraction(TIME=#,1,0)" idX="LiquidMoleFraction(TIME=#,1,0)" />
<Line idY="VapourMoleFraction(TIME=#,1,1)" idX="LiquidMoleFraction(TIME=#,1,1)" />
<Line idY="VapourMoleFraction(TIME=0,1,#)" idX="LiquidMoleFraction(TIME=0,1,#)" />
<Line idY="VapourMoleFraction(TIME=10,1,#)" idX="LiquidMoleFraction(TIME=10,1,#)" />
</Plot2D>
```

Similarly, we may want to generate a phase diagram by plotting, say, Temperature as a function of both the liquid and vapour mole fractions. Assuming the appropriate definition of Temperature, this can be done by:

```
<Plot2D version="1">
  <Line idY="Temperature(TIME=#,0)" idX="LiquidMoleFraction(TIME=#,1,0)" />
  <Line idY="Temperature(TIME=#,0)" idX="VapourMoleFraction(TIME=#,1,0)" />
</Plot2D>
```

Note that it is not necessary that the variables have the same number of dimensions; only that they are defined over the same domain that is specified to be free in the `<Line/>` tag. That is, the `#` symbol should specify the *same* domain in each `<Line/>` tag.

Note also that gPROMS does not check that the values of the fixed domains are identical in each `<Line/>` tag. If they are specified different values, it is almost certain that the graph produced will be physically meaningless.

Note that all of the tags and attributes described above are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

3D Plots

For Variables that are defined over two or more independent domains (including time), 3D plots may be generated using the `<Plot3D>` construct and its associated `<Surface/>` tag. The basic format is:

```
<Plot3D version="1">
  <Surface id="" />
</Plot3D>
```

where the string specified in the `id` attribute defines the variable to be plotted (in this case, only one variable is allowed per plot), against which domains it should be plotted on which axes, and the values to which all other domains should be fixed. Like 2D plots, the `width` and `height` attributes are mandatory and specify the width and height of the plot in pixels. As an example, consider the following Variable definition.

```
VARIABLE
  Temperature AS DISTRIBUTION(Axial, Radial) OF AbsoluteTemperature
```

This Variable therefore has 3 independent domains: time (even in a steady-state simulation), axial and radial. To define a 3D plot, we must select two of the domains to be free and fix the third. For the two free domains, we may also choose which of the cartesian-coordinate axes will be used: x or y. The surface will then be plotted using a standard right-handed cartesian-coordinate system with the x axis horizontally in the plane of the screen/page and the z axis vertically in the plane of the screen/page. The y axis therefore points into the screen/page and is perpendicular to it. Variable values will be plotted on the z axis, with the two free domains on the x and y axes, as specified in the `<Surface/>` tag.

For the above Variable definition, one possible plot is generated with the following xml.

```
<Plot3D version="1">
  <Surface id="Temperature(TIME=#x,#y,0)" />
</Plot3D>
```

Here, the time domain has been specified to be represented by the x axis and the axial domain by the y axis. The values of Temperature plotted are to correspond $r = 0$ in the radial domain. The `#x` string specifies which free domain is represented by the x axis, and the `#y` string behaves similarly.

If the Variable defined above were used in a steady-state simulation, the surface can only be defined in one of two ways:

```
<Plot3D version="1">
  <Surface id="Temperature(TIME=0,#x,#y)" />
</Plot3D>
```

the only other possibility being to swap which axes represent the axial and radial domains.

Note that all of the tags and attributes described above are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

3D Plot Orientation

It is often necessary to adjust the orientation of a 3D plot to show the shape of the surface more clearly. This can be achieved using the `<Rotation/>` tag within the `<Plot3D>` construct. This allows the user to specify the orientation of the plot by using standard rotations about each of the cartesian-coordinate axes. The basic syntax is as follows (using the example presented before).

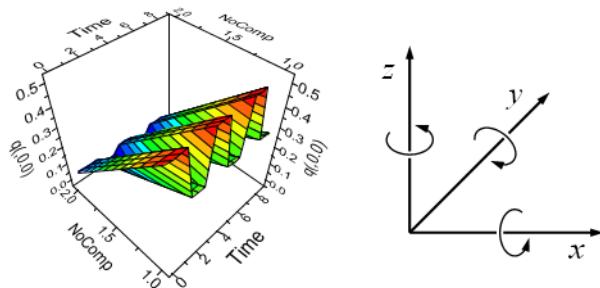
```
<Plot3D version="1">
  <Surface id="Temperature(TIME=0,#x,#y)" />
  <Rotation x="0" y="0" z="0" />
</Plot3D>
```

Each attribute defines the rotation in degrees about its corresponding axis. The values may be positive or negative. The values above (i.e. no rotation) produce a coordinate system with the x and z axes in the plane of the screen/page, with the x axis horizontal. By definition, the y axis therefore points into the screen/page. This is not a particularly useful view, so the default view is to rotate the coordinates 45 degrees about both the x and z axes. In other words, omitting the `<Rotation/>` tag altogether is the same as specifying:

```
<Plot3D version="1">
  <Surface id="Temperature(TIME=0,#x,#y)" />
  <Rotation x="45" y="0" z="45" />
</Plot3D>
```

Of course, any other values may be specified to suit the Variable being plotted. The figure below shows the default rotation on the left and no rotation on the right (along with an indication of the positive direction of rotation for each axis). The plot on the left has time assigned to the x axis and NoComp to the y axis.

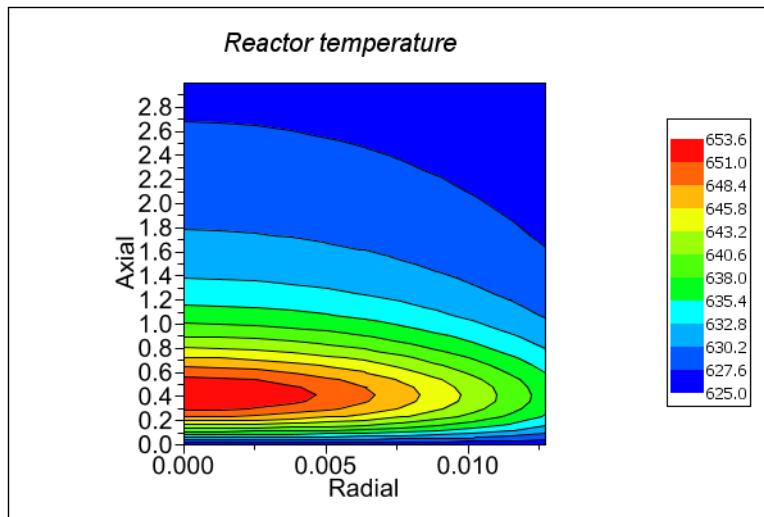
**Figure 10.11. Default Orientation of 3D Plots (left)
and Definition of Coordinates with no Rotation (right)**



Note that all of the tags and attributes described above are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

Contour plots

Contour plots are a special case of 3D plots in which no 3-dimensional surface is plotted but where the contour lines are projected onto the x-y-area. The example below shows the temperature at the exit of a tubular reactor.

Figure 10.12. Example of a contour plot

The xml code for defining this plot looks as follows. The important Surface attributes to set are `mesh` and `shade`, both require the value `false`.

```
<Plot3D width="600" height="400" version="1" border="true">
  <Header label="Reactor temperature">
    <Font name="Times" size="20" style="italic"/>
  </Header>
  <Legend show="true" border="true" anchor="right" orientation="vertical" style="continu
    <Font name="Arial" size="12"/>
  </Legend>
  <Axes>
    <LabelFont name="Arial" size="50"/>
    <NumberFont name="Arial" size="50"/>
    <Axis orientation="x" show="true"/>
    <Axis orientation="y" show="true"/>
    <Axis orientation="z" show="true"/>
  </Axes>
  <Surface id="Reactor.T(TIME=5,#y, #x)" mesh="false" shade="false"
    contours="true" zones="true"/>
    <Rotation x="90" y="0" z="0"/>
</Plot3D>
```

Note that all of the tags and attributes described above are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

Formatting Options

Each of the environments for creating different types of Model Report have a number of tags for specifying how they should be formatted.

- Formatting options for `<PMA_TABLE>`
- Formatting options for `<Plot2D>`
- Formatting options for `<Plot3D>`

Tags can be used in two ways, depending on whether they may contain other tags. If a tag may not contain any other tags, then it can only be used in the "simple tag" form:

```
<TagName attribute1="" attribute2="" ... attributeN="" />
```

However, when other tags need to be included, then the full tag form must be used:

```
<TagName attribute1="" attribute2="" ... attributeN="">
  <!-- contained tags go here -->
</TagName>
```

Unless otherwise stated, attributes and tags are optionally specified and there can be at most one of each tag.

Formatting options for <PMA_TABLE>

The <PMA_TABLE> tag has a number of attributes that specify how the table will look in the report. These are described in the table below. Where there are only a certain number of allowable values for the attribute, these are listed inside brackets, separated by pipes. E.g. [true|false] means that an attribute may only take the values true or false (of course, when specifying the values of attributes, they must always be enclosed in quotes, e.g. attr="true").

Note that all of the tags and attributes described here are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

Table 10.1. Attributes of the <PMA_TABLE> tag

Attribute Name	Description	Default Value	Notes
pmas	Determines which Public Model Attributes are shown.	specified	[all variables parameters, specified] specified means...
border	The border width in pixels.	1	Only non-negative integers allowed.
lineThickness	The thickness of the lines between the cells in pixels.	0	Only non-negative integers allowed.
cellspacing	The cell spacing in pixels.	1	Only non-negative integers allowed.
units	Specifies whether or not to display the units.	true	[true false]
tableAlign	Alignment of table relative to the page.	left	[left center right]
headerAlign	Alignment of table headings.	center	[left center right]
pmaNamesAlign	Alignment of PMA names.	left	[left center right]
pmaValuesAlign	Alignment of PMA values.	left	[left center right]
unitsAlign	Alignment of units.	left	[left center right]
altBGColorMode	Alternate the background colour for each PMA name?	true	[true false]
altBGColor	Alternating background colour.	#DEEFEE	Takes a string defining the colour either as a name or in hexadecimal RGB format preceded by a # character. The allowable names (case insensitive) are: Black (#000000), Green (#008000), Silver (#C0C0C0),

Attribute Name	Description	Default Value	Notes
			Lime (#00FF00), Gray (#808080), Olive (#808000), White (#FFFFFF), Yellow (#FFFF00), Maroon (#800000), Navy (#000080), Red (#FF0000), Blue (#0000FF), Purple (#800080), Teal (#008080), Fuchsia (#FF00FF), Aqua (#00FFFF).
pmaColTitle	Title for PMA column.	Name	
valueTitle	Title for value column.	Value at time \$t	\$t is replaced by the time selected using the slider at the top of the reports window.
unitsTitle	Title for units column.	Units	
numberFormat	Specifies the formatting of numbers in the table.	N/A	See Tables.

The `<Attribute>` tag is a simple tag that specifies which Public Model Attribute to include in the PMA Table. One tag is used for each Variable to be included, which is specified using the mandatory `id` attribute. For example, a single Variable would be tabulated thus:

```
<PMA_TABLE>
  <Attribute id="..." />
</PMA_TABLE>
```

The format for the `id` attribute is similar for each type of Model Report.

In addition to the `<Attribute>` tag, two tags provide formatting options for the header and body font. These are `<HeaderFont>` and `<BodyFont>`, both of which take the following attributes.

Table 10.2. Attributes of the `<HeaderFont>` and `<BodyFont>` tags

Attribute Name	Description	Default Value	Notes
name	The name of the font.	Automatically chosen	
size	The size of the font in points.	Automatically chosen	Only positive integers allowed.
style	The font style.	Automatically chosen	Can be a combination of bold, italic, underline and strikeout, separated by commas. E.g. style=bold, italic.

Formatting options for `<Plot2D>`

The `<Plot2D>` tag has a number of attributes that specify how the graph will look in the report. These are described in the table below. Where there are only a certain number of allowable values for the attribute, these are listed inside brackets, separated by pipes. E.g. [true|false] means that an attribute may only take the values true or false.

Note that all of the tags and attributes described here are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

Table 10.3. Attributes of the <Plot2D> tag

Attribute Name	Description	Default Value	Notes
width	The width of the graph in pixels.	500	Only positive integers allowed.
height	The height of the graph in pixels.	300	Only positive integers allowed.
border	Defines if a border should be drawn around the graph.	false	[true false]
version	The version of the XML plot format.	—	This attribute is mandatory and must be set to 1.

The remainder of the formatting for 2D plots is done using embedded tags within the <Plot2D> tag. These are:

- <Header>
- <Footer>
- <Legend>
- <Axes>
- <Grid>
- <Line>

The <Header> and <Footer> tags define the text at the head and foot of the graph. They both contain one attribute and one tag. The Label attribute is a mandatory attribute and is the string defining the text used for the header/footer. The tag defines the font used for the text. It has the following attributes.

Table 10.4. Attributes of the tag

Attribute Name	Description	Default Value	Notes
name	The name of the font.	Automatically chosen	
size	The size of the font in points.	Automatically chosen	Only positive integers allowed.
style	The font style.	Automatically chosen	Can be a combination of bold, italic, underline and strikeout, separated by commas. E.g. style="bold, italic".

For example, the header might be specified like this:

```
<Plot2D version="1">
  <Header label="Some text to use at the head of the graph.">
    <Font name="Arial" size="12" style="bold"/>
  </Header>
</Plot2D>
```

Or if the font were to be determined automatically, one could specify the header more simply like this:

```
<Plot2D version="1">
  <Header label="Some text to use at the head of the graph."/>
</Plot2D>
```

The <Legend> tag defines the properties of the graph legend, including whether or not it is displayed. It may contain a tag, which defines the font used for the text, and it has the following attributes.

Table 10.5. Attributes of the <Legend> tag

Attribute Name	Description	Default Value	Notes
show	Defines whether or not the legend is visible.	true	[true false]
border	Specifies if a border should be drawn around the legend.	false	[true false]
anchor	The position relative to the graph.	right	[top topRight right bottomRight bottom bottomLeft left topLeft]
orientation	Whether the labels are listed horizontally or vertically.	vertical	[horizontal vertical]
fixSymbolSize	Whether the symbols have a fixed size.	false	[true false]

The <Axes> tag is a full-form tag that contains just 3 sub-tags. These are:

- <LabelFont> specifies the font attributes for the axis label. This tag has the same attributes as the tag.
- <NumberFont> specifies the font attributes for the numbers on the axis. This tag has the same attributes as the tag.
- <Axis> defines each of the axes on the graph. There may be up to 3 <Axis> tags used: one for each of the possible axes x, y and y2. If none are used, all of the axes will take default properties.

The <Axis> tag is a simple tag that contains the following attributes.

Table 10.6. Attributes of the <Axis> tag

Attribute Name	Description	Default Value	Notes
orientation	The axis to which the attributes will apply.	—	Mandatory. [x y y2]
label	The text used to label the axis.	Either "Time" or the id of the first line associated with this axis.	
show	Boolean specifying that the axis is visible.	true	[true false]
min	The minimum extent of the axis.	—	Any real number.
max	The maximum extent of the axis.	—	Any real number.
transform	Applies a transform to the numbers on the axis.	—	Any simple expression containing numbers and the +, -, * and / operators. Operations are performed in sequence; there is no operator precedence and bracketed expressions are not allowed. A typical use of this functionality

Attribute Name	Description	Default Value	Notes
			would be to change the units of measurement on a plot. e.g. If you had Temperature (K) vs. Time (sec) data but you wanted to plot it as Temperature (F) vs. Time (hr) then you would enter /3600 (or /60/60) as the transformation for the x-axis -273.15*1.8+32 as the transformation for the y-axis
log	Defines a logarithmic axis.	false	[true false]
origin	The value at the origin.	Automatically chosen	Any real number.
numbering	The frequency of numbers on the axis.	Automatically chosen	Any real number.
ticks	The frequency of ticks on the axis.	numbering/2	Any real number.
precision	The number of decimal places of the numbers on the axis.	0	Only non-negative integers allowed.
labelRotation	The rotation of the axis label.	0	[0 90 180 270] Rotation is anticlockwise and in degrees.

The `<Grid>` tag defines the properties of any gridlines shown on the graph. There may be up to 2 `<Grid>` tags within the `<Plot2D>` tag, each one defining the horizontal and vertical grid lines. The horizontal grid lines may be associated with either the primary (left) or secondary (right) y axis. It is a simple tag that contains only the following attributes.

Table 10.7. Attributes of the `<Grid>` tag

Attribute Name	Description	Default Value	Notes
orientation	The axis to which the grid lines will be associated.	—	Mandatory. [x y y2]
increment	The interval between grid lines.	Automatically chosen	Only positive real numbers allowed.
pattern	The style of the line drawn.	solid	[none solid longDash dotted shortDash longDash dashDot]
color	The colour of the line drawn.	black	Takes a string defining the colour either as a name or in hexadecimal RGB format preceded by a # character. The allowable names (case insensitive) are: Black (#000000), Green (#008000), Silver (#C0C0C0), Lime (#00FF00), Gray (#808080), Olive (#808000),

Attribute Name	Description	Default Value	Notes
			White (#FFFFFF), Yellow (#FFFF00), Maroon (#800000), Navy (#000080), Red (#FF0000), Blue (#0000FF), Purple (#800080), Teal (#008080), Fuchsia (#FF00FF), Aqua (#00FFFF).
width	The width of the line drawn.	1	Only positive integers allowed.

The <Line> tag is responsible for specifying which Variables are plotted in the graph. One <Line> tag is used for each Variable plotted and there can be as many tags as needed. It is a simple tag that contains only the following attributes.

Table 10.8. Attributes of the <Line> tag

Attribute Name	Description	Default Value	Notes
idY	Variable id for y axis.	—	Mandatory. A string defining the Variable to be plotted on the y axis.
idX	Variable id for x axis (only required for x-y plots).	—	A string defining the Variable to be plotted on the x axis. Only used for x-y plots.
label	A name for this line to appear in the legend.	The name of the Variable	The default value uses only the Variable name and not the full path: e.g. if the full path is Flowsheet.Column.m_Waste, then the default value will be "m_Waste".
axis	Which of the y axes are used primary (y) or secondary (y2).	y	[y y2]
pattern	The style of the line drawn.	solid	[none solid longDash dotted shortDash longDash dashDot]
color	The colour of the line drawn.	Automatically chosen	Takes a string defining the colour either as a name or in hexadecimal RGB format preceded by a # character. The allowable names (case insensitive) are: Black (#000000), Green (#008000), Silver (#C0C0C0), Lime (#00FF00), Gray (#808080), Olive (#808000), White (#FFFFFF), Yellow (#FFFF00),

Attribute Name	Description	Default Value	Notes
			Maroon (#800000), Navy (#000080), Red (#FF0000), Blue (#0000FF), Purple (#800080), Teal (#008080), Fuchsia (#FF00FF), Aqua (#00FFFF).
width	The width of the line drawn.	1	Only positive integers allowed.
symbolShape	The shape of the symbols drawn for each data point on the line.	Automatically chosen	[none dot box triangle diamond star verticalLine horizontalLine cross circle square]
symbolColor	The colour of the symbols drawn for each data point on the line.	Automatically chosen	Takes a string defining the colour either as a name or in hexadecimal RGB format preceded by a # character. The allowable names (case insensitive) are: Black (#000000), Green (#008000), Silver (#C0C0C0), Lime (#00FF00), Gray (#808080), Olive (#808000), White (#FFFFFF), Yellow (#FFFF00), Maroon (#800000), Navy (#000080), Red (#FF0000), Blue (#0000FF), Purple (#800080), Teal (#008080), Fuchsia (#FF00FF), Aqua (#00FFFF).
symbolSize	The size of the symbol at each point plotted for this line.	6	Only positive integers allowed.

Formatting options for <Plot3D>

The <Plot3D> tag has a number of attributes that specify how the graph will look in the report. These are described in the table below. Where there are only a certain number of allowable values for the attribute, these are listed inside brackets, separated by pipes. E.g. [true|false] means that an attribute may only take the values true or false.

Note that all of the tags and attributes described above are *case sensitive*: if they are not typed exactly as shown above, then the report will not be generated and an error message will be displayed instead.

Table 10.9. Attributes of the <Plot3D> tag

Attribute Name	Description	Default Value	Notes
width	The width of the graph in pixels.	600	Only positive integers allowed.

Attribute Name	Description	Default Value	Notes
height	The height of the graph in pixels.	400	Only positive integers allowed.
border	Defines if a border should be drawn around the graph.	false	[true false]
version	The version of the XML plot format.	—	This attribute is mandatory and must be set to 1.

The remainder of the formatting for 3D plots is done using embedded tags within the `<Plot3D>` tag. These are:

- `<Header>`
- `<Footer>`
- `<Legend>`
- `<Axes>`
- `<Surface>`
- `<Rotation>`

The `<Header>` and `<Footer>` tags define the text at the head and foot of the graph. They both contain one attribute and one tag. The `label` attribute is a mandatory attribute and is the string defining the text used for the header/footer. The `` tag defines the font used for the text. It has the following attributes.

Table 10.10. Attributes of the `` tag

Attribute Name	Description	Default Value	Notes
name	The name of the font.	Automatically chosen	
size	The size of the font in points.	Automatically chosen	Only positive integers allowed.
style	The font style.	Automatically chosen	Can be a combination of bold, italic, underline and strikeout, separated by commas. E.g. <code>style="bold, italic"</code> .

For example, the header might be specified like this:

```
<Plot3D version="1">
  <Header label="Some text to use at the head of the graph.">
    <Font name="Arial" size="12" style="bold"/>
  </Header>
</Plot3D>
```

Or if the font were to be determined automatically, one could specify the header more simply like this:

```
<Plot3D version="1">
  <Header label="Some text to use at the head of the graph."/>
</Plot3D>
```

The `<Legend>` tag defines the properties of the graph legend, including whether or not it is displayed. It may contain a `` tag, which defines the font used for the text, and it has the following attributes.

Table 10.11. Attributes of the <Legend> tag

Attribute Name	Description	Default Value	Notes
show	Defines whether or not the legend is visible.	true	[true false]
border	Specifies if a border should be drawn around the legend.	false	[true false]
anchor	The position relative to the graph.	right	[top topRight right bottomRight bottom bottomLeft left topLeft]
orientation	Whether the labels are listed horizontally or vertically.	vertical	[horizontal vertical]
style	Determines the type of legend.	continuous	[continuous stepped]

The <Axes> tag is a full-form tag that contains just 3 sub-tags. These are:

- <LabelFont> specifies the font attributes for the axis label. This tag has the same attributes as the tag.
- <NumberFont> specifies the font attributes for the numbers on the axis. This tag has the same attributes as the tag.
- <Axis> defines each of the axes on the graph. There may be up to 3 <Axis> tags used: one for each of the possible axes x, y and z. If none are used, all of the axes will take default properties.

The <Axis> tag is a simple tag that contains the following attributes.

Table 10.12. Attributes of the <Axis> tag

Attribute Name	Description	Default Value	Notes
orientation	The axis to which the attributes will apply.	—	Mandatory. [x y z]
label	The text used to label the axis.	Either "Time" or the id of the first line associated with this axis.	
show	Boolean specifying that the axis is visible.	true	[true false]
min	The minimum extent of the axis.	—	Any real number.
max	The maximum extent of the axis.	—	Any real number.
transform	Applies a transform to the numbers on the axis.	—	Any simple expression containing numbers and the +, -, *, and / operators. Operations are performed in sequence; there is no operator precedence and bracketed expressions are not allowed. A typical use of this functionality would be to change the units of measurement

Attribute Name	Description	Default Value	Notes
			on a plot. e.g. If you had Temperature (K) vs. Time (sec) data but you wanted to plot it as Temperature (F) vs. Time (hr) then you would enter /3600 (or /60/60) as the transformation for the x-axis -273.15*1.8+32 as the transformation for the y-axis
scale	Scales the axis by a certain amount.	1.0	Only positive real numbers are allowed.

The <Surface> tag is responsible for specifying which Variable will be plotted in the graph. There must be exactly one <Surface> tag in each 3D plot. It is a simple tag that contains only the following attributes.

Table 10.13. Attributes of the <Surface> tag

Attribute Name	Description	Default Value	Notes
id	Variable id.	—	Mandatory. A string defining the Variable to be plotted (on the z axis) and the free domains to be used on the x and y axes.
mesh	Display a wire mesh effect on the surface.	true	[true false]
shade	Include colours on the surface.	true	[true false]
contours	Inlcude contour lines on the surface.	true	[true false]
zones	Divide the surface up into different zones (colours).	true	[true false]

The final tag specifies the orientation of the 3D graph. This is done by giving rotations about each of the axes, relative to a starting orientation, where the x axis is horizontal and in the plane of the screen/paper, the z axis is vertical and in the plane of the screen/paper, and the y axis is perpendicular to and pointing into the screen/paper. The simple tag <Rotation> is used to specify these rotations, and if omitted the default rotations will be used. The <Rotation> tag has just 3 optional attributes:

Table 10.14. Attributes of the <Rotation> tag

Attribute Name	Description	Default Value	Notes
x	Rotation about the x axis, in degrees.	45	Any real number.
y	Rotation about the y axis, in degrees.	0	Any real number.
z	Rotation about the z axis, in degrees.	45	Any real number.

Format of the id, idx and idy attributes

The id, idx and idy attributes effectively define a set of data. A valid id consists of a valid variable name followed by parameters (comma delimited within parentheses) with the first parameter beginning "TIME=". For a

2D or x-y plot, "#" denotes the independent domain. For a 3D plot, "#x" and "#y" denote the independent x and independent y domains respectively. For PMA tables, "#" denotes the time specified by the user (using the slider bar at the top of the report window). If the TIME parameter is omitted, it will be assumed to be "TIME=#", e.g. "`q(a,b)`" = "`q(TIME=#,a,b)`". Wildcards (*) are permitted in PMA tables, 2D plots and x-y plots to avoid using multiple tags to define a range of variables to plot. Some examples are given below.

- Example Variable definitions

- VARIABLE

```
q AS DISTRIBUTION(NoComp, Axial) OF NoType  
r AS DISTRIBUTION(NoComp, Axial) OF NoType
```

- PMA tables

- `<Attribute id="q(TIME=#,a,b)" />`

The value of q at the specified time with NoComp=a, Axial=b.

- `<Attribute id="q(TIME=#,*,b)" />`

the value of q at the specified time with Axial=b, for each element NoComp.

- 2D plots

- `<Line idY="q(TIME=#,a,b)" />`

A single line of q vs TIME with NoComp=a, Axial=b.

- `<Line idY="q(TIME=a,#,b)" />`

A single line of q vs NoComp with TIME=a, Axial=b.

- `<Line idY="q(TIME=a,*,#)" />`

A number of lines of q vs Axial with TIME=a: one for each element of NoComp.

- x-y plots

- `<Line idX="q(TIME=#,a,b)" idY="r(TIME=#,c,d)" />`

A single line of how q (with NoComp=a and Axial=b) varies against r (with NoComp=c and Axial=d) over the whole TIME domain.

- 3D plots

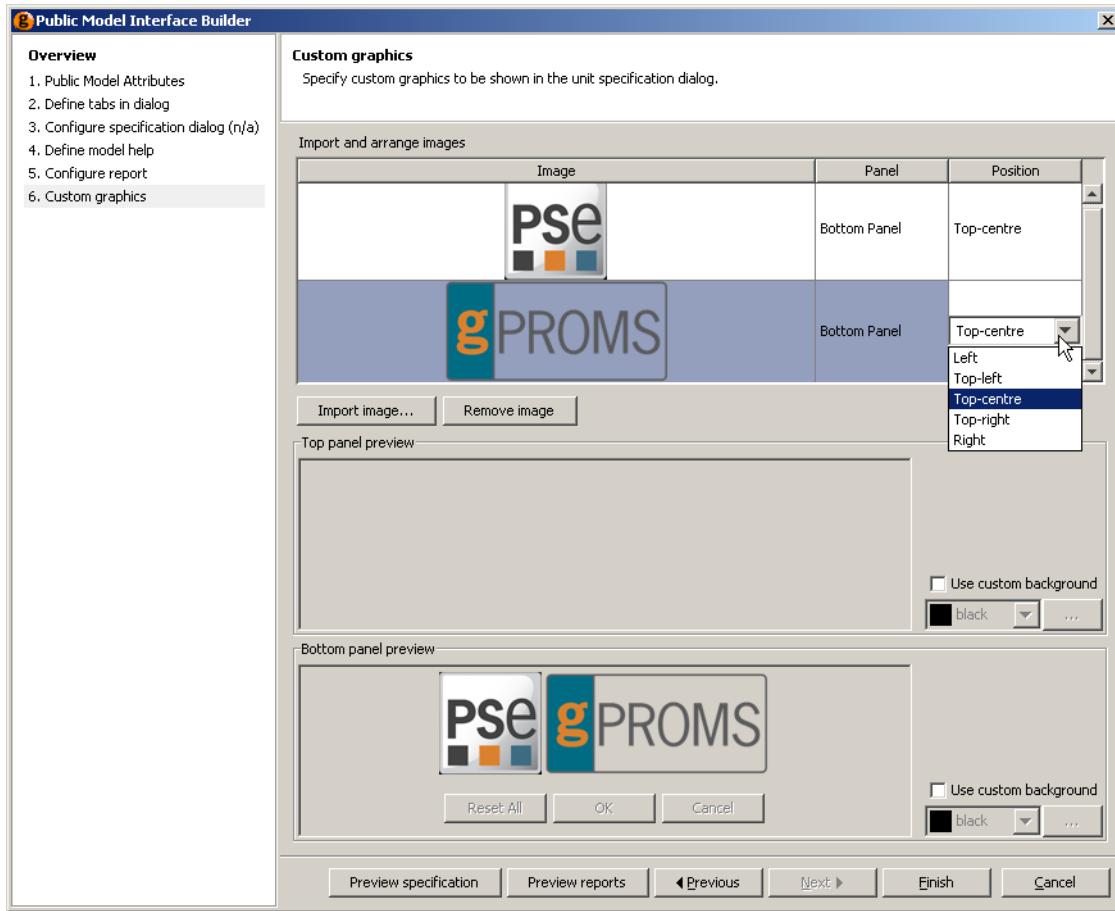
- `<Surface id="q(TIME=#x,a,#y)" />`

A surface of q vs TIME (x axis) and Axial (y axis) with NoComp=a.

Defining custom graphics

Custom graphics allow placing images at the top and the bottom of a dialog, for instance in order to provide them with a company's branding. The following image formats are supported: .gif, .jpg (and .jpeg), .png and .svg.

The controls in this part of the interface builder allow adding or removing images, choosing the alignment and also to set a background colour in RGB format.

Figure 10.13. Example custom graphic specification

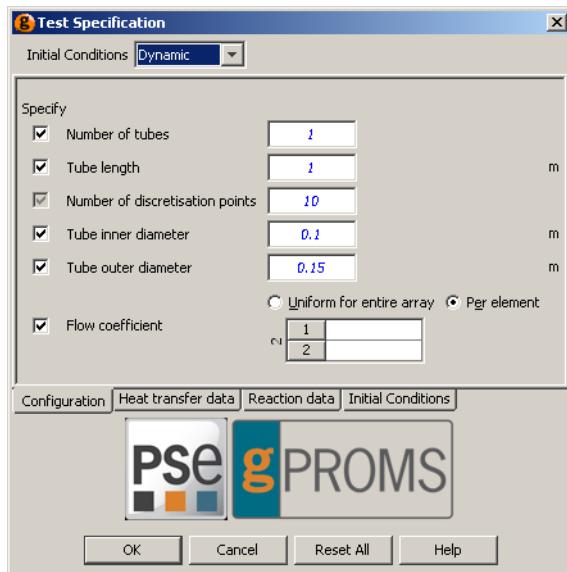
In the example above, two images have been imported and assigned to the bottom panel. The top and bottom panel preview panes show how the images will be aligned on the dialog. Here, both images are set to Top-centre and their position is shown relative to the buttons that will appear at the bottom of the configuration dialog. Of course, any image can be assigned to either the top or bottom panel and aligned using the following options.

Table 10.15. Alignment options

Alignment	Position in panel
Left	Flush left, level with the controls
Top-left	Flush left, above the controls
Top-centre	Centred, above the controls
Top-right	Flush right, above the controls
Right	Flush right, level with the controls

Clicking on the Preview specification button activates a preview dialog. The dialog for the example above is shown below.

Figure 10.14. Test specification dialog



Chapter 11. Defining Schedules

Schedules are used in gPROMS to define operating procedures. An operating procedure can be considered as a recipe that defines periods of undisturbed operation *along with* specified or conditional external disturbances to the system. The Schedule section is the last part of the Process entity (for defining a simulation activity).

Schedules can be generated (and modified) by entering gPROMS language, by using a graphical interface or by using a combination of the two. Both methods are entirely equivalent and interchangeable: when a schedule is modified using the graphical interface, the equivalent change is automatically made to the language and, similarly, changes made to the gPROMS language are automatically applied to the graphical representation of the Schedule.

The Schedule is stored in either a Process or a Task entity and can be viewed by selecting either the Schedule tab or the gPROMS language tab from the Process window. The Schedule tab displays the graphical representation of the Schedule and the gPROMS language tab displays all of the language associated with the Process (i.e. Unit, Set, Assign etc.); the Schedule is located at the end, so one may need to scroll the window to see the Schedule. These two views are shown below for a Process.

Figure 11.1. Graphical Schedule Editor

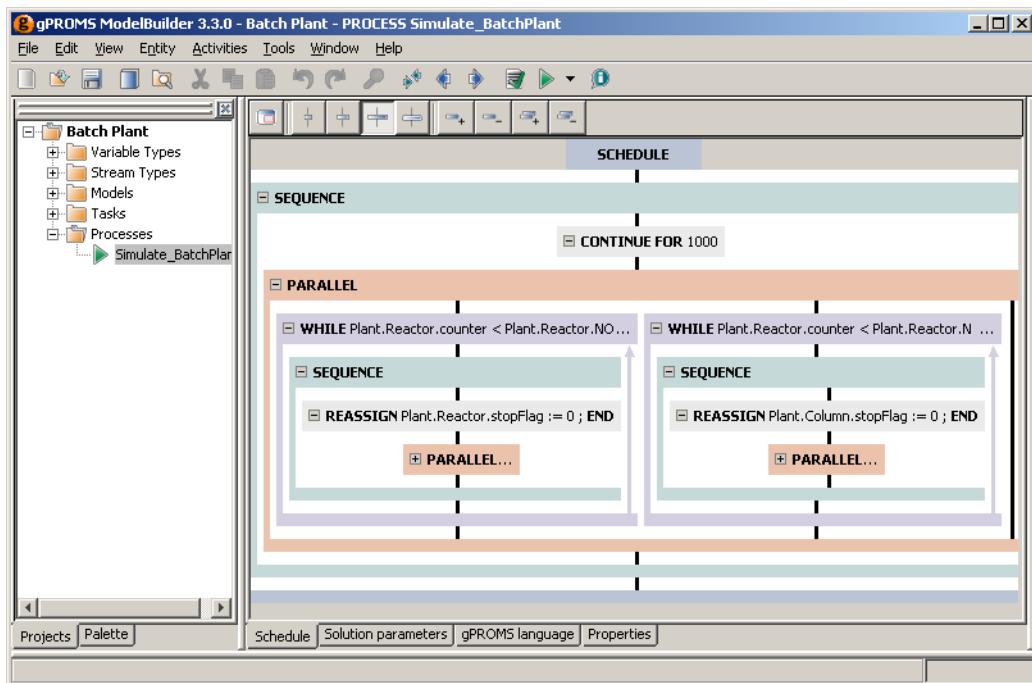


Figure 11.2. Schedule Language Editor

```

gPROMS ModelBuilder 3.3.0 - Batch Plant - PROCESS Simulate_BatchPlant
File Edit View Entity Activities Tools Window Help
[Icons]
Batch Plant
  Variable Types
  Stream Types
  Models
  Tasks
  Processes
    Simulate_BatchPlant

318  SCHEDULE
319
320
321  SEQUENCE
322
323  CONTINUE for 1000
324
325  PARALLEL
326
327  # ***** first task-entity: Operation of the reactor *****
328  WHILE Plant.Reactor.counter < Plant.Reactor.NOCYCLE DO
329    SEQUENCE
330      REASSIGN Plant.Reactor.stopFlag := 0 ; END
331    PARALLEL
332      MonitorWaste (Reactor IS Plant.Reactor)
333      ReplenishFeedA(Reactor IS Plant.Reactor, Column IS Plant.Column)
334      ReplenishFeedB(Reactor IS Plant.Reactor)
335      ReplenishClean(Reactor IS Plant.Reactor)
336    SEQUENCE
337      FillReactor (Reactor IS Plant.Reactor)
338      StartReaction (Reactor IS Plant.Reactor)
339      GenerateDescent (Descent IS Plant.Descent)
340
  1:1 INS
Schedule Solution parameters gPROMS language Properties

```

Schedules are specified using:

- Elementary tasks, which are used to specify external disturbances to the systems (e.g. changing the values of simulation input variables, specifying periods of undisturbed operation etc);
- Timing structures, which combine elementary tasks and specify the manner in which they are executed (sequentially, concurrently, conditionally or iteratively);
- Results-control elementary tasks, which control the way the results are displayed (but do not affect the results themselves); and
- Tasks for creating and using Saved Variable Sets.

The Schedule may also include user-specified Tasks, which are re-usable parts of the operating procedure. Tasks are associated with one or more Models and can be used multiple times within a Schedule and by other Tasks. *See: Defining Tasks.*

Before considering the above elements in detail, one must first be familiar with the procedure of Building a Schedule.

Building a Schedule

There are two main ways to build a Schedule: using the graphical interface or by entering gPROMS language. The former is by far the most convenient and is described here. The gPROMS language for Schedules is covered in the following sections, describing the Tasks in detail.

To begin building a Schedule, one must first create a Process. Let's assume one already exists, which contains all of the specifications for the simulation apart from the Schedule; that is:

- Units are defined,
- Parameters have all been Set,
- Variables have been Assigned to take up any degrees of freedom and
- Initial conditions have been specified

so that the simulation can be initialised. All that remains is to define what should happen during the simulation and when. For example, one can fill a reactor, heat it up, keep the temperature constant while the reactions take place, cool it down and finally empty it. These actions are defined by specifying changes in Assigned Variables and periods of uninterrupted simulation, all by using elementary Tasks.

Before these Tasks can be placed into the Schedule, we must first create a Schedule. To do so, double-click on the Process to open it in the gPROMS editor window. There are four tabs in the Process window: Schedule, Solution parameters, gPROMS language and properties. The gPROMS language tab contains all of the code that defines the elements of the Process listed above. The code for the Schedule will be placed at the end, in a SCHEUDLE section. The graphical interface is shown in the Schedule tab. These two views are shown below.

Figure 11.3. gPROMS language tab with no Schedule

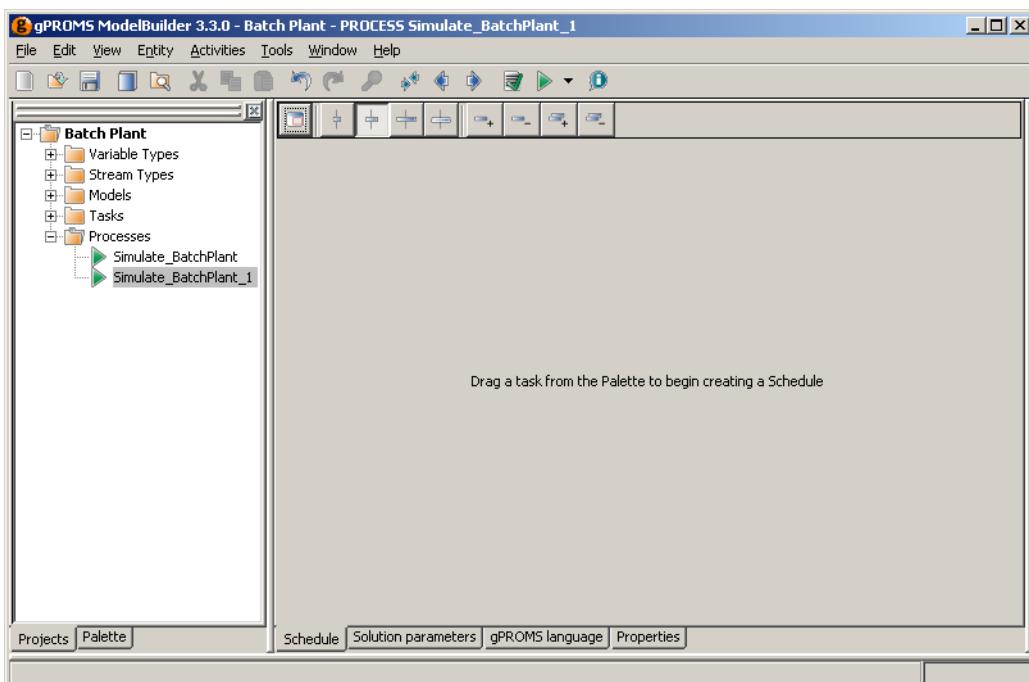
```

gPROMS ModelBuilder 3.3.0 - Batch Plant - PROCESS Simulate_BatchPlant_1
File Edit View Entity Activities Tools Window Help
Projects Palette Schedule Solution parameters gPROMS language Properties
Batch Plant
  Variable Types
  Stream Types
  Models
  Tasks
  Processes
    Simulate_BatchPlant
    Simulate_BatchPlant_1

295      no_Mol(1) = 002 ;
296      no_Mol(2) = 0 ;
297      no_Mol(3) = 2182 ;
298      no_Mol(4) = 956 ;
299      no_Mol(5) = 0 ;
300      total_Enth = 0 ;
301      END
302
303      END # Within Plant.Reactor
304
305      SOLUTIONPARAMETERS
306
307      ReportingInterval := 100 ;
308      DASolver := "DASOLV" [
309          "InitialisationNLSSolver" := "BDNLSOL" [
310              "UseIfSuperstructure" := FALSE;
311          ],
312          "ReInitialisationNLSSolver" := "BDNLSOL" [
313              "UseIfSuperstructure" := TRUE;
314          ],
315      ]
316
317
  317:1 INS

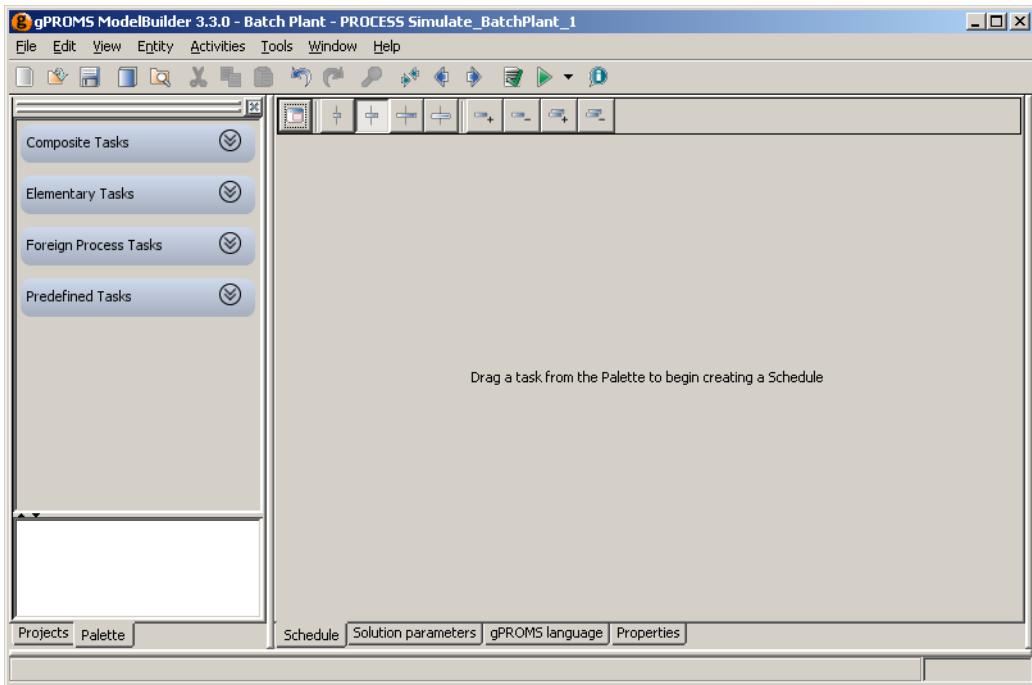
```

Figure 11.4. Schedule tab with no Schedule



To create the Schedule using the graphical interface, a Task needs to be dragged from the Task Palette onto the Schedule window. Therefore, one must first click on the Palette tab in the Project tree. If the Palette tab is not visible, then it can be enabled by selecting Palette from the View menu or by pressing **CTRL+F11**. The Task Palette is shown below.

Figure 11.5. Task Palette



The Task Palette is divided into two panes: the top pane contains all of the available Tasks (arranged in four categories) and the bottom pane contains an explanation of the currently-selected Task. The four categories of Task are:

- Composite Tasks, which combine elementary tasks and specify the manner in which they are executed (sequentially, concurrently, conditionally or iteratively);
- Elementary Tasks, which are used to specify external disturbances to the systems (e.g. changing the values of simulation input variables, specifying periods of undisturbed operation etc);
- Foreign Process Tasks, which control the way the results are displayed (but do not affect the results themselves); and
- Predefined Tasks, which are user-defined reusable Tasks that contain a segment of an operating procedure.

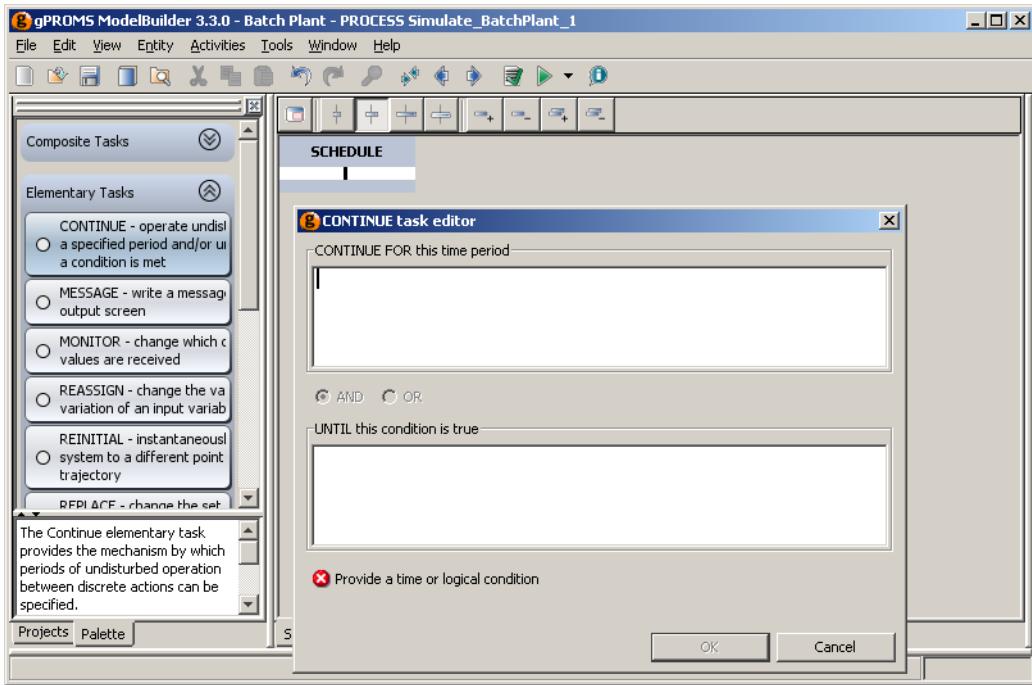
To expand a category, simply left click on its title or on the symbol next to it. All of the available Tasks will then be shown. Left clicking on a task will display further information about it in the window at the bottom of the palette. Left clicking on the category title again or on the symbol will collapse the category.

To create the Schedule, left click on a Task and, while holding the left mouse button down, drag the Task onto the Schedule window. Before the mouse button is released, the mouse pointer will change to to indicate that the task will be copied into the Schedule. When the mouse button is released, the Schedule is created and the Task is placed into the Schedule. Most Tasks, however, need to be configured before they can be added to the Schedule; in these cases, a configuration dialog will appear and it must be completed before the Task is added.

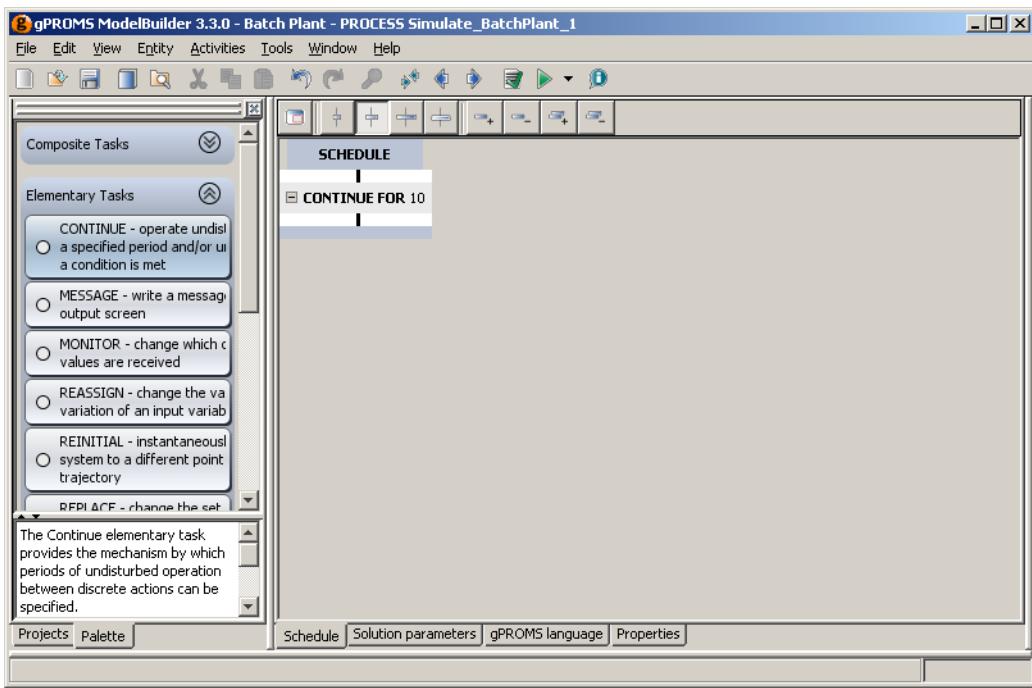
This is demonstrated in the following example. Suppose we only want to simulate the Process for a given amount of time, without changing any of the input specifications. This is done with the Continue Task. Since the Continue

Task instructs gPROMS to simulate the Process for a given amount of time (or until a certain condition is satisfied), this time (or condition) must be specified before the Task can be added to the Schedule. The figure below shows the Schedule and Task configuration dialog just after the Task had been dragged onto the Schedule window and the left mouse button released.

Figure 11.6. Continue Task configuration dialog



Configuration dialogs automatically check syntax, so this one initially states that the configuration will only be complete when a time value is entered in the first text box or a logical condition is entered in the second one. It is also possible to enter values in both boxes and the two conditions will be combined with an AND or OR logical operator, which can be selected using the radio button. In this case, it is disabled because both text boxes are empty. Once the configuration is complete, the OK button will be enabled and left clicking on this will complete the addition of the Task to the Schedule. This is shown in the figure below. (Left clicking on the Cancel button will cancel the addition of the Task, but will leave a blank Schedule in the Schedule window (visible just above the configuration dialog).)

Figure 11.7. Continue Task in a Schedule

Notice also that by left clicking on the Continue Task, the bottom pane of the Task Palette has been populated with an overview of the Continue Task. The scroll bar on the right can be used to scroll through the text and the size of the pane can be adjusted by dragging the divider up or down.

When a Task is added to the Schedule using the graphical interface, the gPROMS language is automatically added to the Process, as can be seen in the language tab below. The Schedule could have been created by typing this code into the Process and the same graphical Schedule would have been generated automatically.

Figure 11.8. Continue Task in a Schedule (gPROMS language tab)

The screenshot shows the gPROMS ModelBuilder interface with the "gPROMS language" tab selected. The code pane displays the following gPROMS language code:

```

297 no_Mol(3) = 2102 ;
298 no_Mol(4) = 956 ;
299 no_Mol(5) = 0 ;
300 total_Enth = 0 ;
301 END
302
303 END # Within Plant.Reactor
304
305 SOLUTIONPARAMETERS
306 ReportingInterval := 100 ;
307 DASolver := "DASOLV" [
308   "InitialisationNLSSolver" := "BDNLSOL" [
309     "UseIfSuperstructure" := FALSE;
310   ],
311   "ReInitialisationNLSSolver" := "BDNLSOL" [
312     "UseIfSuperstructure" := TRUE;
313   ],
314   ]
315 ]
316 ]
317 SCHEDULE
318 CONTINUE FOR 10
319 |

```

The code is numbered from 297 to 319. The "INS" tab is highlighted at the bottom of the code editor.

Returning to the Schedule tab, it can be seen that the Schedule itself is represented in the graphical interface. It contains a black vertical line above and below the Continue Task. These lines are "hot spots" where additional

Tasks can be added. In a blank Schedule (as seen in the screen shot showing the Task configuration dialog), there is just one black line and therefore only one place where a new task can be added. Once a Task has been added, a new one can be added before or after the first one, by dragging a new Task onto one of the lines.

The Continue Task displays the gPROMS language resulting from the specification made in the configuration dialog. In this case, the number 10 was entered in the first text box, specifying that gPROMS should simulate the Process for 10 units of time and then stop. It is possible to hide the details of any Task by left clicking on the  symbol on the left (the details can be shown again by pressing on the  symbol). This allows the user to customise how much detail is shown in the graphical view: as can be seen in the screen shot above, Tasks can be nested within other Tasks such that a complex hierarchy can be built up and it may not be desirable to see all of this detail all of the time. For this screen shot, the details of the Parallel Tasks were hidden so that the whole of the Schedule was visible in the editor. To save space, gPROMS will also only show the first 4 lines of code associated with a Task. An ellipsis (...) is used to indicate that some information is not being shown. There are three ways to see the details: 1. double click on the Task to bring up the configuration dialog; 2. view the Task language by right clicking on the Task and selecting Go to language from the context menu; or 3. move the mouse pointer over the Task and hold it there until a tool tip appears showing the details. You can also adjust the width of the Task boxes by pressing one of the four buttons shown below (see also the Schedule Tab Toolbar).

Figure 11.9. Width Controls



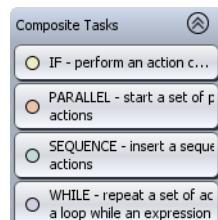
The first three limit the width of the Task boxes to small, medium and large. The last one removes the limit so that the Task boxes will be as wide as the longest visible line of language. The currently-selected option is indicated by the depressed button (the second one in the case above). In the screen shot above, it can be seen that the boxes are too narrow to show all of the lines for some of the tasks and this is indicated by the ellipsis at the end of the line (in the While and Parallel tasks).

Any Task can be selected by left clicking on it. Once selected, a Task can be deleted by pressing the **DEL** key or by right clicking and selecting Delete from the context menu. The Task can also be copied or cut using the context menu. It may be pasted into the Schedule by right clicking on one of the black lines and selecting Paste. *Note that if you delete a Composite Task, then all of the Tasks that it contains will also be deleted.* Pressing the  button or **CTRL+z** will undo any changes made to the Schedule, including the deleting of Tasks. (Pressing the  button or **CTRL+y** will redo any changes that have been undone.)

Tasks can also be reconfigured by double-clicking on them. This will open the Task Configuration dialog, allowing the details of the Task to be modified.

The context menu also provides another way of adding a new Task to an existing Schedule. Right clicking on a black line activates the context menu, which contains sub menus for each of the built-in Tasks: Composite, Elementary and Foreign Process. So to add a new Task using this method, right click on a black line, open the appropriate menu and left click on the Task you want to insert. The result is identical to dragging from the Task Palette: if necessary, a configuration dialog will appear and then the Task will be inserted in the chosen place.

So far, the Schedule we have created is very simple. Most Schedules will be more complex than this, and they may include many Tasks, some occurring after others have finished, some occurring concurrently with others and some Tasks may need to be performed iteratively or only if some condition is met. These structures can be created by using the Composite Tasks that have been mentioned briefly before. The Composite Tasks section of the Task Palette contains the four Tasks that allow Schedules of arbitrary complexity to be built. These are:

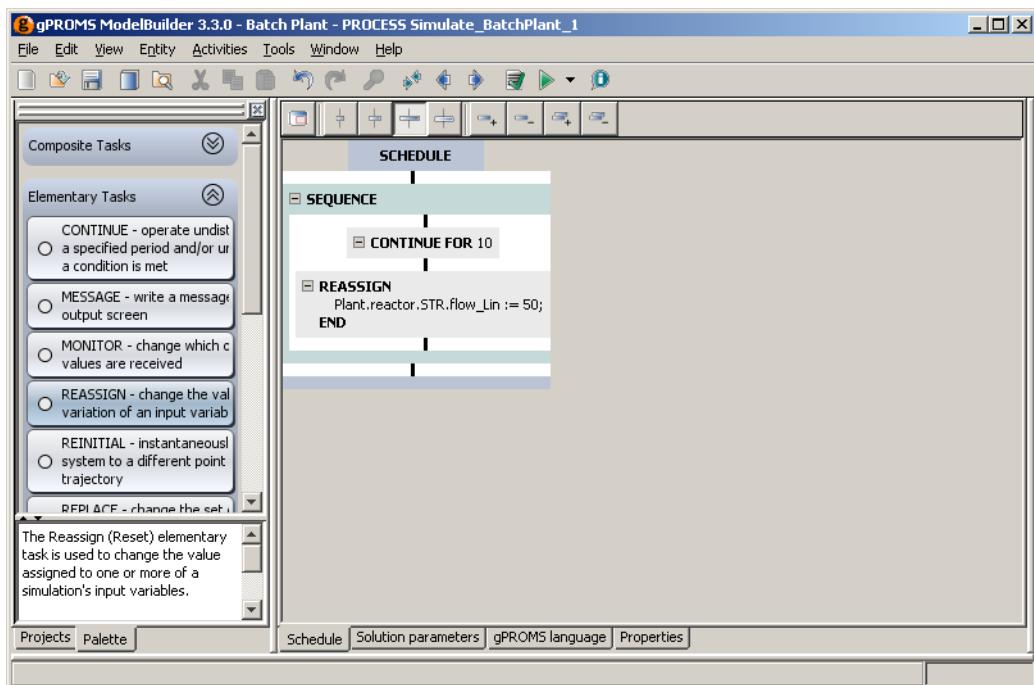


Each of these Tasks can be dragged onto a hot spot in the Schedule and they then provide locations for more Tasks to be added. These Tasks will be described in more detail later (see: Composite tasks). For now, we shall focus on the Sequence Task as the principles covered here apply to all of the above.

Let us proceed with the example given so far. We currently have just one Task in the Schedule: a Continue Task. Suppose that after the 10 units of time, we want to change the value of one of the input Variables. This can be done with the Reassign Task, and so all that need be done is to drag a Reassign Task onto the hot spot below the Continue Task. (Alternatively, we could right-click on the hot spot and choose Reassign from the Add elementary task context menu.

The result of the insertion is shown below (after the Reassign task has been configured — how to do this will be described in the Reassign section).

Figure 11.10. Schedule after a Reassign task was inserted



The first thing to notice is that a Sequence Task has automatically been inserted into the Schedule. This is because if two or more Tasks are to be performed in series, they must be enclosed in a Sequence Task. To save always having to insert the Sequence Task before adding elementary Tasks (such as the Continue and Reassign Tasks here) gPROMS will always insert a Sequence Task if one is needed. This means that you can drag *any* Task onto *any* hot spot and the resulting Schedule will always be valid.

Next, we have changed to width of the Task boxes to show all of the details of the Reassign Task. Here, the Reassign Task changes the value of the `Plant.Reactor.STR.flow_Lin` Variable to 50.

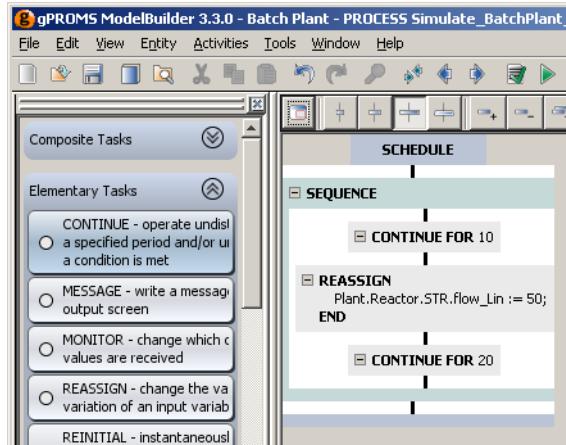
The automatically-generated gPROMS language now looks like this:

```
SCHEDULE
SEQUENCE
    CONTINUE FOR 10
    REASSIGN
        Plant.Reactor.STR.flow_Lin := 50;
    END
END
```

It would have been easy to type this into the gPROMS language tab, but larger more complex Schedules (with all four types of Composite Task being nested in complex arrangements) become harder to follow in this view and this

method is therefore more prone to error. The graphical view is much easier to follow and to modify, particularly if one wants to move or copy Tasks from one place to another, as we shall demonstrate now.

The Schedule currently does nothing new: although the `Flow_Lin` variable changes value, gPROMS stops the simulation immediately afterwards. To see the effect of the change in flowrate, we must add another Continue Task. If we add one after the Reassign Task and set it to simulate for 20 time units, we will have the following.



Now suppose that we want to see what would happen if we started the simulation by Continuing for 20 units, Reassigning the `Flow_Lin` Variable and then Continuing for 10 units of time. We could just double click on the first Task and change its value to 20 and then do the same for the third task, but a quicker and easier way to swap these Tasks over is to move them. To move a Task, left click on it and, while holding the left mouse button down,

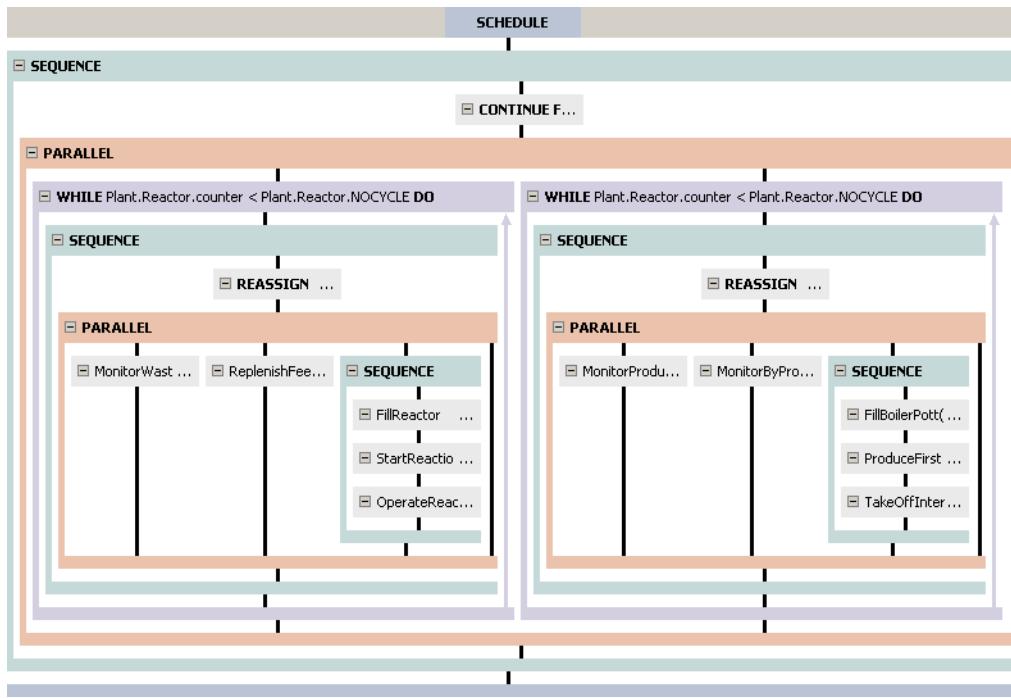
drag it to another hot spot. Before the left mouse button is released, the mouse pointer will change to to indicate that the Task is being moved. Note, this is similar to the pointer when a Task is being added, but without the "+" sign. When the left mouse button is released, the Task will be moved to the new location (note that Tasks cannot be moved if the new location requires the addition of a new Sequence Task — in this case, one must either insert a new Sequence and then move the Task or copy the Task and then delete the original one). Using this method, it is very quick and easy to move Tasks around.

It is also possible to copy Tasks. This is done in a similar way to moving Tasks but by also holding down the **CTRL** key. To copy a Task, drag it to a new hot spot exactly as if it were being moved. The mouse pointer will change to to show that it is being moved. Now, before releasing the left mouse button, hold down the **CTRL**

key. The mouse pointer will now change to to indicate that the Task is being copied. Keeping the **CTRL** key down, release the left mouse button and the duplicate Task will be added to the Schedule. gPROMS will insert a new Sequence Task if necessary. You can change a copy to a move or *vice versa* at any time during a drag: all that matters is the state of the **CTRL** key when the left mouse button is released.

If you prefer not to drag Tasks around, it is also possible to move or copy Tasks using the Cut, Copy and Paste commands in the Edit and context menus or their keyboard shortcuts (**CTRL+x**, **CTRL+c** and **CTRL+v** respectively). Simply right click on the Task, select Cut or Copy from the context menu, then right click on the desired hot spot and select Paste. To use the keyboard shortcuts, left click on the Task, press **CTRL+x** or **CTRL+c**, left click on the desired hot spot and press **CTRL+v**. (The currently-selected hot spot is shown as a blue line instead of a black one.)

It is possible to move, copy or delete multiple Tasks simultaneously. This is done by making multiple selections. To make a multiple selection, select the first Task as usual (by left clicking on it), then hold down the **CTRL** key and select another Task. As long as the **CTRL** key is held down, more Tasks can be added to the selection by left clicking on them. (Note that Tasks cannot be removed from the selection by left clicking on them again.) There is one restriction when making multiple selections: once the first Task is selected, you can only add more Tasks to the selection if those Tasks belong to the same Composite Task as the first one and at the same level in the Task hierarchy. The Schedule below (which is a modified version of the Batch Plant example) will be used to illustrate this.

Figure 11.11. Schedule with example multiple selections

The Continue Task at the top and the large Parallel Task can both be part of the same multiple selection because they are both part of the first Sequence Task. All of the other Tasks are also within the main Sequence Task, but because they are deeper in the hierarchy, they cannot be selected along with the first Continue Task.

The two While Tasks can form a multiple selection because they both belong to the large Parallel Task.

The two small Parallel Tasks cannot form a multiple selection because, even though they are at the same level in the hierarchy, they belong to different Sequence Tasks.

Finally, if we select the `MonitorWast ...` Task, we can also select the `ReplenishFee...` Task and the Sequence next to it, but neither the `FillReactor ...` Task (wrong level) nor the `MonitorProdu...` Task (not in the same Parallel).

Once a multiple selection has been made, it can be moved, copied or deleted just like a single Task. To delete all of the Tasks in a multiple selection (including any Tasks contained within them), simply press the **DEL** key or right click and select Delete from the context menu. To move or copy, make sure the **CTRL** key is held down and then left click and drag one of the Tasks to its new location. Releasing the left mouse button while **CTRL** is still held down will result in a copy; releasing the **CTRL** key first will result in a move. Releasing **CTRL** and pressing **ESC** while the Tasks are being dragged cancels the move/copy and retains the multiple selection.

When the Tasks in the multiple selection have been moved or copied, they will be pasted into the new location in a specific order. First, if they are not copied or moved to a Sequence Task, then one will be inserted automatically and they will be inserted into that. Next, they will be inserted into the Sequence Task in the order that they had in their original Composite Task. That is: if they were originally in a Sequence Task, then their time order will remain the same; if they were in a Parallel Task then the order from left to right in the Parallel Task will become the order from first to last in the Sequence; finally, if they were in an If Task then the Task in the TRUE branch will be inserted before the Task in the ELSE branch.

Just as with any other edit made to the Schedule, a completed move or copy of a multiple selection can be undone by pressing **CTRL+z** or the undo button.

We have seen that when most Tasks are added to the Schedule, a configuration dialog appears. This is because most Tasks need some information to function. In the case of the Continue Task, we needed to specify an amount of time and/or a condition. We also saw that the Reassign Task needs to know which Variables to Reassign and

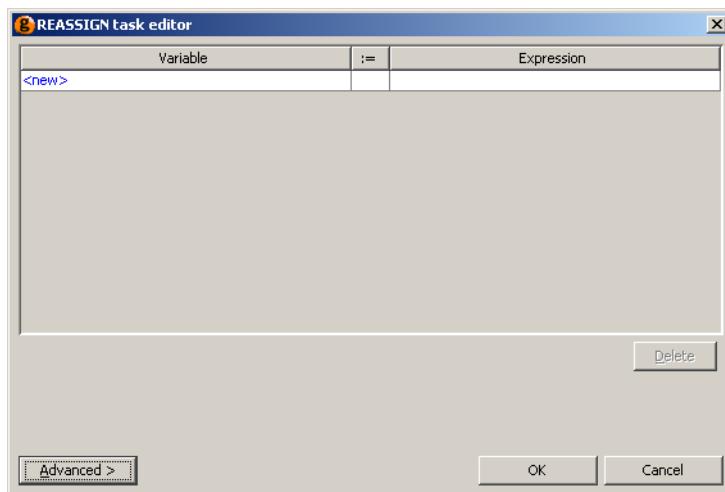
the new values that they should take. Since different Tasks require different data, each configuration dialog will be different. These are discussed in detail in the sections that describe the Tasks. There are, however, some common features that can be described first.

The two features that are common to a lot of Task configuration dialogs are real-time syntax checking and the Advanced view.

All Task configuration dialogs constantly check for errors in the input data. Whenever the data would prevent the Task from working correctly, the OK button is disabled forcing the user to correct the error (or provide the minimum amount of data) before the Task can be inserted or amended.

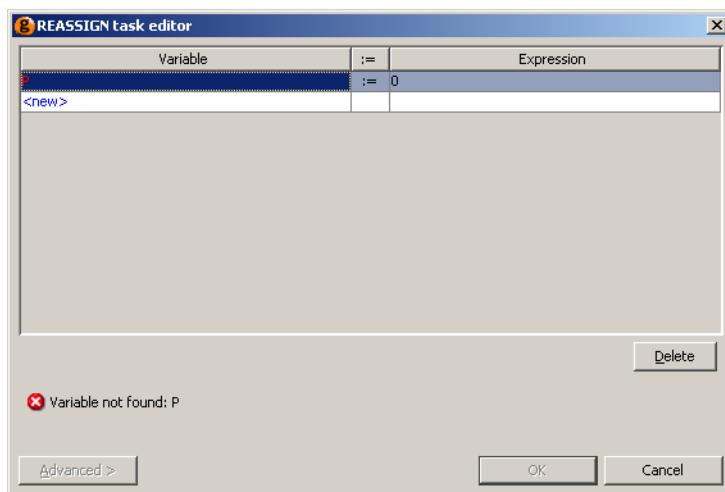
The Reassign Task requires a list of Variables and values to assign to them. When first inserted into the Schedule, the list is empty as is shown in the screen shot below.

Figure 11.12. Initial configuration dialog

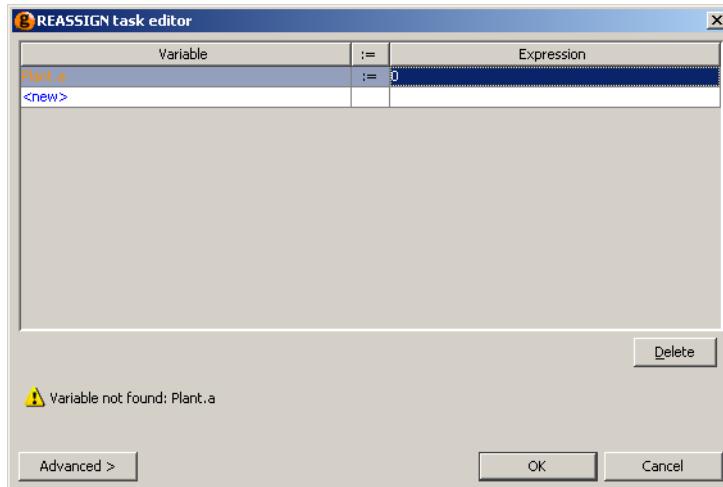


The Reassign Task is allowed to contain an empty list of Variables, so there is no error shown and the OK button is enabled. To add a new Variable, click on the <new> text, enter the path of a Variable and press RETURN. The path will be checked to make sure it is valid, as shown below.

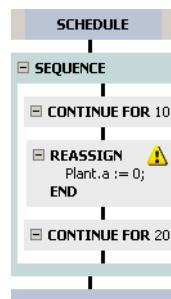
Figure 11.13. Configuration dialog with illegal Variable path



As the path is incorrect, the dialog reports an error and disables the OK button. If a syntactically valid path is entered, but the Variable does not exist, gPROMS gives a warning instead and enables the OK button. This is because one might want to define this Variable after adding the Task.

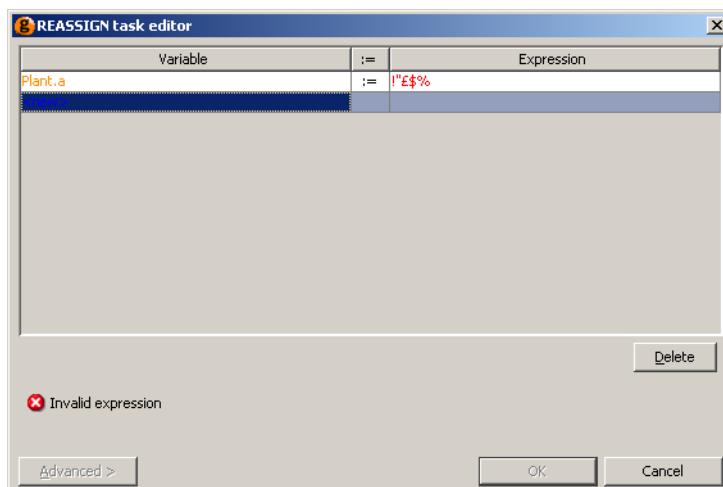
Figure 11.14. Configuration dialog with legal but undefined Variable path

This warning is also shown in the graphical Schedule:

Figure 11.15. Warnings are shown on the graphical Schedule

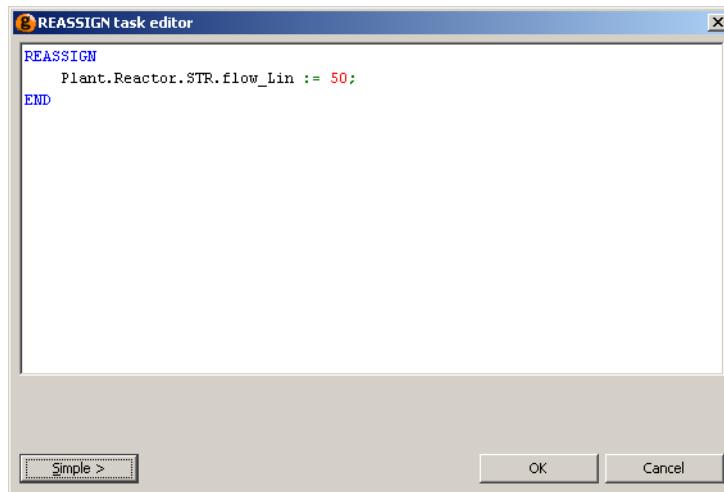
If the Schedule is entered using gPROMS language tab, then syntax errors can occur and they will also be shown in the graphical Schedule (using a ✖ symbol). Double click on the Task (or go back to the gPROMS language tab) to see the error message(s).

Once a legal Variable path has been entered, an expression for the new value must be entered. By default, this is zero but when a new expression is entered, gPROMS checks its syntax and displays the message below if it is illegal. Note also that warnings are highlighted in orange and errors in red.

Figure 11.16. Configuration dialog with illegal expression

When all of the input data are correctly entered, the Advanced button is enabled. This allows you to see the gPROMS language of the Task, as shown below.

Figure 11.17. Configuration dialog showing advanced view



Pressing the Simple button returns to the tabular view.

In summary:

- Schedules can be created using gPROMS language or the graphical interface
 - Both methods are equivalent and can be used interchangeably on the same Schedule
- To create a Schedule
 1. Click on the Schedule tab of a Process
 2. Open the Task Palette
 - if not visible, select Palette from the View menu or press **CTRL+F11**
 3. Drag a Task from the Task Palette onto the Schedule
- Additional Tasks can be dragged from the Task Palette into the Schedule using the hot spots (vertical black lines in the Schedule) or by right clicking on a hot spot and using the context menu to insert a new Task
- For most Tasks, a configuration dialog will appear and need to be completed before the Task is inserted
 - The simple view allows the Task to be configured using text boxes and buttons
 - The advanced view allows the Task to be configured using gPROMS language
 - Both views have real-time syntax checking
 - Double click on existing Tasks in the Schedule to bring up their configuration dialogs
- Composite Tasks allow complex structures to be built up
 - Sequence, Parallel, While and If allow sequential, concurrent, iterative and conditional execution of Tasks
 - A Sequence Task is automatically inserted if needed
- Task information is shown on the Schedule and the level of detail shown is controlled by:
 - Setting the width of Task boxes, using the buttons

- Hiding or showing the details using the or buttons (or by using the Schedule Tab Toolbar)
- Tasks never show more than four lines of language in the graphical Schedule; to see the full details:
 - Move the mouse pointer over the Task to bring up a tool tip that shows all of the language;
 - Double click on the Task and select the Advanced view; or
 - Right click on the Task and select Go to language from the context menu
- Tasks can be selected by left clicking on them
 - multiple selections can be made by holding the **CTRL** key and left clicking on Tasks
 - multiple selections may only comprise Tasks belonging *directly* to the same Composite Task
- Tasks can be moved by dragging them to a new hot spot and copied by dragging with the **CTRL** key held down
 - Works with multiple selections as long as the **CTRL** key is held down
 - The original order is retained and a Sequence is added if necessary
- The Cut, Copy, Paste and Delete context menu items can be used for moving, copying or deleting selected Tasks
- All of the gPROMS language for Schedules is contained in the gPROMS language tab of the Process, within a SCHEDULE section at the end

The next subsection briefly describes the Schedule Tab Toolbar.

The subsequent sections describe in more detail (including how to write gPROMS language):

- Elementary tasks (what to do),
- Timing structures (when to do it),
- Results-control elementary tasks, and
- Tasks for creating and using Saved Variable Sets.

Predefined Tasks are described afterwards. See: *Defining Tasks*.

The Schedule Tab Toolbar

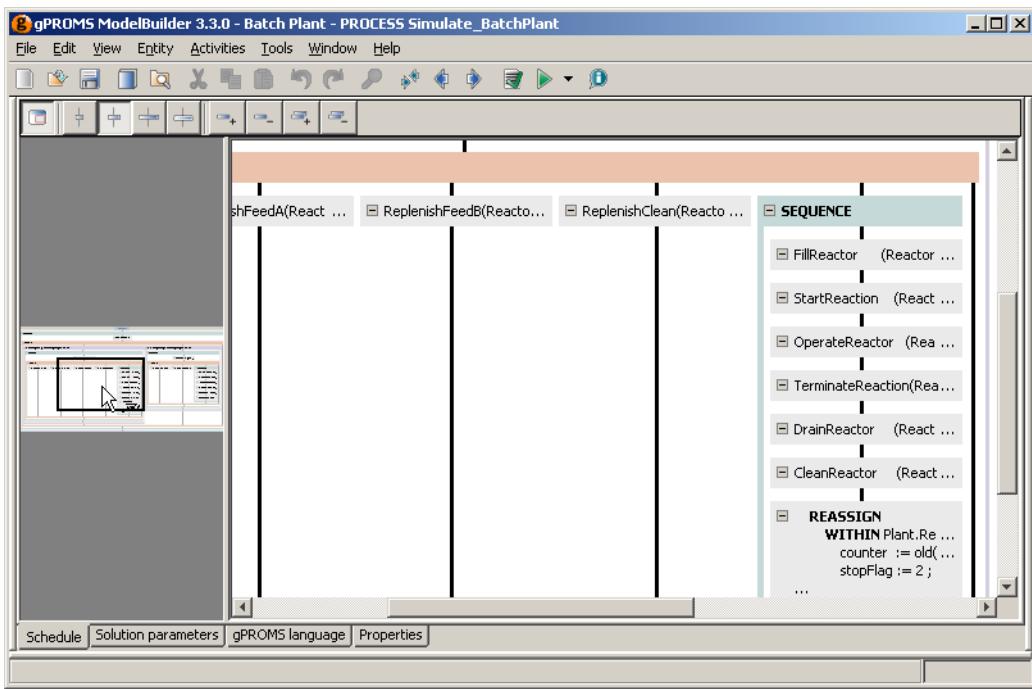
When the Schedule tab is selected, the toolbar below will be visible.

Figure 11.18. Schedule Tab Toolbar



This contains 3 sets of controls.

The first is the overview control. When this button is pressed, an additional pane will be inserted between the Project tree (or Task palette, if this is selected instead) and the Schedule. This pane shows an overview of the Schedule and is useful when the Schedule is so complicated that it takes up more space than can be shown in the Schedule tab. An example of this is shown below (where the Project tree and Palette have been hidden in order to show more detail).

Figure 11.19. Overview pane

The black box on the overview indicates the view shown in the main, right-hand pane. This box automatically moves as you adjust the view in the right-hand pane by dragging the scroll bars. You can also move the black box directly by left clicking on it and dragging it to a new position in the overview (as is being done in the screenshot above). This then automatically changes the view in the large right-hand pane.

The next four buttons, shown below, allow one to adjust the width of the Task boxes shown in the Schedule tab.

Figure 11.20. Width Controls

The first three limit the width of the Task boxes to small, medium and large. The last one removes the limit so that the Task boxes will be as wide as the longest visible line of language. The currently-selected option is indicated by the depressed button (the second one in the screenshot above).

The final set of four controls allow one to expand or collapse the information shown in the task boxes (the equivalent of pressing the **+** and **-** buttons of a particular task).

To expand or collapse an individual Task, left click on it (to select it) and then press either or on the toolbar respectively.

To expand *all* Tasks in the Schedule, press . And to collapse all Tasks, press .

Elementary tasks

The following elementary tasks that can be used to define "what to do" during a gPROMS simulation:

- Reassign
- Switch
- Replace

- Reinitial
- Continue

The Reassign (Reset) elementary task

Model Variables can be Assigned values which can be either fixed or dependent on the simulation time using expressions containing the Time statement. Up to now, Assignments could be changed using the Reset elementary Task. With gPROMS v3.3, the Reassign elementary Task has been introduced and it serves exactly the same purpose as Reset but has a better link to Assign.

Users are encouraged to adapt the Reassign statement in their models to use the more clearly related pair of Assign and Reassign.

Full backward compatibility is maintained and all existing and new models using the Reset elementary Task will continue working as before; they are also properly displayed in the new editor for Graphical Schedules and Tasks.

The syntax for the Reassign task is:

```
REASSIGN
  VariablePath := Expression ;
END
```

where *VariablePath* is the full path to any Variable in the Process and *Expression* is any expression involving constant numerical quantities and the keyword TIME (which represents the simulation time). This means that the expression may involve numbers and Parameters (or functions thereof) but not Variables because they are not inherently constant. When gPROMS refers to a Variable, it refers to the *whole trajectory* of it, so in order to include Variables in a Reassign statement, the OLD() function must be used. This function can only be used in a Schedule and it returns the value of a Variable (or a function involving Variables) at the time immediately before it is used; it has no meaning within Models, because no well-defined values for the variables exist before the simulation commences.

Within statements can be used inside a Reassign task in order to avoid repeating long pathnames.

The examples below demonstrate some applications of the Reassign task.

Example 11.1. Applications of the Reassign task

```
REASSIGN
  V101.Position := 1.0 ;
END

REASSIGN
  WITHIN C101 DO
    Signal := OLD( Bias + Gain * ( Error + IntegralError/ResetTime ) ) ;
  END
END

REASSIGN
  T101.FlowIn := OLD(T101.FlowIn) + 0.1 ;
END
```

In the first example, a Reassign task is used to model the instantaneous opening of a manual valve by a process operator. The Model that corresponds to unit V101 contains a variable called Position, which represents the position of the valve stem, and an equation that relates the flowrate through the valve to the pressure drop across it according to the position of the stem and the inherent characteristics of the valve. The initial position of the valve stem is specified in the Assign section of the corresponding Process. During the simulation, the Reassign task 'reaches' into the model and changes the value of this input variable, just as an operator would walk into the plant

and manipulate the valve. The action is considered to occur in such a small time interval relative to the length of the entire simulation, that it can be modelled as an instantaneous change.

The second example demonstrates how the action of a digital controller at the end of its sampling interval might be modelled. Here, the expression on the right hand side of the assignment is evaluated at the time of execution of the Reassign task. The value of the expression is used to update the value of the control signal instantaneously and according to a proportional-integral control law. This example illustrates the use of the OLD built-in function to refer to the value of the Variables *immediately before* the execution of the Reassign task.

Finally, in the third example the Reassign task is used to impose a step change of magnitude 0.1 on variable T101.FlowIn, representing the input flowrate to a vessel. The OLD function must be used here because the time at which the Reassign Task occurs may not be known *a priori*, so the Value of T101.FlowIn may not be known and cannot be replaced with a literal value.

Using the TIME function in a Reassign

In the Assign section of a Process a Variable value can be made dependent on the simulation time by using the TIME function

```
ASSIGN
  T101.Fin := 20 + 1.2*TIME ;
```

The Reassign elementary task can be used to change this Assignment in a Schedule in the same way as for all other Assignments. In particular, the built-in function OLD can also be used with TIME which is useful in order to avoid discontinuities in input variables. In the following example, a Variable has been Assigned a constant value which is subsequently changed in the Schedule to form a ramp

```
ASSIGN
  T101.Fin := 20;
  ...

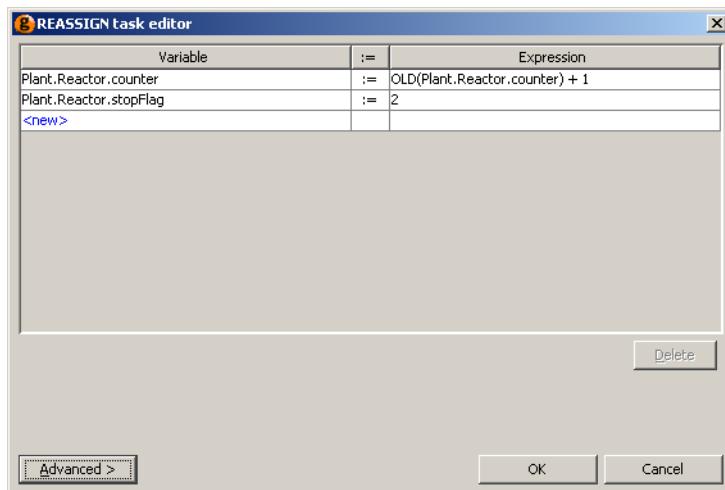
SCHEDULE
  ...
REASSIGN
  T101.Fin := OLD(T101.Fin) + 1.2*(TIME - OLD(TIME));
END
```

It is important to note the difference between using TIME and OLD(TIME). In the example below, the value of Variable A will vary with the simulation time after the Reassign whereas the value of B will remain constant at the value of the simulation time immediately before the Reassign task.

```
REASSIGN
  A := TIME;
  B := OLD(TIME);
END
CONTINUE FOR 100
```

The Reassign Task configuration dialog

When inserting or modifying a Reassign Task using the graphical Schedule interface, the following Task configuration dialog is used.

Figure 11.21. Reassign Task configuration dialog

This dialog contains a list of all of the Variables that are to be Reassign by the Task. To add a new Variable to the list, left click on the cell containing **<new>** and enter the full path of a Variable. Pathname completion can be used at this stage, just as when typing gPROMS language into a Model or a Process. Once the Variable path has been entered press **RETURN** and the associated Expression cell will be set by default to zero. To modify this value, left click on the cell and enter any valid gPROMS expression: as in the examples shown before, this may contain other Variable paths, built-in functions (including **OLD()**) and the **TIME** keyword. As many Variables are required can be added in this way.

To delete a Variable from the Reassign Task, simply select it by left clicking on its row and then press the Delete button.

Once complete, press the OK button.

The Cancel button will close the dialog and discard any changes made to the Task. If the dialog was activated due to the addition of a new Task, then no Task will be added.

The Advanced button can be used to enter gPROMS language. For a new Task, the dialog will contain an empty REASSIGN statement:

```
REASSIGN
END
```

The WITHIN statement may be used in the Advanced view (just as it can be in the gPROMS language tab) if many Variables within the same Unit are to be Reset. The Advanced view also supports pathname completion and copy/paste functionality.

The Switch elementary task

Similar to the Reassign task, the Switch task may be used to alter the value of Selector Variables. Manipulation of a Selector state by a Switch task forces the underlying model to change state as a result of an external action as opposed to a physico-chemical mechanism. Applications include the switching of a pump on or off as shown below, the replacement of a shattered bursting disc by an operator etc.

Example 11.2. Manipulating selector variables using the Switch task

```
# MODEL Pump

VARIABLE
  FlowIn, FlowOut    AS Flowrate
  PressIn, PressOut AS Pressure
  PressRise          AS Pressure

SELECTOR
  PumpStatus         AS (PumpOn,PumpOff)

EQUATION

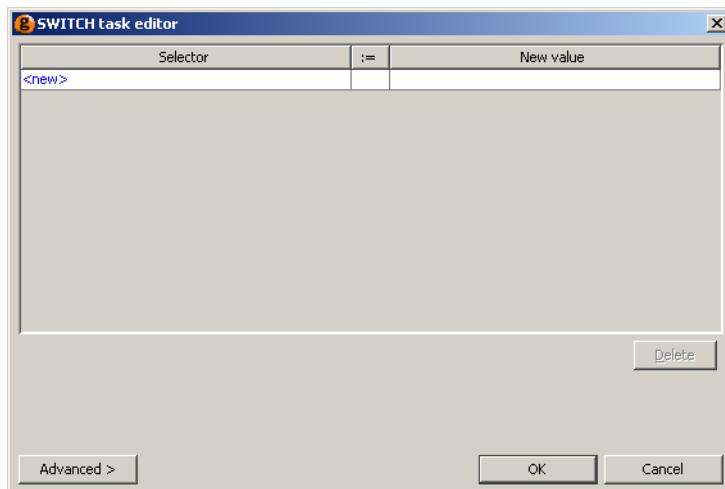
  FlowOut = FlowIn ;
  PressOut = PressIn + PressRise ;
  CASE PumpStatus OF
    WHEN PumpOn : FlowOut = f(PressRise) ;
    WHEN PumpOff : PressRise = 0 ;
  END # Case

# in the SCHEDULE of a Process
SWITCH
  P101.PumpStatus := P101.PumpOn ;
END # Switch
```

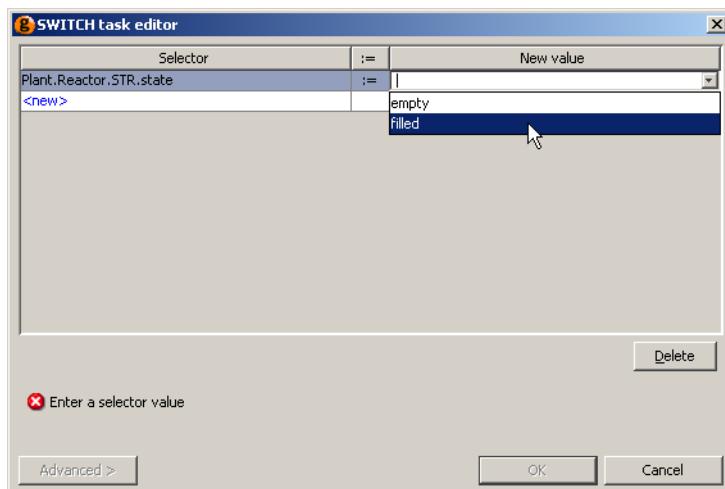
In this example Model Pump has two states, PumpOn and PumpOff, designated by the selector variable Status and representing whether the pump is on or off. When the pump is switched on, the pump characteristic relates the pressure rise across the pump to the flowrate through the pump (note that $f(\text{PressRise})$ is not valid gPROMS language: in this case it is short-hand for some function of the Variable PressRise). When the pump is switched off, the pressure rise is set to zero. Note that no SWITCH statements are present in the CASE statement because no physico-chemical transitions link these two states. Whether the pump is initially switched on or off forms part of the initial condition of each simulation experiment. This information is specified in the SELECTOR section of the corresponding Process. On the other hand, external actions during the simulation are modelled by Switch tasks and cause dynamic changes to this status.

The Switch Task configuration dialog

When inserting or modifying a Switch Task using the graphical Schedule interface, the following Task configuration dialog is used.

Figure 11.22. Switch Task configuration dialog

This dialog contains a list of all of the Selector Variables that are to be Switched by the Task. To add a new Selector Variable to the list, left click on the cell containing <new> and enter the full path of a Selector Variable. Pathname completion can be used at this stage, just as when typing gPROMS language into a Model or a Process. Once the Selector Variable path has been entered press **RETURN**. If a valid Selector Variable path has been entered, the New value cell will now contain a list of possible values one of which *must* be selected from the list box (otherwise a syntax error will be reported — see below). As many Selector Variables are required can be added in this way.

Figure 11.23. Switch Task configuration dialog: selecting a value

To delete a Selector Variable from the Switch Task, simply select it by left clicking on its row and then press the Delete button.

Once complete, press the OK button.

The Cancel button will close the dialog and discard any changes made to the Task. If the dialog was activated due to the addition of a new Task, then no Task will be added.

The Advanced button can be used to enter gPROMS language. For a new Task, the dialog will contain an empty SWITCH statement:

```
SWITCH
END
```

The WITHIN statement may be used in the Advanced view (just as it can be in the gPROMS language tab) if many Variables within the same Unit are to be Switched. The Advanced view also supports pathname completion and copy/paste functionality.

The Replace elementary task

The Replace elementary task 'unAssigns' an input variable (leaving it free to vary) and Assigns a different one in its place. An interesting application of the Replace task is the automatic calculation of the steady-state bias of a controller. In order to determine the bias, a steady-state calculation is performed in which the controller error is set to zero by an input equation, while the bias is free to vary. The bias value obtained by this calculation corresponds to the correct steady-state bias for the controller. Therefore, before dynamic simulation begins, the Replace task shown below can be used to "unAssign" the error variable and Assign the bias variable to its steady-state value. The controller error is then free to fluctuate as disturbances are introduced and the controller attempts corrective action.

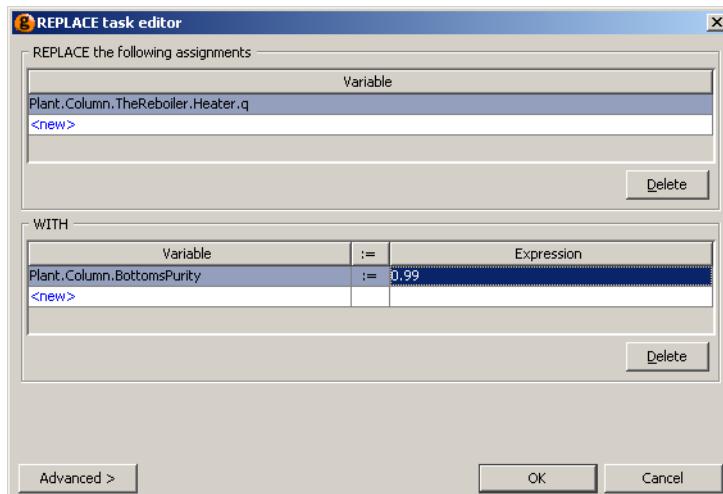
Example 11.3. Automatic calculation of controller bias using a Replace task

```
REPLACE
  PI101.Error
  WITH
    PI101.Bias := OLD(PI101.Bias) ;
  END
```

The Replace Task configuration dialog

When inserting or modifying a Replace Task using the graphical Schedule interface, the following Task configuration dialog is used.

Figure 11.24. Replace Task configuration dialog



This dialog contains a list of all of the Assigned Variables that are to be Replaced by the Task and a list of replacement Assignments. To add a new Assigned Variable to the list, left click on the cell in the top half of the dialog containing **<new>** and enter the full path of an already-Assigned Variable. Pathname completion can be used at this stage, just as when typing gPROMS language into a Model or a Process. Press **RETURN** when done. Add more Variables by repeating this process until all of the Variables that need to be Replaced have been entered.

The bottom half of the dialog contains a list of Variables that are to be Assigned in replacement of the Variables listed above. This part of the dialog behaves exactly the same as the Reassign dialog. The only restriction is that this part of the dialog must contain exactly the same number of Variable Assignments as Variables listed in the top half (otherwise the problem will be under or over specified, and gPROMS will report an error.).

To delete a Variable from the either of the lists, simply select it by left clicking on its row and then press the appropriate Delete button.

Once complete, press the OK button.

The Cancel button will close the dialog and discard any changes made to the Task. If the dialog was activated due to the addition of a new Task, then no Task will be added.

The Advanced button can be used to enter gPROMS language. For a new Task, the dialog will contain an empty REPLACE statement:

```
REPLACE  
WITH  
END
```

The WITHIN statement may be used in the Advanced view (just as it can be in the gPROMS language tab) if many Variables within the same Unit are to be Switched. The Advanced view also supports pathname completion and copy/paste functionality.

The Reinitial elementary task

Both the Reassign and Replace elementary tasks introduce discontinuities in the simulation. Although these discontinuities may affect the values of input and/or algebraic variables, they do not normally affect the values of differential variables. The latter usually represent quantities that are conserved according to the laws of physics (e.g. mass, energy, momentum etc.) and are therefore continuous across such discontinuities; gPROMS follows this assumption and normally expects the values of the differential variables before the discontinuity to be the same as those just after the discontinuity. The Reinitial elementary task makes it possible to introduce discontinuities in the differential variables themselves. Of course, once we drop the continuity assumption, we need to provide some other information to replace it.

Example 11.4. Applications of the Reinitial task

```
REINITIAL  
  PI101.IntegralError  
WITH  
  PI101.IntegralError = 0 ;  
END  
  
REINITIAL  
  R101.HoldUp(1),  
  R101.HoldUp(2)  
WITH  
  R101.HoldUp(1) = 2 * OLD(R101.Holdup(1)) ;  
  R101.X(2) = 0.3 ;  
END
```

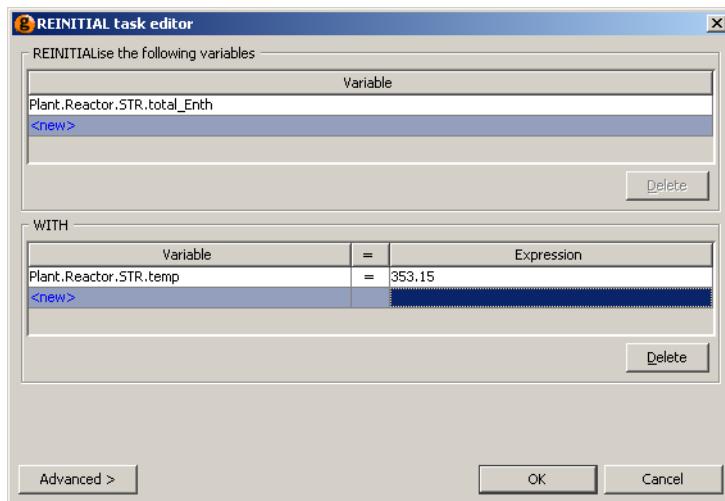
Two examples of the application of the REINITIAL task are shown in the gPROMS code above. In the first example, the integral error of a PI controller is reset to zero. The execution of this task will result in a reinitialisation calculation in which the usual assumption concerning the continuity of differential variable PI101.IntegralError will be replaced by the equation in the second clause of the REINITIAL task. The latter simply states that the value of PI101.IntegralError after the discontinuity is zero. Note that this is a general equation and not just an assignment, which is why we do **not** write:

```
PI101.IntegralError := 0 ;
```

This is consistent with the treatment of general initial conditions in gPROMS. In the second example, the holdups of components A and B in a chemical reactor change by instantaneous additions of material. The amounts added are such that, in the final mixture, the holdup of A is doubled while the mass fraction of B is 0.3. Note again that the condition specified is a general equation involving any variables in the problem and not just the ones that are reinitialised. Naturally, the number of differential variables in the first clause of a REINITIAL task must match the number of equations in the second clause.

The Reinitial Task configuration dialog

When inserting or modifying a Reinitial Task using the graphical Schedule interface, the following Task configuration dialog is used.

Figure 11.25. Reinitial Task configuration dialog

This dialog contains a list of all of the differential Variables that are to be Reinitialised by the Task and a list of new initial conditions. To add a new differential Variable to the list, left click on the cell in the top half of the dialog containing *<new>* and enter the full path of a Variable. Pathname completion can be used at this stage, just as when typing gPROMS language into a Model or a Process. Press **RETURN** when done. Add more Variables by repeating this process until all of the Variables that need to be Reinitialised have been entered.

The bottom half of the dialog contains a list of initial conditions that are to be used to reinitialise the system. This part of the dialog behaves exactly the same as the Reassign dialog, although its function is fundamentally different: these are additional equations to be used for reinitialisation; not assignments of degrees of freedom. This part of the dialog must contain exactly the same number of equations as Variables listed in the top half (otherwise the initialisation problem will be under or over specified, and gPROMS will report an error.). When using the Simple view of the dialog, these initial conditions must be of the form *<Variable> = <Expression>*. Use the Advanced view or the gPROMS language tab of the Process to enter more general initial conditions (of the form *<Expression> = <Expression>*).

To delete a Variable from the either of the lists, simply select it by left clicking on its row and then press the appropriate Delete button.

Once complete, press the OK button.

The Cancel button will close the dialog and discard any changes made to the Task. If the dialog was activated due to the addition of a new Task, then no Task will be added.

The Advanced button can be used to enter gPROMS language. For a new Task, the dialog will contain an empty REINITIAL statement:

```
REINITIAL
WITH
END
```

The WITHIN statement may be used in the Advanced view (just as it can be in the gPROMS language tab) if many Variables within the same Unit are to be Switched. The Advanced view also supports pathname completion and copy/paste functionality.

The Continue elementary task

The execution of all elementary tasks described so far takes place instantaneously with respect to the simulation clock. The Continue elementary task provides the mechanism by which periods of undisturbed operation between discrete actions can be specified. We have already used the CONTINUE task in its simplest form:

CONTINUE FOR *TimePeriod*

This specifies a period of undisturbed process operation, starting from when the Continue task is encountered and extending until the simulation clock has advanced *TimePeriod* time units. In fact, as well as being a real number, *TimePeriod* may alternatively be a real expression involving any quantities that the schedule has access to. For example:

```
# Continue for 100 time units
CONTINUE FOR 100

# Continue for period equal to the sampling interval
CONTINUE FOR C101.SamplingInterval
```

Alternatively, the period of undisturbed process operation can be specified implicitly, in terms of a logical condition:

CONTINUE UNTIL *LogicalCondition*

In this case, simulation continues until *LogicalCondition* becomes true. Again, *LogicalCondition* can be of arbitrary complexity and can involve any quantities that the schedule has access to. For example:

```
# Continue until required conversion has been achieved
CONTINUE UNTIL R101.Conversion > 0.95

# Continue until reactant holdups have been exhausted
CONTINUE UNTIL R101.HoldUp(1) < Epsilon AND R101.HoldUp(2) < Epsilon
```

The two forms described above may also be combined in a single CONTINUE task through the use of AND and OR operators:

```
CONTINUE FOR TimePeriod AND UNTIL LogicalCondition
CONTINUE FOR TimePeriod OR UNTIL LogicalCondition
```

Here, the period of undisturbed operation extends until the simulation clock has advanced *TimePeriod* time units and/or until *LogicalCondition* becomes true, respectively. For instance,

```
CONTINUE FOR 100 OR UNTIL R101.Conversion > 0.95
```

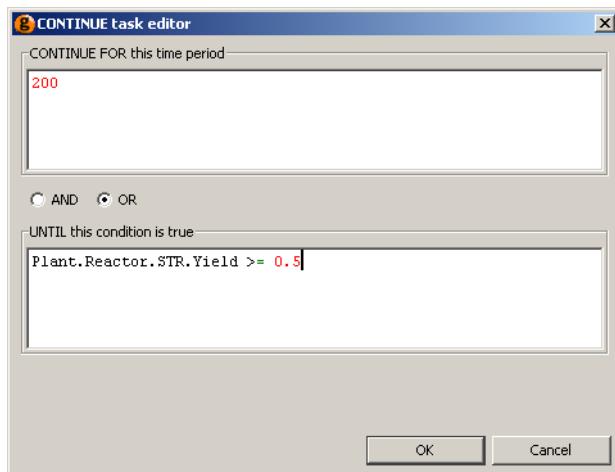
advances the simulation for *at most* 100 time units even if the reactor conversion never reaches the required value, while

```
CONTINUE FOR 100 AND UNTIL R101.Conversion > 0.95
```

advances the simulation for *a minimum of* 100 time units and then waits for the reactor conversion to reach the required value.

The Continue Task configuration dialog

When inserting or modifying a Continue Task using the graphical Schedule interface, the following Task configuration dialog is used.

Figure 11.26. Continue Task configuration dialog

This dialog contains two text boxes, at least one of which must contain a valid entry.

The first box may contain a number or an expression that results in a number . This is used to provide the amount of simulation time the Continue Task will use to advance the simulation. The gPROMS language produced is:

```
CONTINUE FOR contents of first box
```

The second box may contain any logical expression and is the equivalent of:

```
CONTINUE UNTIL contents of second box
```

which causes the simulation to advance until the value of the expression becomes FALSE.

If both boxes contain valid expressions, then they will be combined into one statement using the value determined by the radio button in the middle (which is only enabled when both boxes are complete). If the AND button is selected, the following language is generated.

```
CONTINUE FOR contents of first box AND UNTIL contents of second box
```

There is no Advanced view for the Continue Task. To enter gPROMS language directly, use the gPROMS language tab for the Process or right click on the Continue Task and select Go to language from the context menu.

The Stop elementary task

Stop is a simple elementary tasks that may be used to halt a simulation (perhaps in conjunction with a conditional statement) The syntax for STOP is:

```
STOP
```

There is no configuration dialog for the Stop Task as no further information is required.

Specifying the relative timing of multiple tasks

Having discussed the elementary tasks that define "what to do", we now introduce the following timing statements that describe "how/when" to do something:

- Sequence

- Parallel
- If
- While

These are combined with the elementary tasks to create complex operating procedures.

Sequential execution — Sequence

Sequential execution begins with the first task and only proceeds to the next task when execution of the preceding task has terminated. Sequential execution of a series of tasks is specified by enclosing them within a Sequence structure. The execution of a Sequence structure is complete when the execution of the last task in the structure has terminated. The gPROMS code below shows a Process for a simulation experiment involving a multi-component mixing tank. Unit T101 is a tank with two input streams, containing a mixture of components A, B and C. The values of the flowrates and component mole fractions of the inlet streams are specified in the Assign section. The outlet valve is closed. Initially, the tank contains 1000kg of component A, with additional components B and C to make up a volume of 1.5m³. The initial amount of component C is twice that of component B. The schedule of operation in the gPROMS code below contains only a Continue task, thus defining a period of continuous operation with a duration of 120 time units.

Example 11.5. Mixing tank Process

```
# PROCESS SimpleSim

UNIT
T101 AS MixingTank

SET # Parameter values
WITHIN T101 DO
    NoComp := 3 ;
    NoInput := 2 ;
    ValveConstant := 10 ;
    CrossSectionalArea := 1 ; # m2
    Density := [ 950, 1000, 900 ] ; # kg/m3
END # Within

ASSIGN # Degrees of freedom
WITHIN T101 DO
    # First inlet stream
    Fin(1) := 5 ;
    Xin(1,) := [ 0.12, 0.21, 0.67 ] ;
    # Second inlet stream
    Fin(2) := 15 ;
    Xin(2,) := [ 0.98, 0.01, 0.01 ] ;
    # Outlet stream valve fully closed
    ValvePosition := 0.0 ;
END # Within

INITIAL # Initial conditions
WITHIN T101 DO
    HoldUp(1) = 1000 ;
    2 * Holdup(2) = HoldUp(3) ;
    TotalVolume = 1.5 ;
END # Within

SCHEDEULE
CONTINUE FOR 120
```

The gPROMS code below illustrates how a more complicated operating procedure may be defined by using a SEQUENCE structure in the SCHEDULE section. The execution of this simulation experiment will result in the following:

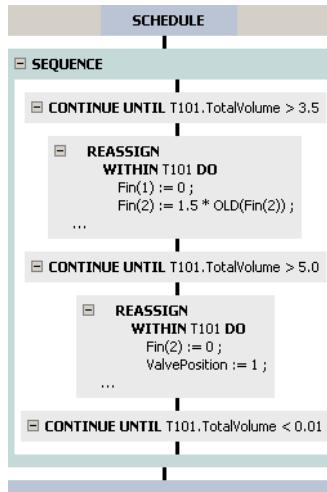
1. Simulation begins. Based on the input equations specified in the ASSIGN section and the initial conditions specified in the INITIAL section, consistent initial values are determined for all variables in the system.
2. The first CONTINUE UNTIL task is executed. Simulation proceeds until the volume of liquid in the tank exceeds 3.5m^3 .
3. The first REASSIGN task is executed. The flowrate of the first inlet stream is set to zero, while that of the second inlet stream is increased by 50%.
4. The second CONTINUE UNTIL task is executed. Simulation proceeds until the volume of liquid in the tank exceeds 5m^3 .
5. The second REASSIGN task is executed. The flowrates of both inlet streams are set to zero. The outlet valve is opened completely.
6. The third CONTINUE UNTIL task is executed. Simulation proceeds until the tank drains.

Example 11.6. Mixing tank Process — tasks in Sequence

```
# PROCESS SeqSim  
...  
SCHEDULE  
SEQUENCE  
  
    # Fill up tank to 3.5 m3  
    CONTINUE UNTIL T101.TotalVolume > 3.5  
  
    # Turn off first inlet stream and  
    # increase the flowrate of the second by 50%  
    REASSIGN  
        WITHIN T101 DO  
            Fin(1) := 0 ;  
            Fin(2) := 1.5 * OLD(Fin(2)) ;  
        END # Within  
    END # Reassign  
  
    # Fill up tank to 5 m3  
    CONTINUE UNTIL T101.TotalVolume > 5.0  
  
    # Turn off second inlet stream and  
    # open the outlet valve completely  
    REASSIGN  
        WITHIN T101 DO  
            Fin(2) := 0 ;  
            ValvePosition := 1 ;  
        END # Within  
    END # Reassign  
  
    # Drain tank  
    CONTINUE UNTIL T101.TotalVolume < 0.01  
  
END # Sequence
```

The equivalent graphical representation is shown below.

Figure 11.27. Mixing tank Process — graphical representation of tasks in Sequence



There is no configuration dialog for the Sequence Task as all of the information about the order of its constituent Tasks is contained in the graphical representation.

Concurrent execution — Parallel

Tasks to be executed in parallel are enclosed within a Parallel structure. Execution of all tasks begins simultaneously and proceeds concurrently. The execution of a Parallel structure is completed when *all* tasks have terminated. The gPROMS code below demonstrates the use of concurrent tasks in specifying an operating policy for the mixing tank example. The operating policy is in fact the same as in the gPROMS code above. However, here, the operating policies for the two inlet and the outlet streams are specified separately with three SEQUENCE structures. These are then enclosed in a PARALLEL structure, so that the three policies are executed concurrently.

Example 11.7. Mixing tank Schedule — tasks in Parallel

```
SCHEDULE

PARALLEL

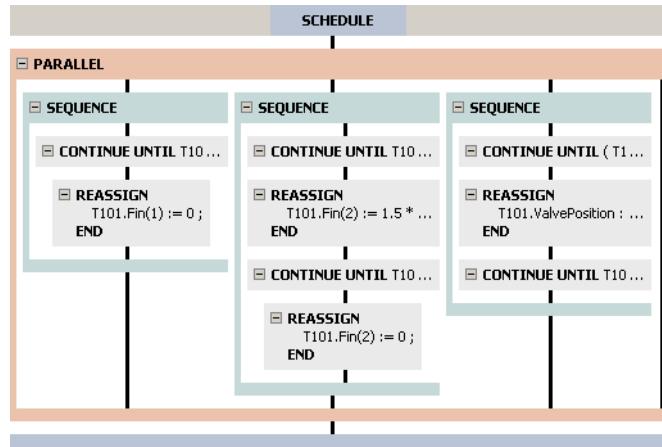
# Operating policy for first inlet stream
SEQUENCE
    # Fill up tank to 3.5 m3
    CONTINUE UNTIL T101.TotalVolume > 3.5
    # Turn off first inlet stream
    REASSIGN
        T101.Fin(1) := 0 ;
    END # Reassign
END # Sequence

# Operating policy for second inlet stream
SEQUENCE
    # Fill up tank to 3.5 m3
    CONTINUE UNTIL T101.TotalVolume > 3.5
    # Increase the flowrate of the second inlet stream by 50%
    REASSIGN
        T101.Fin(2) := 1.5 * OLD(T101.Fin(2)) ;
    END # Reassign
    # Fill up tank to 5 m3
    CONTINUE UNTIL T101.TotalVolume > 5.0
    # Turn off second inlet stream and
    REASSIGN
        T101.Fin(2) := 0 ;
    END # Reassign
END # Sequence

# Operating policy for outlet stream
SEQUENCE
    # Wait until both inlet streams have been turned off
    CONTINUE UNTIL ( T101.Fin(1) < 0.01 ) AND ( T101.Fin(2) < 0.01 )
    # Open the outlet valve completely
    REASSIGN
        T101.ValvePosition := 1 ;
    END # Reassign
    # Drain tank
    CONTINUE UNTIL T101.TotalVolume < 0.01
END # Sequence

END # Parallel
```

The equivalent graphical representation is shown below.

Figure 11.28. Mixing tank Process — graphical representation of Tasks in Parallel

There is no configuration dialog for the Parallel Task as all of the information about its constituent Tasks is contained in the graphical representation.

The black vertical line on the far right is the hot spot for inserting a new Task to be performed in Parallel with the existing 3 Sequences.

Conditional execution — If

In many circumstances, the correct external actions to apply to a system cannot be fully determined *a priori* and must be established from decisions that can only be made while the simulation is in progress. For instance, consider a batch operation involving a series of elementary processing steps applied to a batch of material. Once all steps are completed a decision is made as to whether the batch is acceptable, should receive further processing or should be discarded. This decision depends only on the quality of the batch, so the result can only be established after the preceding steps have been completed.

The If conditional structure enables selection between alternative actions based on the current status of a system. In common with most programming languages, it comprises an If clause, an optional Else clause and a logical condition. If the logical condition is true when the If structure is encountered, the contents of the If clause are executed; otherwise, the contents of the Else clause are executed. As with all other timing structures, conditional structures can be nested in arbitrary manner. The gPROMS code below shows the application of the If structure to 'clipping' a digital control signal before sending it off to a control valve. If, at the time of execution, the signal proves to be greater than 1.0 or less than 0.0, the stem position is set to 1.0 and 0.0 respectively. Otherwise, the stem position is set to the value indicated by the control signal.

Example 11.8. Application of the If conditional structure

```

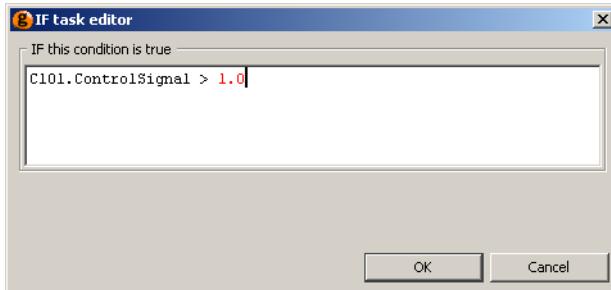
SCEDULE

...
IF C101.ControlSignal > 1.0 THEN
  REASSIGN V101.Position := 1.0 ; END
ELSE
  IF C101.ControlSignal < 0.0 THEN
    REASSIGN V101.Position := 0.0 ; END
  ELSE
    REASSIGN V101.Position := OLD(C101.ControlSignal) ; END
  END # If
END # If

...
  
```

When using the graphical interface, inserting an If Task will activate the following Task configuration dialog.

Figure 11.29. If Task configuration dialog

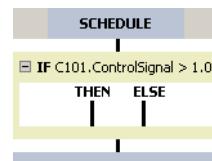


Enter a valid logical expression in the text box (e.g. C101.ControlSignal > 1.0) and press the OK button. gPROMS checks the syntax of the expression and only enables the OK button when it is valid.

There is no Advanced view of the configuration dialog for the If Task.

Once a valid expression has been provided, the If Task will be inserted and will look like this:

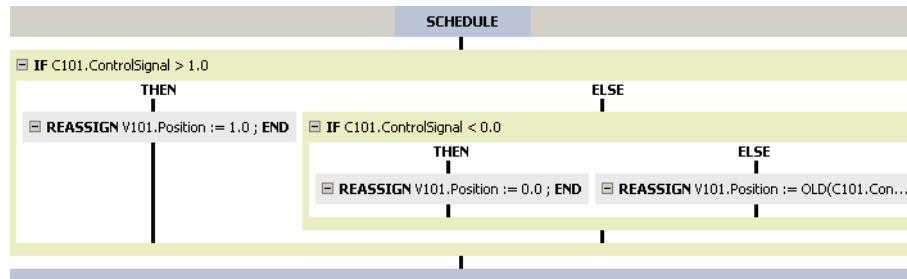
Figure 11.30. A new If Task



Drag new Tasks onto the THEN hot spot to provide the operating policy to be performed if the condition is TRUE. The ELSE branch contains the *optional* operating policy when then if condition is FALSE.

The graphical representation of the example above is shown below.

Figure 11.31. Graphical representation of the If Task



Iterative execution — While

Many processing systems are characterised by the repetitive nature of external actions required to achieve the desired operation. For example, periodic processes, such as pressure swing or temperature swing adsorption, are usually brought to and maintained at a 'cyclic steady-state' by a sequence of external actions that is applied repeatedly. Also, the action of a digital control system on a process can be considered to consist of a regular cycle between continuous operation, sampling and implementation of discrete actions.

The While iterative structure permits the repeated execution of the tasks it encloses for as long as a logical condition is satisfied. When the While structure is first encountered, the logical condition is examined. If it is satisfied, the enclosed tasks are executed. The condition is then examined again and, if still satisfied, the enclosed tasks are executed once more. This process continues until the condition is no longer satisfied, at which point the execution of the While structure is completed. Note that, if the condition is not satisfied initially, the execution of the While structure terminates immediately. The gPROMS code below illustrates the use of a WHILE structure in specifying

the operation of a digital PI controller. While the conversion in the reactor is below 0.95, the controller repeatedly goes through an inactive step of 5 time units (CONTINUE task), followed by a sampling and calculation step (REASSIGN task), followed by a clipping and implementation step (IF structure).

Example 11.9. Application of the While iterative structure

```
SCHEDULE
```

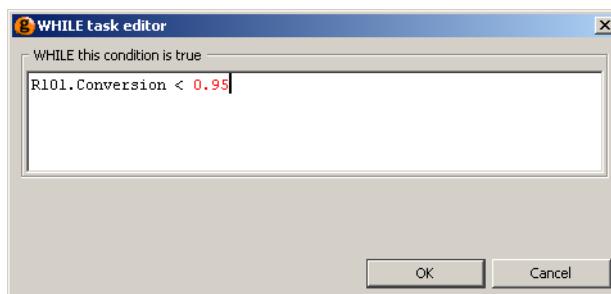
```
...
```

```
WHILE R101.Conversion < 0.95 DO
    SEQUENCE
        # Continuous operation
        CONTINUE FOR 5
        # Sampling and calculation
        REASSIGN
            C101.Error := 150.0 - Sensor101.Measurement ;
            C101.IntegralError := C101.IntegralError + 5.0*C101.Error ;
            C101.ControlSignal := 0.5 + 1.2*(C101.Error +
                                         C101.IntegralError/20.0) ;
        END # Reassign
        # Clipping and implementation
        IF C101.ControlSignal > 1.0 THEN
            REASSIGN
                V101.Position := 1.0 ;
            END
        ELSE
            IF C101.ControlSignal < 0.0 THEN
                REASSIGN
                    V101.Position := 0.0 ;
                END
            ELSE
                REASSIGN
                    V101.Position := OLD(C101.ControlSignal) ;
                END
            END # If
        END # If
    END # Sequence
END # While
```

```
...
```

When using the graphical interface, inserting a While Task will activate the following Task configuration dialog.

Figure 11.32. While Task configuration dialog

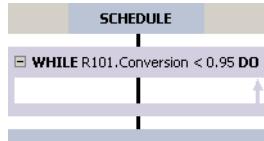


Enter a valid logical expression in the text box (e.g. `R101.Conversion < 0.95`) and press the OK button. gPROMS checks the syntax of the expression and only enables the OK button when it is valid.

There is no Advanced view of the configuration dialog for the While Task.

Once a valid expression has been provided, the While Task will be inserted and will look like this:

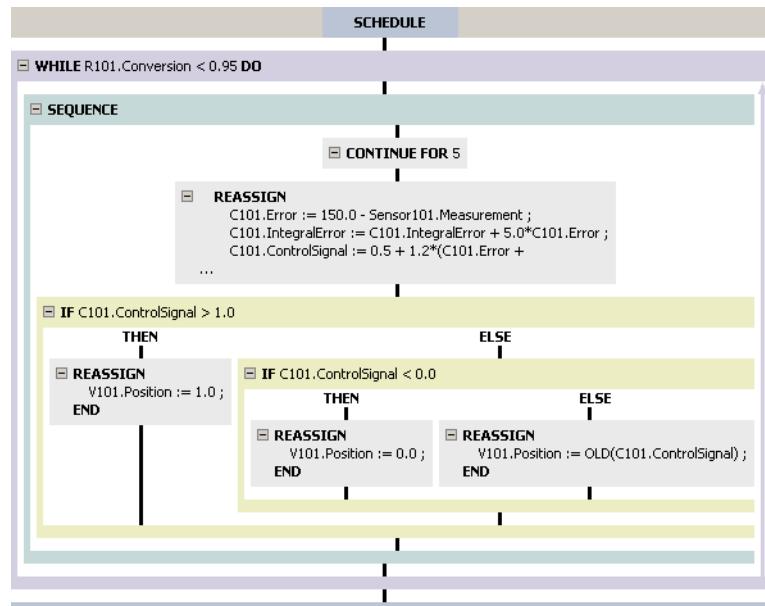
Figure 11.33. A new If Task



The While Task may only contain a single Task. Any Task can be dragged onto the hot spot for the While Task. To include more Tasks, they must be contained in one of the other Composite Tasks, so drag a Sequence, Parallel or If Task into the While Task and then drag new Tasks into the Composite Task. (A quicker way to include a Sequence Task is to drag the first Elementary Task into the While Task and then to drag the second Elementary Task into it after the first: gPROMS will then automatically insert the required Sequence Task).

The graphical representation of the example above is shown below.

Figure 11.34. Graphical representation of the While Task



Result control elementary tasks

The "what to do" elementary tasks influence the numerical results of a simulation (e.g. Reassign changes the value of a degree of freedom, thereby changing the results of the simulation). We now consider the following useful "result control" elementary tasks that influence the generation of results of a simulation, and not the results themselves:

- Message
- Monitor
- Resetresults

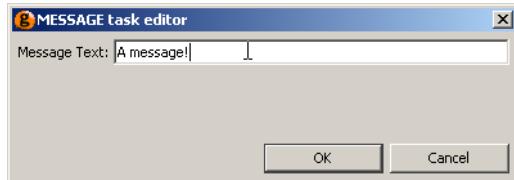
The message elementary task

Message is a simple elementary tasks that may be used to write a message to the screen. The syntax for MESSAGE is:

```
MESSAGE "text"
```

When using the graphical interface, the Task configuration dialog for the Message Task is used to specify the message text:

Figure 11.35. Message Task configuration dialog



Simply enter the desired text (without the quotes) in the text box and press the OK button.

The Monitor elementary task

Normally, during a gPROMS simulation the values of all variables at each reporting interval are sent to the Output Channel in order to be plotted. The Monitor task may be used to restrict the amount of data that is sent, and may be useful for a number of reasons:

- For large distributed models, which may consist of tens of thousands of variables, only a small proportion may be of particular importance and it may sometimes be useful to prevent gPROMS from sending all of these variables. One such example is chromatographic processes, where only the effluent profiles may be of importance. In this case, many of the variables are of secondary importance and could be suppressed from the gPROMS output.
- Restricting the output from gPROMS may be useful in other circumstances: for example, periodic adsorption processes require many cycles of operation before a periodic steady state is achieved. If the modeller is only interested in the steady-state conditions, then the output from gPROMS may be disabled until the final cycle.
- Finally, restricting the data that are sent results in much smaller files (large distributed models may require several Megabytes of storage).

The above situations can be dealt with in two ways, depending on whether variables should be suppressed permanently or only at certain times. The Monitor section of the Process is used to specify which variables are to be monitored during the simulation; those that are not specified are permanently suppressed. If the Monitor section is omitted, then all variables are monitored. The syntax for the MONITOR section is as follows:

```
UNIT
...
MONITOR
  VariablePathPattern ;
...
SET
...
```

where *VariablePathPattern* is the full pathname of the variable to be monitored. Asterisks (*) and percent signs (%) can be used as wild cards to specify ranges of Variables that are to be monitored. Asterisks match any *sequence* of characters and percent signs match any *single* character. Any Variable paths that match the string expressions in the MONITOR section are included in the results. Some examples of *VariablePathPattern* are:

```
MONITOR
  *          ; # monitor everything! (same as not including a MONITOR section
  aaa.*      ; # monitor all Variables and Units in aaa
```

```
aa%          ; # monitor all Variables and Units begining with aa and ending
              # in any other character, e.g. aaa, aab, aac, aa0, aa_ etc.

aaa.v*       ; # monitor all Variables and Units in aaa that begin with a v

aaa.*.y(*,2) ; # monitor all Variables y that belong to any Unit of aaa
              # (or any subunits thereof), provided that they are arrays of
              # dimension > 1; monitor only the elements with the last index = 2

*.x*         ; # all variables starting with x would be monitored in all units
              # also, any units starting with x would also be monitored entirely
```

Note that for distributed variables (i.e. those that depend on a DISTRIBUTION_DOMAIN), the indices must be integers and depend on the numerical method applied to the domain. For each distributed variable, gPROMS will generate an indexed variable with the same number of dimensions as the number of DISTRIBUTION_DOMAINs that the variable depends on. The length of each dimension is equal to $NE \times O + 1$ for OCFEM and $NE+1$ for finite difference methods, where NE is the number of elements and O is the order of the method. For example, if the variable DV1 is defined by:

```
DV1          AS DISTRIBUTION(x,y) OF NoType
```

where the DISTRIBUTION_DOMAINs x and y are Set to the following methods:

```
x := [ OCFEM, 3, 5 ] ;
y := [ BFDM, 2, 20 ] ;
```

then the maximum values for the indices of DV1 are 16 ($5 \times 3 + 1$) and 21 ($20+1$) respectively.

During the simulation, the output of all variables that are specified in the Monitor section can be toggled using the MONITOR task. The syntax for this is:

```
MONITOR ON
```

to enable monitoring, and:

```
MONITOR OFF
```

to disable monitoring. Note that this is a Task that can only appear in the Schedule of a Process and is distinct from the MONITOR section of the Process.

One final use of the MONITOR Task is to change the frequency at which results are sent to the Output Channel(s). This is done by:

```
MONITOR FREQUENCY NumericalValue
```

where *NumericalValue* is a number or an expression that results in a number.

An example of the MONITOR task is shown in the gPROMS code below, where the task DoSomeCycles operates the process until cyclic steady stage is achieved, then DoOneCycle operates the process for a single cycle after monitoring has been enabled.

Example 11.10. Example of the MONITOR task

```
SCHEDULE
SEQUENCE
  MONITOR OFF
  DoSomeCycles ;
  MONITOR ON
  DoOneCycle ;
END
```

Another example of the MONITOR task, illustrating the FREQUENCY keyword, is shown next. In this example, the first Task manipulates the inputs of the system slowly so that a reporting interval of 10 is more than enough to observe the dynamics. Then, the FastOperation Task creates much faster dynamics, which are too fast to be seen clearly with a reporting interval of 10. The MONITOR task changes the reporting interval to a more suitable value. The benefit of this approach, compared with simply setting the ReportingInterval to 1 in the SOLUTIONPARAMETERS section, is that the resulting Case is much smaller.

```
SOLUTIONPARAMETERS
  ReportingInterval := 10 ;

SCHEME
  SEQUENCE
    SlowOperation ;
    MONITOR FREQUENCY 1
    FastOperation ;
  END
```

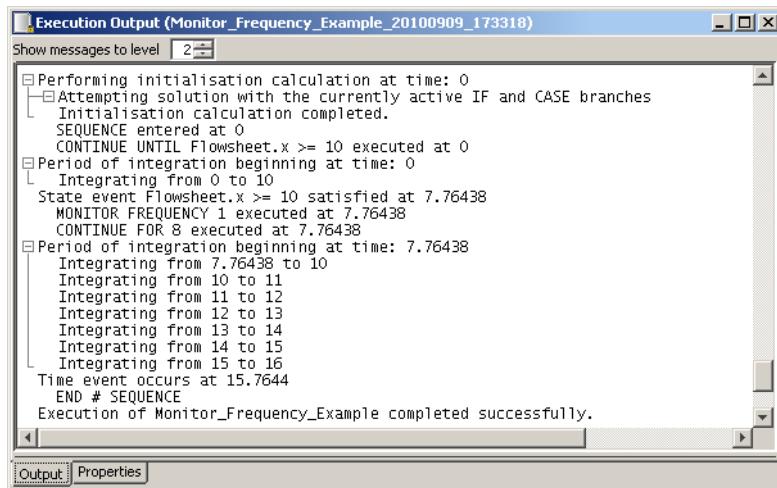
where SlowOperation and FastOperation are Tasks that respectively produce slow and fast dynamics in the simulation.

Exactly when the reporting interval is updated depends on when the MONITOR Task is encountered. gPROMS will always continue to the end of the current reporting interval before updating. The example below illustrates precisely what happens.

```
SOLUTIONPARAMETERS
  ReportingInterval := 10;

SCHEME
  SEQUENCE
    CONTINUE FOR 7
    MONITOR FREQUENCY 1
    CONTINUE FOR 8
  END
```

Figure 11.36. Output from the example Schedule illustrating MONITOR FREQUENCY



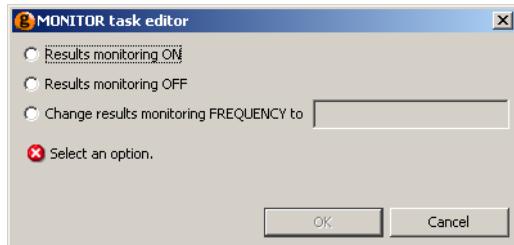
As can be seen, gPROMS starts at time, $t = 0$ and begins integration with the reporting interval equal to 10, so gPROMS outputs data at $t = 0$ and the next set of data are due at $t = 10$. At $t = 7.76$, the Continue Task ends, so a set of data is sent to the output channel at this time (because data are always sent when a discontinuity occurs). The reporting interval is updated to every 1 unit of time but this will not change until the next scheduled reporting time, $t = 10$, so gPROMS then integrates from 7.76 to 10. At $t = 10$ another set of data is sent to the output channel and the new reporting interval takes effect: gPROMS now integrates from 10 to 11, and so on.

The reason for this behaviour is clear: if gPROMS were to update the reporting interval immediately, then data would be sent to the output channel at times 0, 7.76, 8.76, 9.76 etc., which is not very elegant.

The Monitor Task configuration dialog

When inserting or modifying a Monitor Task using the graphical Schedule interface, the following Task configuration dialog is used.

Figure 11.37. Monitor Task configuration dialog



The Monitor Task configuration dialog allows one to turn monitoring off or on, or to specify a monitoring frequency. Only one option can be selected. To turn on monitoring *and* set a new value for the monitoring frequency, simply insert two Monitor Tasks.

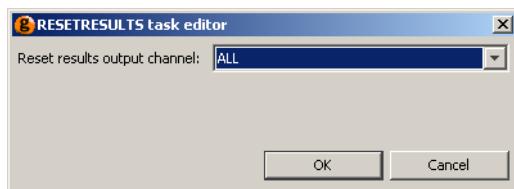
The Resetresults elementary task

The `RESETRESULTS` may be used in the Schedule section of Processes or Tasks to discard all previous data that was transmitted to a particular output channel. It may be called using one of the following commands:

```
RESETRESULTS gRMS  
RESETRESULTS gPLOT  
RESETRESULTS gExcelOutput  
RESETRESULTS gUserOutput  
RESETRESULTS ALL
```

When using the graphical interface, the Task configuration dialog for the Resetresults Task is used to specify one of the above options:

Figure 11.38. Message Task configuration dialog



Simply select the desired option using the list box and press the OK button.

The Save and Restore elementary tasks

Occasionally, it may be necessary to use the solution of one simulation in another. gPROMS provides a facility to Save the current values of all or some of the variables in a simulation and to Restore them in (the same) or another simulation through the use of *Saved Variable Sets*. The syntax of the `SAVE` and `RESTORE` tasks are:

```
SAVE <VarType> "V_Set_Name"
```

and

```
RESTORE <VarType> "V_Set_Name"
```

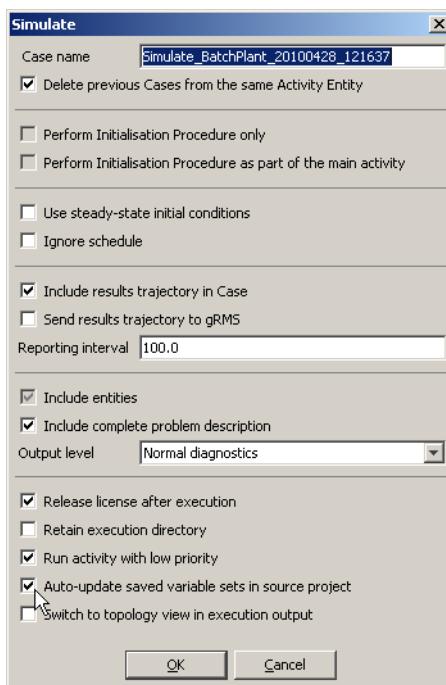
where the optional argument *VarType* can be one of STATE, ALGEBRAIC and INPUT (or any combination of these, separated by commas), and *V_Set_Name* is the name of the *Saved Variable Set* that the variables will be saved in (or restored from). If the *VarType* argument is omitted, then gPROMS will save the values of all variables; whereas arguments STATE, ALGEBRAIC and INPUT instruct gPROMS to save only the values of the state, algebraic or input variables respectively. The *VarType* optional argument works similarly with the Restore task.

Any new *Variable Set* created during a simulation activity using the Save elementary task will be stored in the Results Entity group within the Execution Case. So that the *Variable Set* can be used in conjunction with the Restore elementary task, the *Variable Set* must then be copied into the working project where it will appear in the *Saved Variable Sets Entity* group.

It is also possible to over-write (or modify) an existing *Variable Set* by using the Save elementary task on a *Variable Set* already present in the source project. In this instance, two Saved Variable Sets with the same name will appear in the Execution Case: the original (from the working project) will appear in the *Original Entities* and the new entity created by the Save elementary task will be stored under *Results*.

ModelBuilder can be configured so that the *Saved Variable Set* in the Project is automatically updated. This is done by checking the auto update source project option in the execution dialog that can also be seen in the figure below.

Figure 11.39. Auto Update Source Project Option



Variables may also be Restored from multiple sets, separated by commas:

```
RESTORE "v_set1", "v_set2"
```

Note that, unlike in the PRESET section, when using the Restore Task to restore state Variables, the values of all Selector Variables will be restored as well.

The gPROMS code below illustrates how the SAVE and RESTORE tasks could have been used in the example problem presented in the Monitor section. Rather than solving the problem in one Process, with Monitor used to show only the last cycle of operation, here we can use two Processes: one to establish the cyclic steady state and to save the variables, and the second to simulate a single cycle using as initial conditions the values of the variables at the end of the simulation of the first Process. One advantage of this approach is that the variables can be plotted against the *local* time for the cycle (i.e. the cycle starts at time = 0) as opposed to the global time of the whole simulation (where the start of the cycle will be at some arbitrary time).

Example 11.11. Application of the Save and Restore Tasks.

```
# the Schedule of one Process or Task
SCHEME
SEQUENCE
MONITOR OFF
DoSomeCycles ;
SAVE STATE "CyclicSteadyState"
END

# the Schedule of another Process or Task
SCHEME
SEQUENCE
MONITOR OFF
RESTORE STATE "CyclicSteadyState"
MONITOR ON
DoOneCycle ;
END
```

When Save or Restore Tasks are inserted into the Schedule using the graphical editor, the following configuration dialogs are used.

Figure 11.40. Save Task configuration dialog

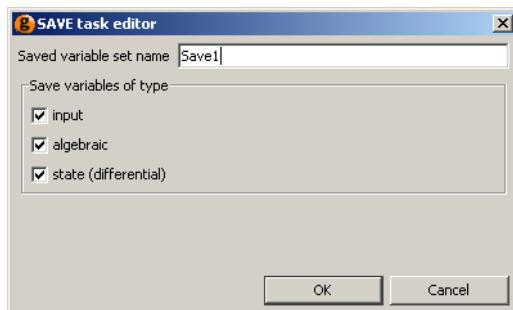
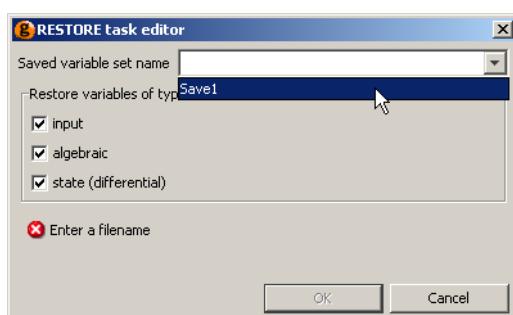


Figure 11.41. Restore Task configuration dialog



When configuring a Save Task, the name of the *Saved Variable Set* must be entered in the text box. The types of Variables stored in the *Saved Variable Set* are specified by checking or unchecking the boxes next to the Variable types: input, algebraic and state (differential). These can be set in any combination.

The Restore Task is configured similarly to the Save Task. The only exception is that the name of the *Saved Variable Set* must be specified by choosing an option from the list box. The list box will only contain the names of the *Saved Variable Sets* present in the Project.

Chapter 12. Defining Tasks

A Task forms a re-usable part of the operating procedure; it is associated with one or more Models and can be used multiple times within a Schedule and by other Tasks.

A Task entity is defined by three sections: Task Parameter declarations, (optional) Task Variable declarations and a Schedule where the Task's operating procedure is expressed in terms of the Task Parameters and Variables.

Overall, the structure of a Task definition is the following:

```
PARAMETER
  ... Parameter declarations ...

VARIABLE
  ... Local variable declarations ...

SCHEDULE
  ... Schedule declaration ...
```

The Variable and Schedule sections of a Task

The Variable section is used to declare local variables. They can only be used within the Task in which they are declared. Task Variables are the equivalent of local subroutine Variables and as such are calculated by the Task. They should not be confused with Model Variables and are NOT associated with Variable Types instead they are declared to be of type INTEGER or REAL.

The Schedule section defines the operating policy implemented by the Task. It is based on the same language used to define the Schedule section in Process Entities, the only difference being that a Task Schedule has access to the local variables declared in the Variable section. The values of the latter can be manipulated by using assignment statements.¹

¹Changing the value of a Task Variable does not require a RESET statement; this only applies to Model Variables.

Example 12.1. Task for a digital PI control law

```
# TASK DigitalPI

VARIABLE
    Error, IntegralError, ControlSignal AS REAL

SCHEDULE
SEQUENCE
    IntegralError := 0 ;
    WHILE TIME < 1000 DO
        SEQUENCE
            CONTINUE FOR 5.0
            Error := 150.0 - Sensor101.Measurement ;
            IntegralError := IntegralError + 5.0*Error ;
            ControlSignal := 0.5 + 1.2 * ( Error + IntegralError/20.0 ) ;
            IF ControlSignal > 1.0 THEN
                RESET Valve201.Position := 1.0 ; END
            ELSE
                IF ControlSignal < 0.0 THEN
                    RESET Valve201.Position := 0.0 ; END
                ELSE
                    RESET Valve201.Position := OLD(ControlSignal) ; END
                END # If
            END # If
        END # Sequence
    END # While
END # Sequence
```

This example shows a TASK that models the action of a digital PI controller. Three local variables are declared in the VARIABLE section, namely Error, IntegralError and ControlSignal. In the SCHEDULE section, an assignment statement initialises IntegralError to zero. Then, the repeated action of the controller is specified within a WHILE structure. This is executed until a termination condition is satisfied (in this case, when 1000 time units have passed on the simulation clock). The action of the controller is itself a sequence of elementary Tasks. First, a CONTINUE task is used to enforce a period of undisturbed operation (5 time units). After this, sampling takes place. The signal of a temperature sensor is used to update the controller Error and IntegralError and a ControlSignal is calculated. An IF structure is used to clip the signal which is then implemented it through a RESET task.

In essence, Tasks are user-defined tasks. Once declared, they are equivalent to elementary tasks and can be used in Process Schedules or even within the Schedules of other Tasks. For instance,

```
SCHEDULE
PARALLEL
    DigitalPI
    CONTINUE FOR 1000
END # Parallel
```

executes the digital control law in parallel with the operation of the rest of the process.

The Parameter section of a Task

The Digital PI control example, although useful for grouping a series of elementary tasks together, has a big disadvantage: it is extremely specific. First of all, it refers to a unique sensor/valve pair, Sensor101 and Valve201 respectively. Moreover, the sampling interval (5 time units) and controller tuning parameters (150.0, 0.5, 1.2, 20.0) are expressed as constant values. Finally, the task always terminates after 1000 time units have elapsed and is thus appropriate for a simulation of that length only. If it were necessary to apply the same operating procedure to a different sensor/valve pair possibly using different tuning parameters for the controller, a new Task

would have to be declared. This is clearly unsatisfactory. In most instances, we want to be able to declare Tasks that are independent of the details of an individual simulation.

For instance, we want to be able to define a Task that switches 'a' pump on and another that switches 'a' pump off. 'A' is used to indicate that the actual pump on which the Tasks act remains unspecified until the moment they are used in a particular simulation experiment. Similarly, we want to be able to define a Task for 'a' digital controller and only specify the sensor/valve pair it uses and the values for its tuning parameters when the Task is actually used in a simulation experiment.

This is achieved by using Task parameters. Upon declaration, a Task can be parameterised with respect to an arbitrary number of parameters. The actual values of these parameters have to be specified only when the Task is actually used in a specific simulation experiment.

Task parameters are declared in the Parameter section. Declared parameters may be of any of the following types:

- INTEGER, REAL or LOGICAL constants. These are used to parameterise a TASK with respect to, for instance, controller tuning parameters, event durations etc.
- INTEGER_EXPRESSION, REAL_EXPRESSION or LOGICAL_EXPRESSION. These are used to parameterise a TASK with respect to, for instance, logical conditions for the conditional and iterative structures etc.
- MODEL. These are used to parameterise a TASK with respect to the actual Models on which it acts.

Example 12.2. Task to switch on a pump

```
# TASK SwitchPumpOn

PARAMETER
    Pump AS MODEL GenericPump

SCHEDULE
    RESET
        Pump.Status := Pump.Open ;
    END # Reset
```

This example shows a task that switches a pump on. Once this Task has been defined, it can be used in a Schedule section. For instance,

```
SCHEDULE
...
SwitchPumpOn(Pump IS Plant.P201)
...
```

will switch on pump Plant.P201, while

```
SCHEDULE
...
SEQUENCE
    SwitchPumpOn(Pump IS Plant.P205)
    SwitchPumpOn(Pump IS Plant.P206)
    SwitchPumpOn(Pump IS Plant.P207)
END # Sequence
...
```

will, in sequence, switch on pumps Plant.P205, Plant.P206 and Plant.P207.

Note that, when executing a Task that contains parameters, the proper list of arguments must be given along with the name of the Task. Tasks that contain parameters can be thought of as the equivalent of subroutines or

functions in high-level programming languages. Variables declared in the Variable section are the equivalent of local subroutine variables. On the other hand, the Parameter section is the equivalent of a function prototype. It defines the number and type of arguments that a Task accepts as arguments. A 'call' to the Task then includes a list of all the Parameters declared in the Task and values for each of them.

Example 12.3. Parameterised Task for a digital PI control law

```
# TASK DigitalPI

PARAMETER
    SetPoint, Bias, Gain, IntegralTime AS REAL
    SamplingInterval AS REAL
    TerminationCondition AS LOGICAL_EXPRESSION
    Sensor AS MODEL GenericSensor
    Valve AS MODEL GenericValve

VARIABLE
    Error, IntegralError, ControlSignal AS REAL

SCEDULE
    SEQUENCE
        IntegralError := 0 ;
        WHILE NOT TerminationCondition DO
            SEQUENCE
                CONTINUE FOR SamplingInterval
                Error := SetPoint - Sensor.Measurement ;
                IntegralError := IntegralError + SamplingInterval*Error ;
                ControlSignal := Bias + Gain*( Error +
                    IntegralError/IntegralTime ) ;
                IF ControlSignal > 1.0 THEN
                    RESET Valve.Position := 1.0 ; END
                ELSE
                    IF ControlSignal < 0.0 THEN
                        RESET Valve.Position := 0.0 ; END
                    ELSE
                        RESET Valve.Position := OLD(ControlSignal) ; END
                    END # If
                END # If
            END # Sequence
        END # While
    END # Sequence
```

This example presents the correct version of the digital controller Task. The Parameters include real constants that determine the various tuning parameters and the sampling interval, a logical expression that determines the termination of control, and model parameters that determine the sensor/valve pair on which the controller is used.

This Task is much more reusable. It can be used for any sensor/valve pair in a simulation experiment and different tuning parameters for the controller can be specified without rewriting the Task. For instance,

```
SCEDULE
...
PARALLEL
    DigitalPI
        ( SetPoint      IS 150.0,
          Bias         IS 0.5,
          Gain         IS 1.2,
          IntegralTime IS 20.0,
          SamplingInterval IS 5.0,
```

```
TerminationCondition IS Plant.T101.TotalVolume > 5.0,
Sensor           IS Plant.Sensor101,
Valve            IS Plant.Valve205 )

DigitalPI
( SetPoint        IS 10.0,
Bias             IS 0.8,
Gain              IS 2.6,
IntegralTime     IS 50.0,
SamplingInterval IS 1.0,
TerminationCondition IS Plant.R101.Temperature > 80.0,
Sensor           IS Plant.Sensor103,
Valve            IS Plant.Valve207 )

END # Parallel
...
```

will initiate two digital control procedures in parallel, acting on two different sensor/valve pairs. The two procedures also have different controller tuning characteristics and a different logical expression determining their termination.

Hierarchical Task Construction

A complex operation on one or more items of process equipment can usually be decomposed into lower-level, simpler operations. Each of the lower-level operations may in turn be decomposed in other, more primitive operations, the decomposition continuing until all operations can be described in terms of elementary manipulations of the underlying models made possible by elementary tasks. Similarly to hierarchical sub-model decomposition, this *hierarchical sub-task decomposition* defeats complexity by restricting the scope of the problem considered at any point to a manageable level.

Hierarchical sub-task decomposition in gPROMS is possible because previously declared Tasks may be used within other, higher-level Tasks and is greatly facilitated by the fact that suitably parameterised Tasks may be reused several times in different parts of an operation.

Example 12.4. Low-level Task to operate a reactor

```
# TASK OperateReactor

PARAMETER
  Reactor          AS MODEL StirredReactor
  SR               AS REAL
  StartTemperature AS REAL
  Terminationcondition AS LOGICAL_EXPRESSION

SCHEDULE
SEQUENCE
RESET
  Reactor.SteamRate := SR ;
END
CONTINUE UNTIL Reactor.Temperature > StartTemperature
RESET
  Reactor.SteamRate := 0 ;
END
CONTINUE UNTIL TerminationCondition
END # Sequence
```

Consider, for instance, the gPROMS code above containing the `OperateReactor` TASK. It specifies an operating procedure for performing a reaction in a reactor of type `StirredReactor` (a parameter of the TASK). The operating procedure is simple, involving the execution of four elementary tasks in sequence. First,

the steam supply rate to the reactor is set to a value SR. Operation then continues until the temperature in the reactor has exceeded a predefined limit StartTemperature. Finally, the steam supply is cut off and operation continues until a TerminationCondition is satisfied. In addition to the reactor unit, SR, StartTemperature and TerminationCondition are also parameters of the TASK, of type REAL, REAL_EXPRESSION and LOGICAL_EXPRESSION respectively.

Example 12.5. High-level Task to operate a reactor train

```
# TASK OperateReactorTrain

PARAMETER
    Plant AS MODEL ReactorTrain

SCHEDULE
PARALLEL
    PerformReaction
        ( Reactor           IS Plant.R1,
          SR                IS 35.3,
          StartTemperature   IS 70.0,
          TerminationCondition IS Plant.R1.Conversion(1) > 0.95 )
    PerformReaction
        ( Reactor           IS Plant.R2,
          SR                IS 10.0,
          StartTemperature   IS 40.0,
          TerminationCondition IS Plant.R2.Temperature > 120.0 )
END # Parallel
```

The gPROMS code above illustrates how the OperateReactor TASK is used to define a higher-level Task, namely OperateReactionTrain. Two OperateReactor tasks are invoked in parallel to model the operation of two reactors. Parameterisation also permits the specification of different values for the operating parameters of the two reactors.

Building Tasks using the graphical interface

Just as it is possible to construct a Schedule of a Process using a graphical interface, it is also possible to build new user-defined Tasks graphically. The following tabs provide a graphical interface for building (or modifying) user-defined Tasks and are entirely equivalent to typing in gPROMS language.

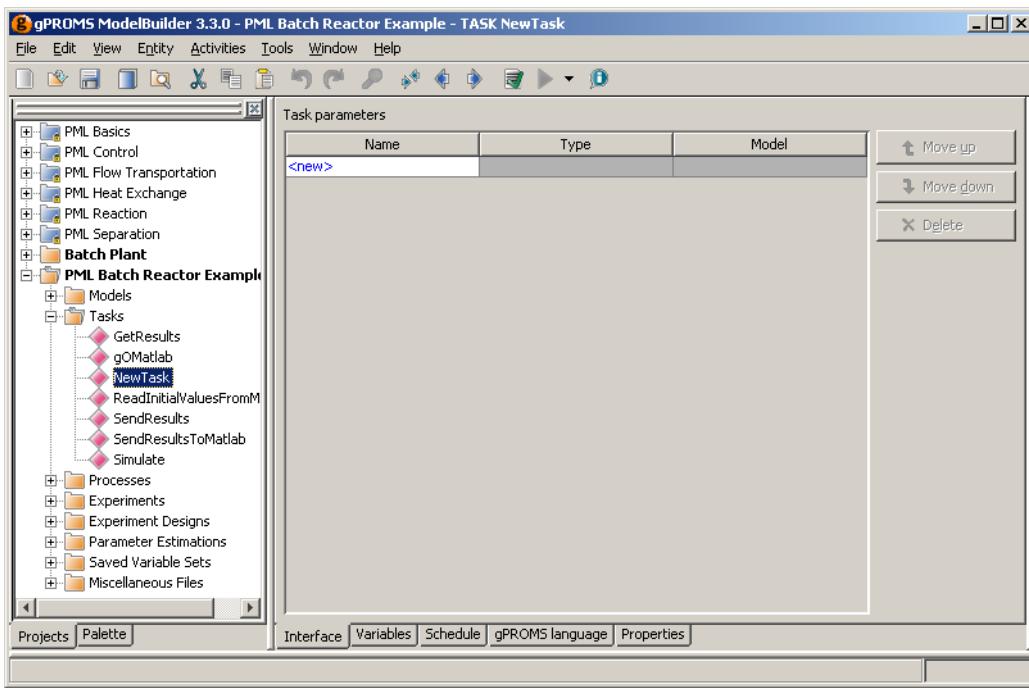
- Interface, which is equivalent to the PARAMETER section
- Variables, which is equivalent to the VARIABLE section
- Schedule, which is equivalent to the Schedule section

Either or both methods can be used interchangeably: modifications made using one of the three tabs above will automatically result in the same changes to the appropriate section of the gPROMS language tab and *vice versa*.

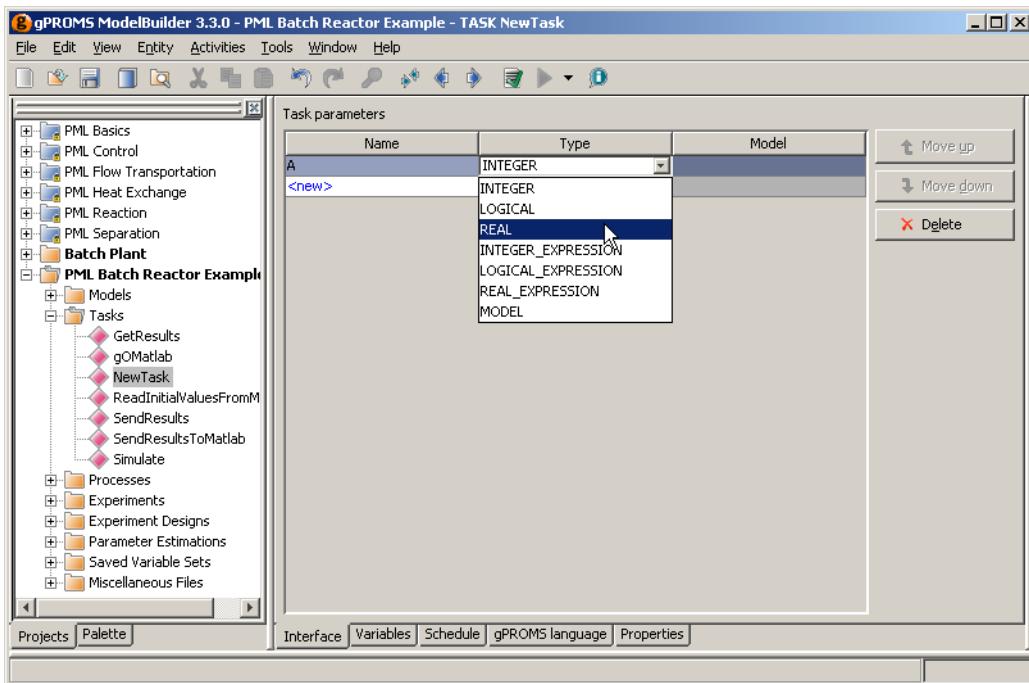
These three tabs are described next. You should be familiar with Defining Schedules (in particular, using the graphical interface) before reading the documentation on the Schedule tab.

Using the Interface tab

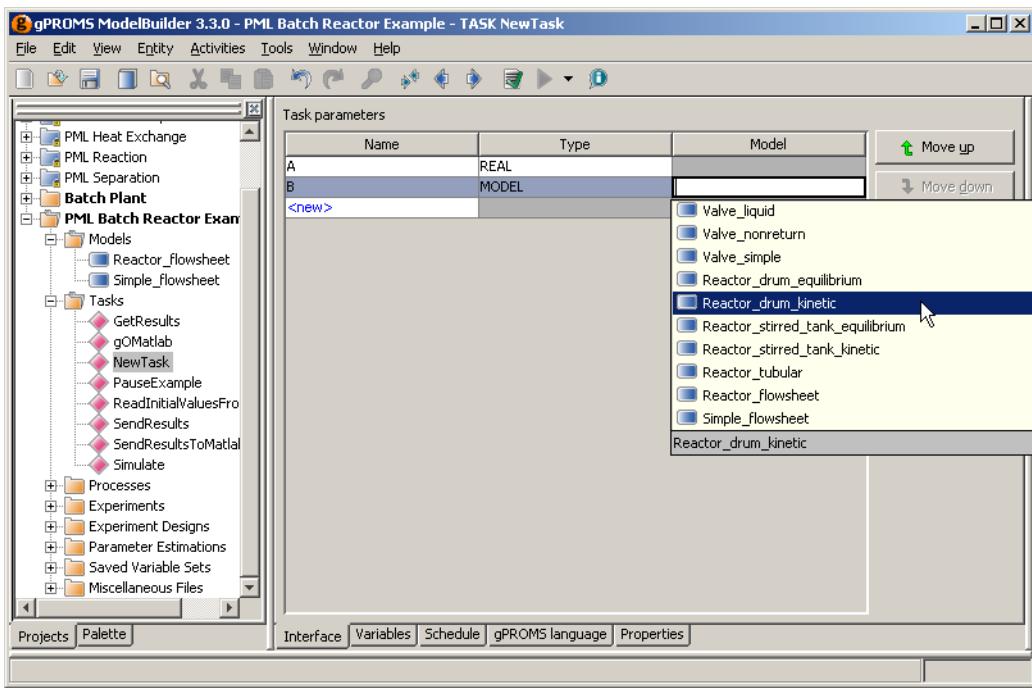
After inserting a new Task in the Project (right click on Tasks in the Project tree, select New entity..., provide a name and click OK), left click on the Interface tab and the following will be shown.

Figure 12.1. New Task Interface tab

The Interface tab contains a list of all of the Parameters in the Task. To add a new Parameter, left click on the <new> cell and enter a name for the new Parameter. Then the type can be chosen from the list box, as shown below.

Figure 12.2. Adding a new Parameter

MODEL Parameters require a further specification: left click in the model cell and type the name of a Model. A list box containing all existing Models in the Project can be activated by pressing **CTRL+SPACE**. This is shown below.

Figure 12.3. Adding a MODEL Parameter

The order of the Parameters can be changed by selecting the Parameter and pressing the Move up or Move down buttons. Parameters can be removed from the Task by selecting a Parameter and pressing the Delete button.

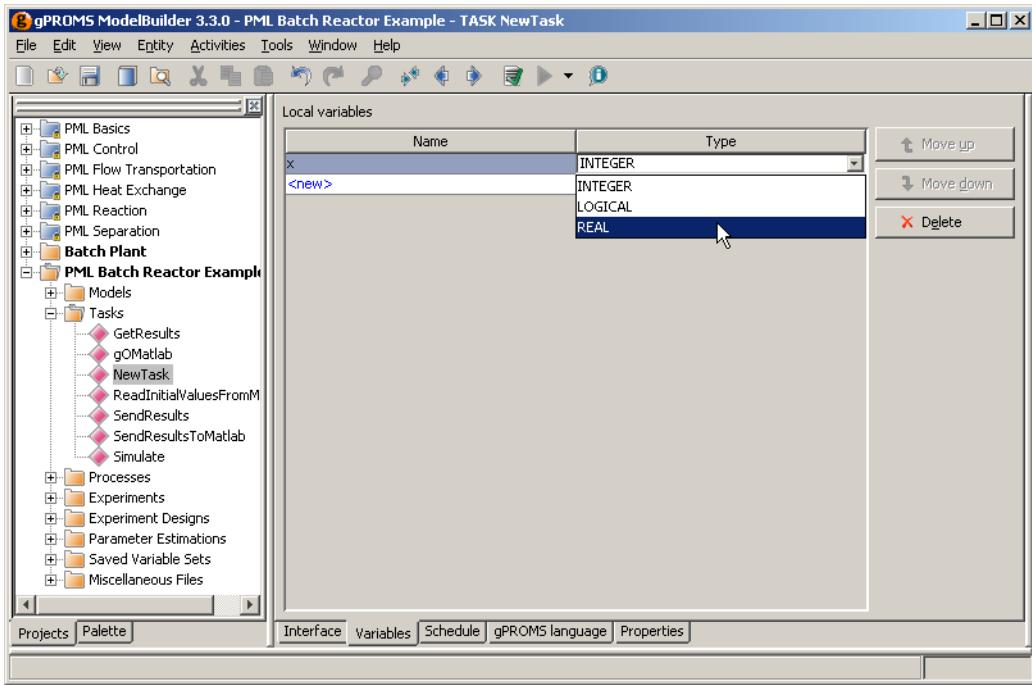
For this example, the gPROMS language tab now contains:

```
PARAMETER
A AS REAL
B AS MODEL Reactor_drum_kinetic
```

Once all of the Parameters have been specified, the Variables tab can be selected in order to define any local Variables for the Task.

Using the Variables tab

The Variables tab contains a list of all of the local Variables in the Task. To add a new local Variable, click on the <new> cell and enter a name for the new Variable. Then the type can be chosen from the list box, as shown below.

Figure 12.4. Adding a new local Variable

The order of the local Variables can be changed by selecting the Variable and pressing the Move up or Move down buttons. Local Variables can be removed from the Task by selecting a Variable and pressing the Delete button.

For this example (including the Parameters defined before), the gPROMS language tab now contains:

```
PARAMETER
  A AS REAL
  B AS MODEL Reactor_drum_kinetic
VARIABLE
  x AS REAL
```

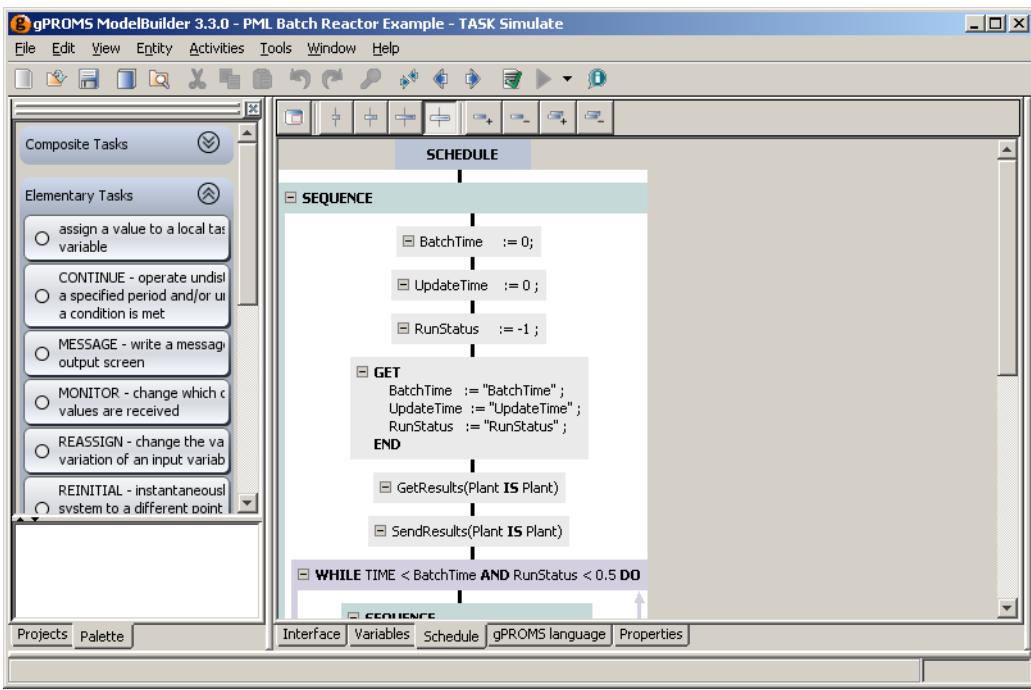
Once all of the local Variables have been specified, the Schedule tab can be selected in order to define the operating policy for the Task.

Using the Schedule tab

Task Schedules are constructed in exactly the same way as Process Schedules (see Defining Schedules), with one additional feature: when the Schedule tab of a Task is open, the Task palette will contain one extra elementary Task for assigning the value of a local Variable (and this will also be added to the context menu).

The use of user-defined Tasks in Schedules is also described here. This was deferred from the section on Defining Schedules because user-defined Tasks had not been described at that point.

The screen shot below shows the Simulate user-defined Task from the PLM Batch Reactor example, along with the Task palette.

Figure 12.5. Simulate user-defined Task

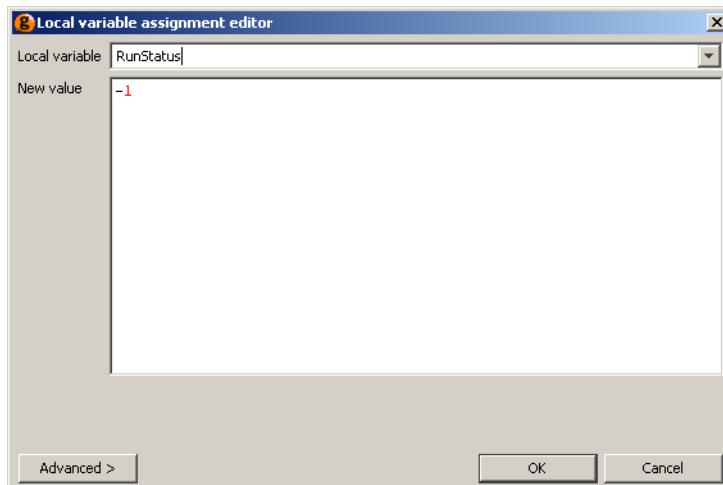
The first three Tasks in the outer Sequence are local Variable assignment Tasks.

To insert a new Assign local variable Task, left click on the Task in the Task palette and drag it onto a hot spot in the Schedule. Alternatively, right click on a hot spot and select Local variable assignment from the Add elementary task context menu. When this is done, a Task configuration dialog will appear.

To configure the Task, select a local Variable from the list box and then enter an expression for its new value in the text box below. Pressing the OK button completes the addition of the Task.

The Advanced view shows the equivalent gPROMS language.

The screenshot below shows the configuration dialog for the third Task in the Schedule above.

Figure 12.6. Local variable assignment Task configuration dialog

The next Task in the Schedule (the GET Task) is a Foreign Process Task. These are described in Using Foreign Processes.

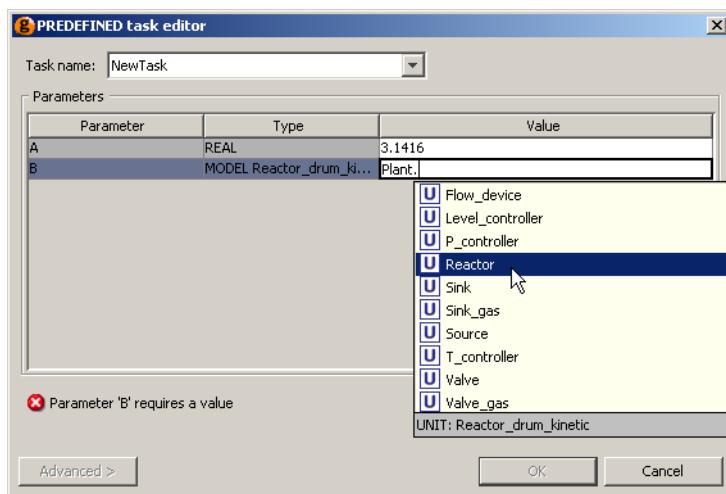
The two Tasks following the GET Task are user-defined Tasks that have been inserted into the Schedule. User-defined Tasks can be inserted into a Schedule using the Task palette or the context menu. The Predefined Tasks section of the Task palette contains a list of all predefined Tasks, as shown below.

Figure 12.7. Task Palette for user-defined Tasks



Predefined Tasks are inserted into the Schedule by dragging them from the palette to the Schedule.² When this is done, a configuration dialog will appear allowing the Parameters of the Task to be specified. The dialog for our new Task is shown below.

Figure 12.8. Completing the Task configuration dialog for a predefined Task



Once all of the Parameters have been specified correctly, you can press the OK button and the Task will be inserted.

The Advanced view shows the gPROMS language:

```
NewTask(A IS 3.1416, B IS Plant.Reactor)
```

²Unlike built-in Tasks, predefined Tasks cannot be inserted into the Schedule using the context menu.

Intrinsic Tasks

When discussing the Parameter section within a Task, we considered an example where there were two digital PI controllers. The Task for each controller must be called in the Process section in order to activate the controller and specify its tuning parameters. This small example of just two controllers requires a reasonable amount of code to be written in the Schedule section of the Process. More complex Models, where there might be tens or even hundreds of controllers, may lead to a large schedule section with much repeated code. Specifying all of these tasks is not only time consuming but also prone to error. Since these Tasks must be enabled for each and every controller, it is possible to automate the specification of these Tasks in the Schedule of a Process. More generally, one can associate a number of Tasks with any Model, so that each instantiation of the Model automatically (and invisibly) adds the Tasks to the Schedule section. These are called Intrinsic Tasks and are nothing more than a declaration in the Model of which (already defined) Tasks should be automatically included in the Schedule, thus automating the laborious manual procedure.

As an example of the use of Intrinsic Tasks, let us assume that we want to model a plant with three reactors that are structurally identical but are used for different duties. This means that the plant Model will contain three instances of the same reactor Model but with different properties. Now if the reactor Model contains three control loops, e.g. for pressure, temperature and level, the following Schedule would be required to model the controllers using ordinary Tasks. (For brevity, some parameters have been omitted.)

```
SCHEDULE
...
PARALLEL
  # Controllers for Reactor1
  DigitalPI
    ( SetPoint           IS 373.0,
      Bias              IS 0.5,
      Gain              IS 1.2,
      Sensor            IS Plant.Reactor1.TemperatureSensor,
      Valve              IS Plant.Reactor1.CoolingWaterValve )

  DigitalPI
    ( SetPoint           IS 10.0,
      Bias              IS 0.8,
      Gain              IS 2.6,
      Sensor            IS Plant.Reactor1.PressureSensor,
      Valve              IS Plant.Reactor1.PressureReliefValve )

  DigitalPI
    ( SetPoint           IS 1.0,
      Bias              IS 0,
      Gain              IS 2,
      Sensor            IS Plant.Reactor1.LevelSensor,
      Valve              IS Plant.Reactor1.LiquidOutletValve )

  # Controllers for Reactor2
  DigitalPI
    ( SetPoint           IS 425.0,
      Bias              IS 1,
      Gain              IS 3,
      Sensor            IS Plant.Reactor2.TemperatureSensor,
      Valve              IS Plant.Reactor2.CoolingWaterValve )

  DigitalPI
    ( ...
      Sensor            IS Plant.Reactor2.PressureSensor,
      Valve              IS Plant.Reactor2.PressureReliefValve )

  DigitalPI
    ( ...
      Sensor            IS Plant.Reactor2.LevelSensor,
      Valve              IS Plant.Reactor2.LiquidOutletValve )
```

```
# Controllers for Reactor3
...
END # Parallel
...
```

Clearly, there is a lot of repeated code that is mostly unnecessary apart from the need to specify different tuning parameters. The use of Intrinsic Tasks is ideal in this type of situation. To implement Intrinsic Task, one first has to define them in the Model itself, which is illustrated below for the reactor example.

```
# MODEL Reactor

PARAMETER
...
TemperatureSetpoint AS REAL
TemperatureGain      AS REAL
...
...
EQUATION
...
INTRINSIC_TASK
DigitalPI
( SetPoint           IS TemperatureSetPoint,
  Bias              IS TemperatureBias,
  Gain              IS TemperatureGain,
  Sensor            IS TemperatureSensor,
  Valve             IS CoolingWaterValve )
DigitalPI
( SetPoint           IS PressureSetPoint,
  Bias              IS PressureBias,
  Gain              IS PressureGain,
  Sensor            IS PressureSensor,
  Valve             IS PressureReliefValve )
DigitalPI
( SetPoint           IS LevelSetPoint,
  Bias              IS LevelBias,
  Gain              IS LevelGain,
  Sensor            IS LevelSensor,
  Valve             IS LiquidOutletValve )

# END of Model Reactor
```

Now, each instance of the Model Reactor will automatically have DigitalPI Tasks enabled in the Schedule section of the Process without the user needing to provide them. Of course, the set points and tuning parameters will need to be specified (unless defaults are provided and are suitable) but these would have to be specified in any case. So the Schedule section could be a simple as:

```
SCHEDULE
CONTINUE FOR 100
```

and the controller Tasks will be added, in parallel with the user-defined Schedule, by gPROMS when the Process is executed.

Note that since ordinary Tasks are only active in dynamic Simulation activities, Intrinsic Tasks are also limited to dynamic Simulation activities. In other words, if a Process contains dynamic Models with Intrinsic Tasks, they will be ignored if there is no Schedule section defined in the Process or if the Ignore schedule option of the Execution Dialog is checked.

In the above examples, the names of a number of Units within the Model were passed to the Model Parameters of the Task. It may also be necessary to pass the Model itself as an argument to the Task. The `This_Unit` keyword is used for this purpose, as illustrated below.

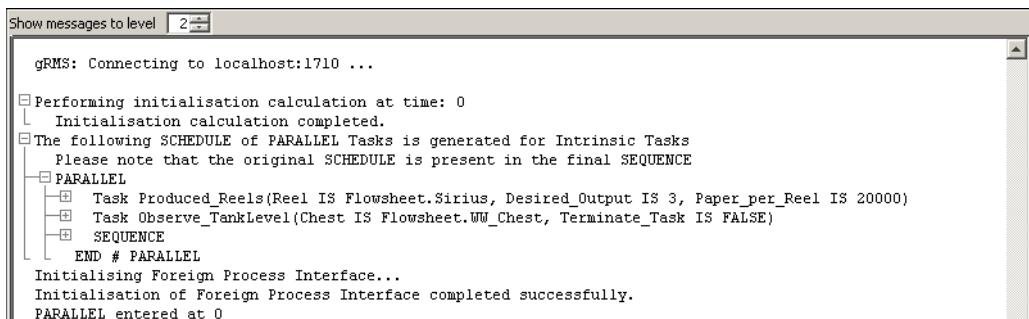
```
# MODEL A_model
...
INTRINSIC_TASK
Task1(
    theModel IS This_Unit,
    aParameter IS 10 )
```

In this example, any instances of `A_model` will automatically have their names passed as arguments to the `Task1` Tasks (which are automatically generated in parallel with the user-defined Schedule).

Viewing the Schedule Generated by Intrinsic Tasks

The final Schedule is reported by gPROMS in the execution output, so that you can check that the Intrinsic Tasks are behaving as intended. After the simulation has completed, scroll the Execution Output window up until you find the line "The following SCHEDULE of PARALLEL Tasks is generated for Intrinsic Tasks". This will be just after the initiation has been completed. Below this line, the Intrinsic Tasks that were added to the Schedule will be displayed. To see the detailed Schedule, simply click on the "+" symbols to expand the various elements of the Tasks. These two views are shown in the figures below (for a different example).

Figure 12.9. Execution Output Indicating the Inclusion of Intrinsic Tasks



The screenshot shows the 'Execution Output' window of gPROMS. At the top left, there is a 'Show messages to level' dropdown set to '2'. The main area contains the following text:

```
gRMS: Connecting to localhost:1710 ...
[+] Performing initialisation calculation at time: 0
  [-] Initialisation calculation completed.
[+] The following SCHEDULE of PARALLEL Tasks is generated for Intrinsic Tasks
  Please note that the original SCHEDULE is present in the final SEQUENCE
  [-] PARALLEL
    [-] Task Produced_Reels(Reel IS Flowsheet.Sirius, Desired_Output IS 3, Paper_per_Reel IS 20000)
    [-] Task Observe_TankLevel(Chest IS Flowsheet.WW_Chest, Terminate_Task IS FALSE)
    [-] SEQUENCE
      [-] END # PARALLEL
    Initialising Foreign Process Interface...
    Initialisation of Foreign Process Interface completed successfully.
  PARALLEL entered at 0
```

Figure 12.10. Execution Output Showing the Detailed Schedule for Intrinsic Tasks

```

gRMS: Connecting to localhost:1710 ...

[...]
PARALLEL
  Task Produced_Reels(Reel IS Flowsheet.Sirius, Desired_Output IS 3, Paper_per_Reel IS 20000)
    SEQUENCE
      WHILE (Reel.Produced_Reels < Desired_Output) DO
        SEQUENCE
          CONTINUE UNTIL Reel.Paper_on_Reel >= Paper_per_Reel
          REINITIAL
          Reel.Paper_on_Reel
          WITH
            Reel.Paper_on_Reel = 0.0 ;
          END
          RESET
          Reel.Produced_Reels := OLD(Reel.Produced_Reels) + 1.0 ;
          END
        END # SEQUENCE
      END # WHILE
    STOP
  END # SEQUENCE
Task Observe_TankLevel(Chest IS Flowsheet.WW_Chest, Terminate_Task IS FALSE)
  PARALLEL
    SEQUENCE
      SEQUENCE
        CONTINUE FOR 100
        RESET
        Flowsheet.WW_Pump.Dialog_Input_Flow := 3 ;
        END
        CONTINUE UNTIL Flowsheet.WW_Pump.Inlet.Protected_Downstream > 0.5
        RESET
        Flowsheet.WW_Pump.Dialog_Input_Flow := 0.5 ;
        END
        CONTINUE FOR 1000
        RESET
        Flowsheet.ModuleJet.Slice_Opening := 0.008 ;
        END
      END # SEQUENCE
    STOP
  END # SEQUENCE

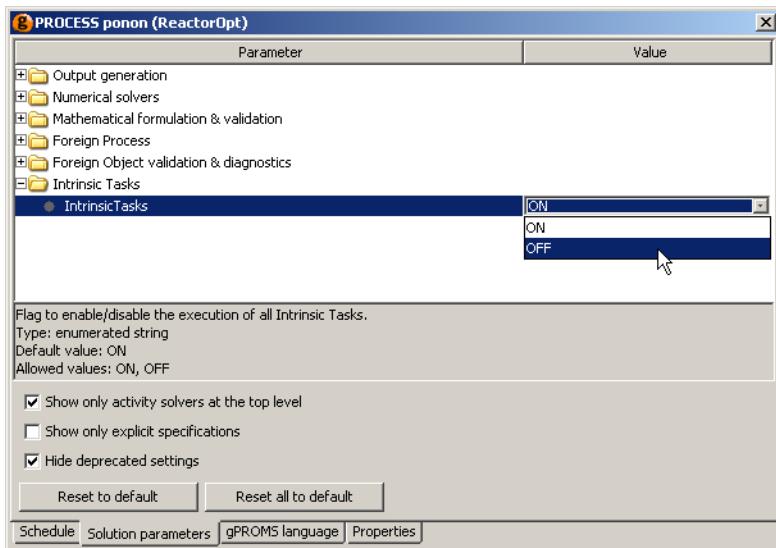
```

The first Sequence shown was defined in the Produced_Reels Task that was specified as an Intrinsic Task: hence, it was automatically placed in the final Schedule. The Sequence nested inside the second Sequence is the whole Schedule from the Process, so everything else was generated automatically. Note that, since much of the Schedule is automatically created, there is no guarantee that these Schedules will terminate, so gPROMS adds a Stop Task to the end of the user-defined Schedule.

Controlling the Use of Intrinsic Tasks

So far, the examples on Intrinsic Tasks have assumed that these Tasks should always be enabled for *every* instance of a Model containing Intrinsic Tasks. Although this is the default behaviour, one can easily select which Model instances should have their Intrinsic Tasks enabled. There are a number of ways to achieve this.

First, all Intrinsic Tasks can be switched off by editing the process properties. In this case, no matter what specifications are made in the Models and Process, no Intrinsic Tasks will be used and the user will have to specify the use of Tasks manually. To do this, open the Process entity and left click on the Solution Parameters tab. Double click on (or click on the "+" symbol next to) the Intrinsic Tasks folder. Now you can change the setting from ON to OFF by clicking on ON and selecting OFF from the list.



Finer control over the use of Intrinsic Tasks can be achieved by defining their use whenever a Model is instantiated. To do this, the Intrinsic Tasks solution parameter of the Process must be ON. Then, there are three options for instantiating a Model (A is the name of a Model defined in the gPROMS project):

```
UNIT
  A      AS A
  A_off AS A INTRINSIC_TASKS OFF
  A_on   AS A INTRINSIC_TASKS ON
```

These three specifications work as follows.

Instantiating a model with the INTRINSIC_TASKS OFF option forces gPROMS not to use any of the Intrinsic Tasks defined for that Model instance.

In contrast, instantiating a Model with the INTRINSIC_TASKS ON option turns on all Intrinsic Tasks for the Model instance.

Finally, if no specification is made (the first example above), then the behaviour of the Model instance will be the same as the Model instance within which it is contained. If it is a top-level model instance, then the default behaviour is for the Intrinsic Tasks to be enabled. So, the behaviour of a particular Model instance will be passed down the Model hierarchy until an explicit instantiation takes place, which will then override the behaviour of the parent Model.

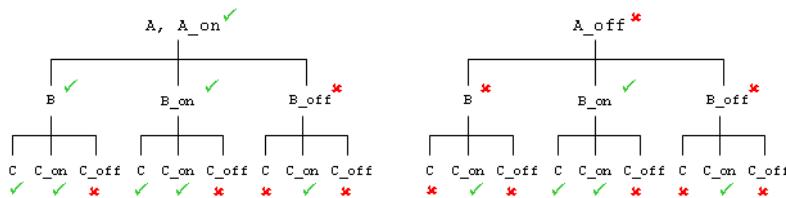
To illustrate the behaviour of Models (and sub Models) instantiated in this way, let us assume that the three Model instances of Model A are made in a Process. Model A then contains three instances of a Model B:

```
UNIT
  B      AS B
  B_off AS B INTRINSIC_TASKS OFF
  B_on   AS B INTRINSIC_TASKS ON
```

Finally, Model B also contains three different instances of Model C:

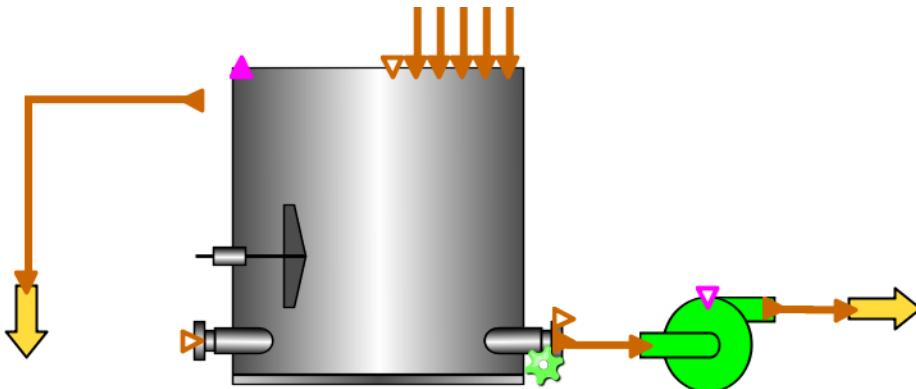
```
UNIT
  C      AS C
  C_off AS C INTRINSIC_TASKS OFF
  C_on   AS C INTRINSIC_TASKS ON
```

This then produces the following Model-instance hierarchy.

Figure 12.11. Illustration of Intrinsic Task control

The ticks and crosses next to each Model instance indicate whether or not intrinsic tasks are enabled for that Model instance. Since the default behaviour for top-level Models is for Intrinsic Tasks to be enabled, A and A_on both have their tasks enabled. Therefore, each of the Model instances within A will have the same properties as those within A_on. The main feature is that the *_on instances always have Intrinsic Tasks enabled, *_off instances are always disabled and the instances with the default specification always behave as the Model instance above.

ModelBuilder also allows these specifications to be made via the graphical interface. Click on the Topology tab and then right click on the Unit you want to specify. The context menu contains an item called Intrinsic Tasks.... Moving the mouse over this item, enables a list containing the three possible settings for the Unit. Left clicking on one of these options sets the value for this Unit. Units with disabled Intrinsic Tasks are indicated by a red cog image on the Unit; those with enabled Intrinsic Tasks by a green cog; and if the default specification is made, no cog is shown. If you then switch back to the gPROMS language view, you will see that the code has changed to reflect the choice made. An example of a Unit with enabled Intrinsic Tasks is shown below.

Figure 12.12. Example of a Unit with enabled Intrinsic Tasks

To reiterate, control over which Model instances use Intrinsic Tasks can occur only when the Process solution parameter Intrinsic Tasks is ON; if it is OFF, then none of the Intrinsic Tasks are enabled and they must be included explicitly in the Schedule.

Chapter 13. Stochastic Simulation in gPROMS

gPROMS can be used to perform stochastic simulations. The prime reason for considering stochastic simulation is to determine how the distributions of key output Variables are influenced by the distributions of the input Variables. In order to do so, you will learn how to do the following:

- Assign random numbers to Parameters and Variables
- Perform multiple simulations and plot their results in the form of probability density functions

An example of the output that can be achieved from a stochastic simulation in gPROMS is shown below

Figure 13.1. Values assigned to the temperature for each scenario.

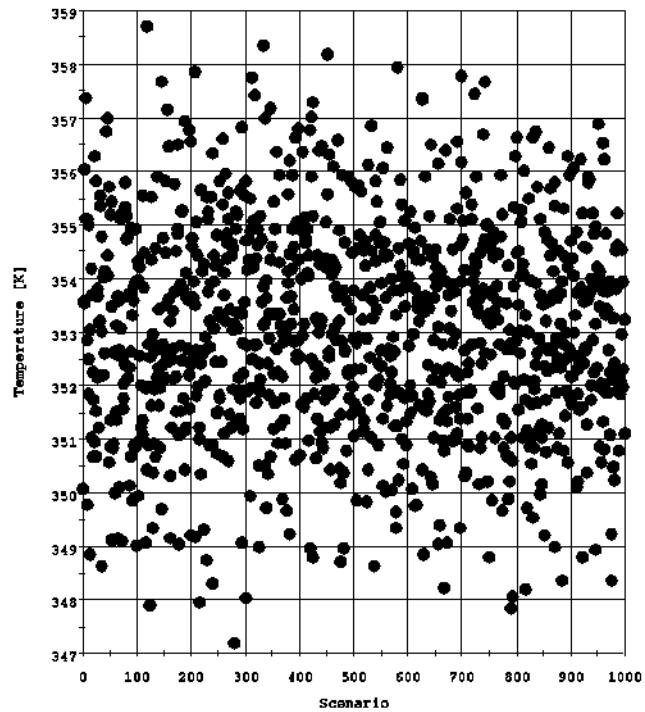
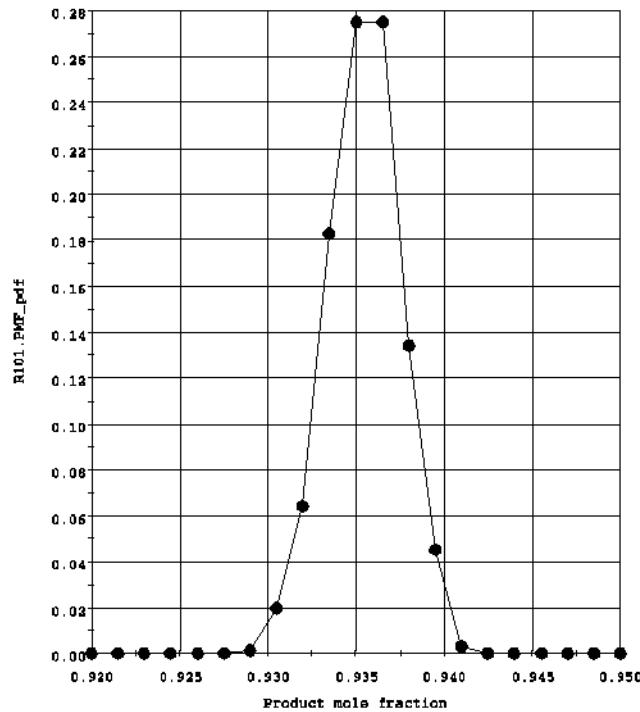
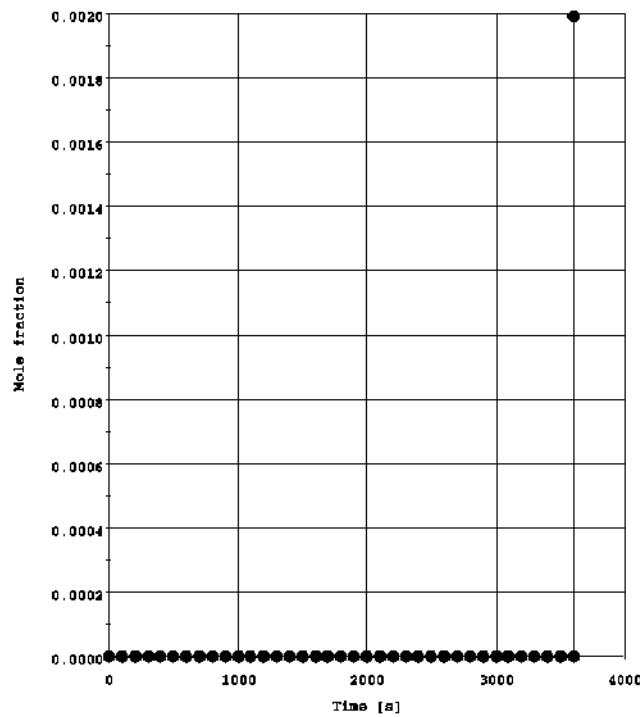


Figure 13.2. Probability density function for the product mole fraction.**Figure 13.3. Standard deviation of the product mole fraction**

Assigning random numbers to Parameters and Variables

Parameters and Variables can be given random values in the Set and Assign sections, respectively, of a Process Entity in the same way that they are given deterministic values. Instead of assigning a literal value or expression to the parameter or variable, special functions are used that return values sampled from the distribution. The syntax is shown below.

```
...
SET
Identifier := DistributionFunction( ArgList ) ;
...
ASSIGN
Identifier := DistributionFunction( ArgList ) ;
...
```

The functions *DistributionFunction* each require a different set of arguments *ArgList*. The available functions are described in table below.

Table 13.1. Probability distribution functions available in gPROMS.

Function	Arguments	Example
Uniform	<i>lower, upper</i>	UNIFORM(0,1) returns a uniformly distributed number in the range [0,1]. <i>lower < upper</i> .
Triangular	<i>lower, mode, upper</i>	TRIANGULAR(1,2,4) returns a number sampled from a triangular distribution with mode 2, lower limit 1 and upper limit 4. <i>lower < mode < upper</i> .
Normal	<i>mean, stddev</i>	NORMAL(3,0.25) returns a value sampled from a normal distribution with mean 3 and standard deviation 0.25. <i>stddev > 0</i> .
Gamma	<i>alpha, beta</i>	GAMMA(3,1) returns a value from the Gamma distribution. <i>alpha, beta > 0</i> .
Beta	<i>alpha, beta, lower, upper</i>	BETA(1.5,5,0,1) returns a value from the Beta distribution. <i>alpha, beta > 0; lower < upper</i> .
Weibull	<i>alpha, beta</i>	WEIBULL(4,1) returns a value from the Weibull distribution. <i>alpha, beta > 0</i> .

Once Parameters and Variables have been given stochastic values, they behave exactly as though they had been assigned deterministic values: i.e. Parameters remain constant and are not calculated by a simulation and the Variables remain at their Assigned values unless re-assigned in a Reset statement. Any Variable may be Reset, as usual, using a literal or an expression (using the *Old* operator if this involves other Variables or by assigning a new random number. Note that Variables and Parameters can only ever be assigned 'point' values; they are not assigned distributions. Furthermore, each time a variable is Reset to a value from a distribution, it is given a different value, even if the distribution function's arguments are the same. For example, in the following segment of a Schedule

section, the variable Random is assigned two different values from the Normal distribution: one time it may be assigned 0.23 then 0.07; another time it may be assigned 0.01 then 0.36.

```
...
SCHEDULE
SEQUENCE
...
RESET
Random := NORMAL(0,1) ;
END
...
RESET
Random := NORMAL(0,1) ;
END
...
END
```

One further issue that should be noted is that gPROMS will always *seed* the random number generator with the same number each time a simulation is started. This means that the results of a stochastic simulation are reproducible.

Plotting results of multiple stochastic simulations

In order to examine how the distributions of key output Variables are influenced by the distributions of the input Variables, we will describe how you can combine multiple simulations in a single process and then use the results to evaluate metrics (such as the mean, variance, etc.) of the output Variables. Thereafter, we will outline a method that allows you to plot the probability density functions of the output Variables.

Combining multiple simulations

Given a model with some uncertain inputs, a series of simulations can be combined into a single process by introducing a new higher-level Model. The original model is included in the new one as an array of Units, as shown below.

```
# MODEL ModelUncertain
...
VARIABLE
Input      AS InputVarType    # uncertain input variable
Output     AS OutputVarType   # important output variable
...
# MODEL Combined
PARAMETER
NoScenarios   AS             INTEGER
InputMean      AS             REAL
InputStdDev    AS             REAL
UNIT
Scenarios      AS ARRAY(NoScenarios) OF ModelUncertain
```

The input Variables for each scenario of ModelUncertain then need to be specified as follows.

```
# PROCESS StochSim

UNIT
StSim AS Combined

...
ASSIGN
WITHIN StSim DO
FOR i := 1 TO NoScenarios DO
    Scenarios(i).Input := NORMAL(InputMean, InputStdDev) ;
END
END

...
```

Note that each input Variable is Assigned a different value from the same distribution. This could also have been done with Parameters, but parameter propagation cannot be used in this way: this would result in all Parameters being set the same value, because the parameter in the higher-level model will be assigned randomly and then that particular value will be propagated to the scenarios. Of course, any inputs that are common to the system (such as design constants or precisely known operating Parameters) can be included in the higher-level model along with equations linking them to the scenarios. This reduces the complexity of the Schedule section.

Plotting probability density functions

Now all of the scenarios are together in one Process, but it is not easy to plot them together in one graph. Rather than having to select each Variable from each scenario instance, it would be much easier to be able to select the whole distribution. This can easily be done as follows.

```
# MODEL Combined

PARAMETER
NoScenarios AS INTEGER
InputMean AS REAL
InputStdDev AS REAL

UNIT
Scenarios AS ARRAY(NoScenarios) OF ModelUncertain

VARIABLE
Input AS ARRAY(NoScenarios) OF InputVarType
Output AS ARRAY(NoScenarios) OF OutputVarType

OPmean AS NoType # mean of Output
OPvariance AS NoType # variance of Output

EQUATION
FOR i := 1 TO NoScenarios DO
    Input(i) = Scenarios(i).Input ;
    Output(i) = Scenarios(i).Output ;
END

OPmean = SIGMA(Output)/NoScenarios ;
OPvariance = SIGMA( (Output - OPmean)^2 )/NoScenarios ;
```

Now, all of the scenarios can be plotted on a single graph by selecting a single Variable in gRMS. Notice also that the mean and variance of the output can easily be calculated.

Finally, it is often useful to be able to plot the probability density function (pdf) of the output. In general, for each Variable this requires two new Variables a distribution domain and three Parameters. However, if two Variables are in the same interval they can share the same distribution domain and Parameters. This is shown below.

```
# MODEL Combined

PARAMETER
  NoScenarios      AS INTEGER
  InputMean        AS REAL
  InputStdDev      AS REAL

  NoInt_OP         AS INTEGER DEFAULT 20 # number of intervals for distribution
  Upper_OP         AS REAL      DEFAULT 3 # upper bound on distribution
  Lower_OP         AS REAL      DEFAULT 1 # lower bound on distribution

DISTRIBUTION_DOMAIN
  Dist_OP          AS (Lower_OP:Upper_OP) # distribution over which
                                              # Output will be plotted

UNIT
  Scenarios        AS ARRAY(NoScenarios) OF ModelUncertain

VARIABLE
  Input            AS ARRAY(NoScenarios) OF InputVarType
  Output           AS ARRAY(NoScenarios) OF OutputVarType

  OPmean           AS                      NoType # mean of Output
  OPvariance       AS                      NoType # variance of Output

# temp variable to count occurrences of Output in a particular interval:
  OPacc            AS DISTRIBUTION(Dist_OP, NoScenarios) OF NoType

# pdf function for Output:
  OP_pdf           AS DISTRIBUTION(Dist_OP) OF                  NoType

EQUATION
  FOR i := 1 TO NoScenarios DO
    Input(i) = Scenarios(i).Input ;
    Output(i) = Scenarios(i).Output ;
  END

  OPmean = SIGMA(Output)/NoScenarios ;
  OPvariance = SIGMA( (Output - OPmean)^2 )/NoScenarios ;

  FOR i := Lower_OP TO Upper_OP DO
    FOR j := 1 TO NoScenarios DO
      IF i - (Upper_OP-Lower_OP)/NoInt_OP/2 <= Output(j) AND
         Output(j) < i + (Upper_OP-Lower_OP)/NoInt_OP/2 THEN
        OPacc(i,j) = 1 ;
      ELSE
        OPacc(i,j) = 0 ;
      END
    END
    OP_pdf(i) = SIGMA(OPacc(i,))/NoScenarios ;
  END
```

The three new Parameters introduced are NoInt_OP, Lower_OP and Upper_OP. These Parameters define the distribution over which the output Variable will be plotted. NoInt_OP is the number of intervals used for the distribution Dist_OP. This will obviously be used to set Dist_OP:

```
# PROCESS StSim  
...  
SET  
...  
Dist_OP := [BFDM, 1, NoInt_OP] ;
```

The first order, backward finite difference method is all that is required because the distribution domain is essentially behaving as an array. The Parameters Lower_OP and Upper_OP are simply the lower and upper bounds on the domain Dist_OP. The Variable being plotted, Output in this case, must lie in the interval [lower, upper] for each scenario; otherwise, the pdf will become distorted. If the lower and upper bounds are set so that a number of Variables lie in this interval, then all of these Variables can be plotted using the same distribution. The number of intervals should be set appropriately so that the distribution is not too coarse. Finally, the two Variables introduced are OPacc and OP_pdf. Each Variable being plotted will need its own pair of Variables. OPacc(i,j) is set to 1 if the value of Output(j) (the value in scenario j) lies in interval i of the distribution domain. OP_pdf(i) therefore represents the number of scenarios in which Output has a value in interval i. This is divided by the number of scenarios to normalise the pdf. Plotting the pdf of a state Variable can slow down the simulation significantly (due to the many discontinuities, and therefore re-initialisations, encountered as the values of the Variables switch between intervals). This can be remedied by introducing one further Variable, as illustrated below for the example already considered:

```
# MODEL Combined  
...  
VARIABLE  
...  
# temporary Output variable = 0 until end of simulation, then = Output  
OutputEnd AS ARRAY(NoScenarios) OF OutputVarType  
...  
EQUATION  
FOR i := 1 TO NoScenarios DO  
    Input(i) = Scenarios(i).Input ;  
    Output(i) = Scenarios(i).Output ;  
END  
...  
FOR i := Lower_OP TO Upper_OP DO  
    FOR j := 1 TO NoScenarios DO  
        IF i - (Upper_OP-Lower_OP)/NoInt_OP/2 <= OutputEnd(j) AND  
            OutputEnd(j) < i + (Upper_OP-Lower_OP)/NoInt_OP/2 THEN  
            OPacc(i,j) = 1 ;  
        ELSE  
            OPacc(i,j) = 0 ;  
        END  
    END  
    OP_pdf(i) = SIGMA(OPacc(i,))/NoScenarios ;  
END
```

```
# PROCESS StochSim  
...
```

```
MONITOR
  StSim.Output(*) ;
  StSim.Input(*) ;
  StSim.OPmean ;
  StSim.OPvariance ;
  StSim.OP_pdf ;

  ...
  ...

ASSIGN
  WITHIN StSim DO
    OutputEnd := 0 ;
  ...
END

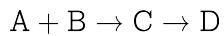
  ...

SCEDULE
  SEQUENCE
  ...
  RESET
    StSim.OutputEnd := OLD(StSim.Output) ;
  END
END
```

So, OutputEnd is 0 throughout the simulation and the If conditions are only evaluated at initialisation. Only at the end of the simulation is OutputEnd changed, at which point all of the If statements are re-evaluated and OP_pdf recalculated. Finally, note that the output has been restricted to only those Variables of importance by using the Monitor section. This reduces the amount of data sent to the output channel (e.g. gRMS). Although this is not necessary, it recommended for moderate to large problems (even small problems output large quantities of data when the number of scenarios is large).

Stochastic Simulation Example

In this section we illustrate the important techniques of stochastic simulation in gPROMS using a simple model of an isothermal batch reaction. The following reactions occur in the reactor, D being the desired product.



The reactor initially contains 10m^3 of an equimolar mixture of A and B. The temperature is held constant at 353K and the reaction is allowed to progress for 1 hour. The reaction rates are assumed to follow Arrhenius's law.

Stochastic gPROMS process model

A simple, generic model for an isothermal liquid-phase CSTR is used to model the process

```
# MODEL LiquidPhaseCSTR

PARAMETER
  # Number of components
  NoComp          AS INTEGER
  # Number of reactions
  NoReac          AS INTEGER
  Density         AS ARRAY(NoComp) OF REAL
```

```
# Reaction data (Arrhenius law)
ArrhConstant      AS ARRAY(NoReac) OF                      REAL
ActivationEnergy   AS ARRAY(NoReac) OF                      REAL

# Reaction orders
Order             AS ARRAY(NoComp, NoReac) OF            INTEGER

# Component stoichiometric coefficients
Nu               AS ARRAY(NoComp, NoReac) OF            INTEGER

# Gas constant
R                AS                                     REAL

VARIABLE
Fin              AS                                     MolarFlowrate
Xin              AS ARRAY(NoComp) OF                  MolarFraction
Fout             AS                                     MolarFlowrate
X                AS ARRAY(NoComp) OF                  MolarFraction
HoldUp           AS ARRAY(NoComp) OF                  Moles
C                AS ARRAY(NoComp) OF                  MolarConcentration
T                AS                                     Temperature
TotalHoldup      AS                                     Moles
TotalVolume       AS                                     Volume
ReactionConstant AS ARRAY(NoReac) OF                NoType
Rate             AS ARRAY(NoReac) OF                NoType

EQUATION
# Material balance
FOR i := 1 TO NoComp DO
    $HoldUp(i) = Fin*Xin(i) - Fout*X(i) + TotalVolume*SIGMA(Nu(i,)*Rate) ;
END

# Reaction rates
FOR j := 1 TO NoReac DO
    ReactionConstant(j) = ArrhConstant(j) * EXP(-ActivationEnergy(j)/R/T) ;
    Rate(j) = ReactionConstant(j) * PRODUCT(C^Order(j)) ;
END

# Total volume and total holdup
TotalVolume = SIGMA(Holdup/Density) ;

TotalHoldup = SIGMA(HoldUp) ;

# Molar fractions and concentrations
Holdup = X * TotalHoldup ;

Holdup = C * TotalVolume ;
```

Now we assume the that temperature of the reaction may change from batch to batch. This can be modelled using a normal distribution with a mean of 353K and a standard deviation of 2K. To see the effect of this, we need to introduce a new composite Model to include a number of scenarios:

```
# MODEL Stochastic_LiquidPhaseCSTR

PARAMETER

# define common PARAMETERS here so their values can be propagated
```

```

# to each scenario
# -----
NoComp          AS           INTEGER
NoReac          AS           INTEGER
Density         AS ARRAY(NoComp) OF    REAL
ArrhConstant    AS ARRAY(NoReac) OF   REAL
ActivationEnergy AS ARRAY(NoReac) OF   REAL
Order           AS ARRAY(NoComp,NoReac) OF INTEGER
Nu              AS ARRAY(NoComp,NoReac) OF INTEGER
R               AS           REAL
# -----

NoScenarios     AS           INTEGER
NoInt_PMF       AS           INTEGER DEFAULT 20
Upper_PMF       AS           REAL      DEFAULT 1
Lower_PMF       AS           REAL      DEFAULT 0.8

DISTRIBUTION_DOMAIN
Dist_PMF        AS (Lower_PMF:Upper_PMF)

UNIT
Scenarios       AS ARRAY(NoScenarios) OF LiquidPhaseCSTR

VARIABLE
T               AS ARRAY(NoScenarios) OF Temperature
ProdMolFrac     AS ARRAY(NoScenarios) OF MolarFraction

PMFmean         AS           NoType
PMFvariance     AS           NoType
PMFstddev       AS           NoType

# temp variable to count occurrences of Output in a particular interval:
PMFacc          AS DISTRIBUTION(Dist_PMF,NoScenarios) OF NoType

# pdf function for Output:
PMF_pdf         AS DISTRIBUTION(Dist_PMF) OF           NoType

EQUATION
FOR i := 1 TO NoScenarios DO
    T(i) = Scenarios(i).T ;
END

PMFmean = SIGMA(ProdMolFrac)/NoScenarios ;
PMFvariance = SIGMA( (ProdMolFrac - PMFmean)^2 )/NoScenarios ;

FOR i := Lower_PMF TO Upper_PMF DO
    FOR j := 1 TO NoScenarios DO
        IF i - (Upper_PMF-Lower_PMF)/NoInt_PMF/2 <= ProdMolFrac(j) AND
            ProdMolFrac(j) < i + (Upper_PMF-Lower_PMF)/NoInt_PMF/2 THEN
            PMFacc(i,j) = 1 ;
        ELSE
            PMFacc(i,j) = 0 ;
        END
    END
    PMF_pdf(i) = SIGMA(PMFacc(i,))/NoScenarios ;
END

```

We have defined new distributed Variables to contain the values of the Variables of interest in each scenario. These are T for the temperature and ProdMolFrac for the mole fraction of the product D (*i.e.* x_4). Again, Parameters are defined that describe the upper and lower limits of the distribution and its coarseness. Finally, Variables are defined for the mean, variance and standard deviation of the product mole fraction. The equations are the same as were described before, except that there is no equation for the standard deviation or to relate the variable ProdMolFrac to the X(4) Variables in each scenario. While we could include the equation for the standard deviation in this model, by using the equation:

```
PMFstddev^2 = PMFvariance ;
```

this tends to slow the simulation down. The alternative used here is to Assign PMFstddev to a temporary value in the Process section and to Reset it at the end of the simulation using:

```
SCHEDULE
SEQUENCE
...
RESET
xxx.PMFstddev := SQRT(OLD(xxx.PMFvariance)) ;
END
END
```

The final difference is the missing equation relating ProdMolFrac to Scenarios().X(4). This is because we are plotting a pdf of a dynamic variable and want to avoid slowing the simulation but are demonstrating a different approach to the one described before (where the additional 'End' variable was used). Here, we can avoid this additional variable simply by Assigning ProdMolFrac itself and then Resetting at the end of the simulation. The disadvantage with this approach is that you cannot plot the mean of the distribution over time; it only contains the correct value at the end of the simulation, when ProdMolFrac gets assigned the correct values. In this example, we were not concerned with plotting the mean, *etc.*, over time and so this approach is an appropriate alternative. The final extract of the gPROMS project, the Process entity, is shown below.

```
# PROCESS Stochastic

UNIT
R101 AS Stochastic_LiquidPhaseCSTR

SET
WITHIN R101 DO
  NoScenarios      := 1000 ; ;
  Upper_PMF        := 0.95 ; ;
  Lower_PMF        := 0.92 ; ;
  NoInt_PMF        := 20 ; ;
  Dist_PMF         := [ BFDM, 1, NoInt_PMF ] ; ;

  NoComp           := 4 ; ;
  NoReac           := 2 ; ;

  Nu               := [ -1, 0,
                      -1, 0,
                      1, -1,
                      0, 1 ] ; ;

  Order            := [ 1, 0,
                      1, 0,
                      0, 1,
                      0, 0 ] ; ;

  R                := 8.31441 ; # kJ/kmol/K
  ArrhConstant     := [ 8E-3, 1E-2 ] ; # m3/kmol s
```

```
ActivationEnergy    := [ 8000, 6000 ] ; # kJ/kmol
Density           := [ 17.48, 17.15, 10.24, 55.56 ] ; # kmol/m3
END

ASSIGN
WITHIN R101 DO
PMFstddev        := 0 ;
FOR i := 1 TO NoScenarios DO
ProdMolFrac(i)   := 0 ;
WITHIN Scenarios(i) DO
Fin              := 0 ;
Fout             := 0 ;
Xin              := [ 0.5, 0.5, 0, 0 ] ;
T                := NORMAL(353, 2) ;
END
END
END

INITIAL
WITHIN R101 DO
FOR i := 1 TO NoScenarios DO
WITHIN Scenarios(i) DO
X(2)            = X(1) ;
X(3)            = 0 ;
X(4)            = 0 ;
TotalVolume     = 10 ;
END
END
END

SCEDULE
SEQUENCE
CONTINUE FOR 3600
RESET
FOR i := 1 TO R101.NoScenarios DO
R101.ProdMolFrac(i) := OLD(R101.Scenarios(i).X(4)) ;
END
END
RESET
R101.PMFstddev := SQRT(OLD(R101.PMFvariance)) ;
END
CONTINUE FOR .01
END
```

Below are some comments on the PROCESS.

- SET: This section illustrates a couple of useful features in gPROMS. The first is that some of the Parameters are having their default values overridden. The second is that all of the Parameters in the lower-level model (LiquidPhaseCSTR) are being propagated.
- ASSIGN: In this section we assign the dummy values to ProdMolFrac and PMFstddev. Also, some of the degrees of freedom of the LiquidPhaseCSTR model are set, e.g. the inlet and outlet flowrates, which are set to zero. Finally, the temperature for each scenario is set a random value from the normal distribution, $N(353,2)$.
- INITIAL: A typical set of initial conditions are used here.
- SCEDULE: This sections illustrates the Resetting of the Variables ProdMolFrac and PMFstddev. Note that because PMFstddev depends on ProdMolFrac, the latter *must* be RESET before the former in a separate RESET

task. If they are RESET in the same task, then PMFstddev will be RESET based on the values in ProdMolFrac from *before* the RESET task.

Finally, on some systems gRMS may not be able to plot the pdf Variables correctly (sometimes the value after the Reset is ignored by gRMS). A simple solution is to include a short Continue at the end of the Schedule. This is not an issue with the Excel output channel, although sending the values of a large number of Variables to Excel takes a considerable length of time. It is therefore recommended that you Monitor only the Variables that are necessary.

Stochastic simulation results

The results of the stochastic simulation are shown in the figures below. The last one also illustrates that in this model, the value of the standard deviation is only correct at the end of the simulation.

Figure 13.4. Values assigned to the temperature for each scenario.

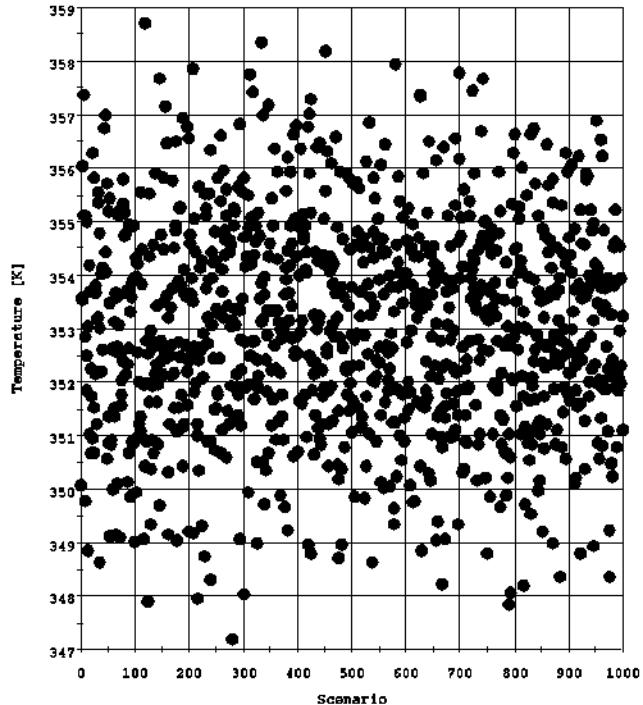
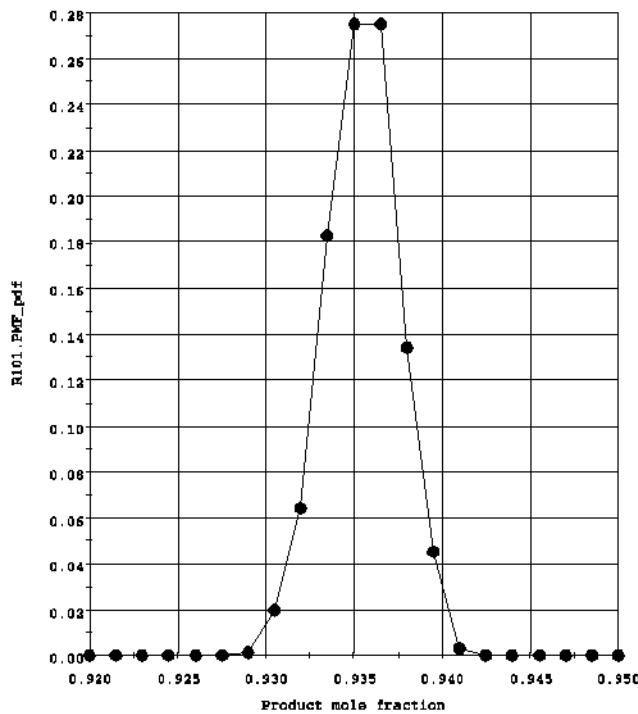
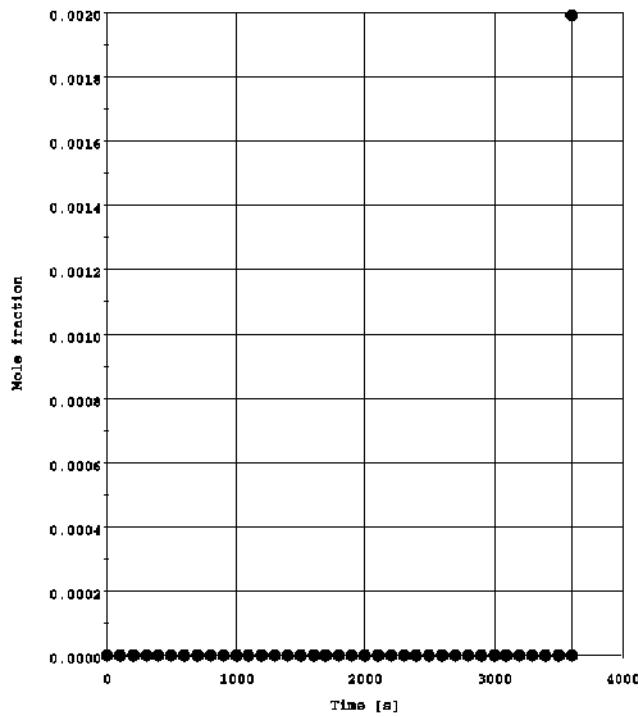


Figure 13.5. Probability density function for the product mole fraction X(4).**Figure 13.6. Standard deviation of the product mole fraction X(4).**

Chapter 14. Controlling the Execution of Model-based Activities

The Process entity is used to describe a simulation activity that is to be carried out by gPROMS using instances of one or more Model entities. The execution of model-based activities involves the solution of different types of mathematical problems. Typically, these are complex problems due to both their size and their nonlinearity. gPROMS provides a number of state-of-the-art mathematical solvers that employ a combination of symbolic, structural and numerical manipulations for the solution of these problems.

There are a number of important features of the Process entity that are related with the solution of the underlying mathematical problems and the handling of the results produced by it:

- The PRESET section describes how you can provide initial guesses for the variables that occur in your model;
- The SOLUTIONPARAMETERS section describes how you can:
 - choose appropriate solvers for different kinds of problems,
 - specify the destination of any results that the solution may produce.

In addition, a detailed description of the mathematical solvers provided as standard within gPROMS. These fall into the following categories:

- solvers for sets of linear algebraic equations;
- solvers for sets of nonlinear algebraic equations;
- solvers for mixed sets of nonlinear algebraic and differential equations;

The description of each solver includes a list of all the parameters that you can use to configure its precise behaviour when applying it to a particular problem.

The PRESET section

At the start of each simulation, gPROMS has to solve a problem known as *initialisation*. For both steady-state and dynamic simulations, gPROMS must first solve a system of algebraic equations (usually nonlinear). This naturally requires initial guesses for all of the variables in order to provide the solution algorithm with a starting point. These initial guesses (and appropriate bounds on the variables) are specified in the Variable Type entities. Usually, specifying the initial guesses in this manner i.e. the same initial guess and bounds for variables of the same type) is sufficient for gPROMS to solve the initialisation problem. Larger, more complex problems, however, may not be suited to this approach and therefore a more flexible method is needed specifying the initial guesses. This is catered for through the Preset section, which allows the default initial guess and bounds of a variable to be overridden.

The syntax for the Preset section is:

```
PRESET      VariablePath  := InitialValue ;
```

or

```
PRESET      VariablePath  := InitialValue : LowerBound : UpperBound ;
```

Within and For statements may also be used in the PRESET section. The PRESET section is usually found within the Process entity, but it may also be included inside a model entity.

Even once a set of suitable initial guesses are found, some problems may take a considerable length of time to solve. This can often be greatly reduced if the solution of the initialisation problem is used to provide the initial

guesses. This can be done in gPROMS using *Saved Variable Sets* by SAVEing the values of all variables after the initialisation and restoring them in the Preset section as shown in the gPROMS code below. In the first Process, a set of initial guesses is used that is sufficient for the initialisation to be solved. The second Process then uses the data in the save file to solve the initialisation more quickly. Note that the second Process may also save the result of the initialisation problem, so that changes can be made to the problem without having to run the first Process again.

Example 14.1. Process used to solve the initialisation problem only

```
# PROCESS InitSim1

...
PRESET
WITHIN aaa DO
  x(1)      := 1 ;
  x(2)      := 1 ;
  x(3:10)   := 0 ;
  y()       := 5 ;
  z         := 10 : 5 : 100 ;
...
END

...
SCHEDULE
SAVE "InitialisationData"
```

Example 14.2. Full Process restoring data from the successful initialisation

```
# PROCESS FullSim

...
PRESET
RESTORE "InitialisationData"
...
SCHEDULE
SEQUENCE
SAVE "InitialisationData"
...
END # sequence
```

Note that *Saved Variable Sets* restored in a RESTORE section do not overwrite the values of any Selector Variables. This is because their values, specified in the INITIALSELECTOR section, are part of the problem definition and therefore must not be modified by a RESTORE.

Multiple *Saved Variable Sets* can be Restored in the PRESET section, along with manually specified initial guesses, as shown in the example below. In all cases, any initial guess provided for a particular variable, either via an explicit specification or via a Restore, will override all earlier initial guesses for the same variable. *Please note* that bounds defined by a variable type will not be overwritten by the bounds in a Saved Variable Set. This means that any Variables that are not included in the *Saved Variable Sets* will have initial guesses and bounds specified by their Variable Types.

```
PRESET
RESTORE "v_set1", "v_set2" ;
RESTORE "v_set3" ;
VariablePath := initialValue ;
```

```
VariablePath := initialValue : LowerBound : UpperBound ;
RESTORE "v_set4", "v_set5" ;
RESTORE "v_set6" ;
```

The SOLUTIONPARAMETERS section

The SOLUTIONPARAMETERS section allows the specification of parameters that affect:

- the results generated by the execution of a model-based activity;
- the mathematical solvers to be used for the execution of a model-based activity;
- the validation and diagnosis of the mathematical models;
- the use of Foreign Processes in a simulation activity¹;
- the behaviour of Foreign Objects associated with a model-based activity;
- the behaviour of Intrinsic Tasks².

The basic syntax for the SOLUTIONPARAMETERS section, along with the default values of the parameters, is shown below:

```
SOLUTIONPARAMETERS
  # parameters concerned with output generation
  gExcelOutput      := OFF      ;
  gPLOT             := OFF      ;
  gRMS              := OFF      ;
  gUserOutput       := OFF      ;
  Monitor           := ON       ;
  OutputLevel       := 1        ;
  ReportingInterval := 0.0     ;
  ScheduleAnnotations := OFF    ;

  # parameters concerned with numerical solvers
  DASolver          := "DASOLV"  ;
  DOSolver          := "CVP_SS"   ;
  EDSolver          := "EXPDES"   ;
  PESolver          := "MAXLKHD"  ;

  # parameters concerned with mathematical formulation and validation
  IdentityElimination      := ON   ;
  IgnoreDAEIndexAnalysis   := OFF   ;
  IndexReduction           := OFF   ;
  PerformStrictDAEStructuralChecks := OFF ;

  # parameters concerned with Foreign Object behaviour
  FOSTatisticsLevel      := 0    ;
  IgnoreAllFODerivatives  := OFF   ;
  LogAllFODerivatives     := OFF   ;
  LogAllFOMethods         := OFF   ;
  TestAllFODerivatives    := OFF   ;
```

¹There is only one FPI Solution Parameter, which specifies the location of the FPI implementation. See Using Foreign Processes for details on how to create an FPI and specify its use in the Solution Parameters.

²The IntrinsicTasks Solution Parameter controls whether or not Intrinsic Tasks are enabled during a simulation activity. See Intrinsic Tasks for details on how to create and use Intrinsic Tasks.

```
# parameters concerned with intrinsic tasks
IntrinsicTasks := ON ;
```

Normally, the above default values are sufficient to solve most problems. However, they may be overridden in the SOLUTIONPARAMETERS section (of the gPROMS language tab) if and when necessary.

Controlling result generation and destination

The following Solution Parameters allow the user to control the generation of results by the execution of a model-based activity, as well as the destination of these results.

- **gExcelOutput:** Enables or disables the Microsoft Excel output channel.

By default, this parameter is switched off. When set to on, output is sent to a file whose stem is the Process entity name plus an index in square brackets to represent the number of times the process has been executed. For example, if the process name was *MyProcess* the first output file generated would be called *MYPROCESS.xls*; the second would be *MYPROCESS[2].xls*; and so on. A different file name can be specified directly in the SOLUTIONPARAMETERS section using the syntax:

```
gExcelOutput := "FileName" ;
```

Note that this specification automatically switches on the output channel: i.e. **gExcelOutput := ON ;**. See Microsoft Excel Output Channel for more details and for some additional options.

- **gPLOT:** Enables or disables the generation of text results files.

By default, this parameter is switched off. When set to on, output is sent to a file whose name is the Process entity name followed by gPLOT. A different file name can be specified directly in the SOLUTION PARAMETERS section using the syntax:

```
gPLOT := "FileName" ;
```

Note that this automatically implies that the gPLOT parameter is switched on.

- **gRMS:** Enables or disables the gRMS output channel.

By default this parameter is switched on. When set to on, output is sent to gRMS, the gPROMS Results Management Service.

Note: This setting is overridden by the settings in the execution control dialog and only applies when an activity is executed outside ModelBuilder, for instance in gO:RUN.

- **gUserOutput:** Enables or disables a user-defined output channel.

The construction of such output channels is described in detail in the gPROMS System Programmer Guide. By default, this parameter is switched off.

- **Monitor:** Sets the initial state for monitoring of variables.

By default, this parameter is switched on. If set to off, no results will be collected during the execution of the model-based activity. However, for dynamic simulation activities, monitoring can be enabled at a later stage by inserting the Monitor elementary task in the simulation Schedule.

- **OutputLevel:** An integer [-1,9] that specifies the diagnostics level reported in the output.

If specified, the OutputLevel defines the initial setting in the Execution Control dialog; otherwise the dialog will be initialised with the default value of Normal diagnostics. Currently used values are -1 (Silent), 0 (Solver diagnostics only) and 1 (Normal diagnostics), with higher values reserved for future use (values greater than 1 behave identically to 1). The effects of this parameter on execution diagnostics are summarised in the table below.

- ReportingInterval: Specifies the reporting interval for results.

This is the frequency at which variable values are transmitted to the output channel(s) during a dynamic simulation activity. This parameter does not have a default value. When a simulation activity is initiated, the ReportingInterval can be entered in a dialog box that appears before the simulation activity is performed. The text box will already contain a value for the ReportingInterval, which will be equal to the value specified by the ReportingInterval Parameter in the Process. If this specification is omitted, then the value will be equal to the default value specified in the Model Builder preferences. In either case, the value in the dialog box can be modified by the user before the simulation activity is started.

- ScheduleAnnotations: Displays unique identifying annotations on each Task in the Schedule.

Allowed values are ON and OFF (default).

Table 14.1. Effects of Output level on execution diagnostics

Output Level	-1 (Silent)	0 (Solver diagnostics only)	≥ 1 (Normal diagnostics, Extra – level n)
Diagnostics for system construction, index reduction and structural info, schedule execution, STN switching etc.	Off	Off	On
Diagnostics of individual solvers	Off	On — according to the individual solver settings	On — according to the individual solver settings

Controlling the behaviour of Foreign Objects

The following Solution Parameters allow the user to control the behaviour of Foreign Objects associated with the execution of a model-based activity:

- FOStatisticsLevel: An integer in the range [0, 2]

0	No statistics
1	Cumulative statistics on the CPU usage of all Foreign Object methods and derivatives executed during any activity
2	Detailed statistics on the CPU usage of all Foreign Objects methods and derivatives executed during any activity

- IgnoreAllFODerivatives: ON or OFF

If ON, ignores the analytical derivatives calculated by all Foreign Objects associated with a model-based activity. gPROMS uses numerical perturbations instead.

- LogAllFODerivatives: ON or OFF

If ON, details of both input and output arguments to all Foreign Object derivative calls will be written to the Execution Output.

- LogAllFOMethods: ON or OFF

If ON, details of both input and output arguments to all Foreign Object method calls will be written to the Execution Output.

- TestAllFODerivatives: ON or OFF

If ON, compares the analytical derivatives calculated by all Foreign Objects associated with a model-based activity against those calculated from numerical perturbations. Details of which comparisons fail this test are written to the file DerivativeFailure.txt which will be present in the *Results* folder of the Execution Case after execution.

Choosing mathematical solvers for model-based activities

gPROMS supports four main types of model-based activity, namely:

- Simulation
- Optimisation - refer to the gPROMS Optimisation Guide.
- Parameter Estimation - refer to the gPROMS Model Validation Guide
- Experiment Design - refer to the gPROMS Model Validation Guide

Each one of these activities can be based on either steady-state or dynamic models.

gPROMS provides a range of state-of-the-art proprietary solvers for the execution of different types of activity. Albeit sufficiently general to handle the dynamic case, these solvers are designed to automatically detect whether a particular problem is, in fact, a steady-state one and to take this into account in its solution. gPROMS also supports an open software architecture regarding mathematical solvers. This basically means that third-party solvers can be used within gPROMS without any modifications either to the gPROMS software or to the models written in it. Detailed information on this topic can be found in the gPROMS System Programmer Guide. The configuration of the solver for all activity types is entered in the SOLUTION PARAMETERS section of the Process entity:

- DASolver specifies the solver to be used for Simulation activities³;
- DOSolver specifies the solver to be used for Optimisation activities - refer to the *gPROMS Advanced Users Guide*.⁴;
- PESolver specifies the solver to be used for Parameter Estimation activities
- EDSolver specifies the solver to be used for Experiment Design activities

Note that a Process entity may contain specifications for all four types of solver irrespective of the kind of activity for which it is actually used.

The value of each of the above four parameters is actually a string identifying the solver to be used, enclosed in double quotes. For example, the syntax:

```
DASolver := "SRADAU";  
DOSolver := "DYNOPT";
```

would be used to indicate that:

- dynamic simulation is to be performed with the SRADAU solver, one of the standard gPROMS dynamic simulation solvers;
- dynamic optimisation should use a (hypothetical) third-party dynamic optimisation solver called DYNOPT.

Note that the name of the solver is *always* enclosed in double quotes.

³The 'DA' in DASolver stands for 'differential-algebraic'; this reflects the fact that the main mathematical operation involved in performing dynamic simulation activities is the solution of mixed sets of differential and algebraic equations.

⁴The 'DO' in DOSolver stands for 'dynamic optimisation'; this reflects the fact that all standard optimisation solvers in gPROMS are designed for the general case of optimisation of systems under transient conditions.

Configuring model validation and diagnosis

Before executing a model-based activity, gPROMS can perform various checks on and modifications to the mathematical formulation of the problem. These are summarised below.

- IdentityElimination: ON (default) or OFF

If set to ON, the solver will attempt to reduce the size of the problem internally by removing equations of the form $x = y$, and substituting all occurrences of one of these variables with the other. Such equations are often introduced in gPROMS models by stream connectivity equations. This may result in faster solution time although at the current stage of development the costs of creating and using the reduced system sometimes outweigh the benefits, particularly when many IF and CASE conditions are present.

- IgnoreDAEIndexAnalysis: ON or OFF (default)

Determines whether or not gPROMS attempts to (re)initialise a system if the index is determined to be greater than 1.

- IndexReduction: ON or OFF (default)

Specifies whether or not gPROMS will perform automatic index reduction for high-index models. This Solution Parameter applies to all four activities. See High-Index DAE systems for more details.

- PerformStrictDAEStructuralChecks: ON or OFF (default)

If ON, gPROMS to perform a check of the structure of the DAE system following the first initialisation and following each reinitialisation.

This option is useful because unchecked structural errors can lead to different symptoms (such as an error reported by the Linear Algebra solver) which can be hard to diagnose. It can be switched on during Model development in order to detect Modelling errors before they result in (harder to diagnose) numerical errors. It is particularly useful for Models containing IF or CASE statements.

Once the Model has been well tested, this option can be turned off, as it may have some computational overhead for complex models, particularly those that contain IF or CASE statements that change branch frequently during simulation. When a (re)initialisation fails a strict DAE structural check will be performed even if PerformStrictDAEStructuralChecks := OFF.

Configuring the mathematical solvers

A mathematical solver for a model-based activity, such as dynamic simulation or optimisation, is usually a complex piece of software. Its precise behaviour and performance in solving any particular problem is controlled by a number of *algorithmic parameters*. For example, the quality of the results produced by a dynamic simulation solver (and also the computational effort required) can be controlled by adjusting one or more error tolerances. Each algorithmic parameter will normally have a default value which is chosen to lead to good (if not optimal) performance for a wide range of problems; this default will be used unless the user specifies a different value. The set of algorithmic parameters recognised by two different solvers -- even of the same type -- will generally be different. gPROMS provides a general mechanism for specifying algorithmic parameter values of five distinct types:

- integer algorithmic parameters (e.g. the maximum permitted number of iterations);
- real algorithmic parameters (e.g. the error tolerances);
- logical algorithmic parameters (e.g. whether a certain feature of the solver is to be used or not);
- string algorithmic parameters (e.g. the name of a file to receive special output generated by the solver);
- enumerated algorithmic parameters; these are strings (enclosed in double quotes) that can take only certain values (e.g. "OFF", "MEDIUM", "HIGH") which are recognised by the solver;

- solver algorithmic parameters; these are strings (enclosed in double quotes) that specify sub-solvers to be used by the solver, as explained in detail below.

For example, the following syntax would be used to specify that a dynamic simulation should be performed using the SRADAU solver with an output level of 2, an absolute error tolerance of 10^{-8} , and with the generation of a special diagnostics output file switched on:

```
DASolver := "SRADAU" [ "OutputLevel"      := 2;
                        "AbsoluteTolerance" := 1E-8;
                        "Diag"              := TRUE ] ;
```

A complete list of all the parameters associated with the SRADAU solver is given. The important things to note here are:

- the name of the algorithmic parameter is *always* enclosed in double quotes, as is the name of the solver itself;
- the values of algorithmic parameters of type string, enumerated and solver (not shown in the above example) must be enclosed in double quotes;
- any algorithmic parameters not specified here will retain their default values.

Specifying solver-type algorithmic parameters

Some of the algorithmic parameters used to configure solvers may be solvers themselves. For example, solving a set of differential and algebraic equations typically requires the solution of a number of mathematical sub-problems involving sets of either nonlinear or linear algebraic equations. Thus, a differential-algebraic equation solver will normally need to make use of both a nonlinear equation solver and a linear equation solver. We will refer to these as the 'sub-solvers' associated with this solver. Some mathematical solvers have built in sub-solvers that they always use for their operation. On the other hand, more advanced solvers may allow their users to specify the sub-solver to be used. This can be done via an algorithmic parameter. For instance, consider the following extended form of the example specification of the dynamic simulation solver:

```
DASolver := "SRADAU" [ "OutputLevel"      := 2;
                        "AbsoluteTolerance" := 1E-8;
                        "Diag"              := TRUE;
                        "LASolver"          := "MA28";
                        "InitialisationNLSolver" := "SPARSE";
                        "ReinitialisationNLSolver" := "SPARSE" ] ;
```

This specifies that the SRADAU solver should use the MA28 solver for the solution of any sets of linear algebraic equations that it needs to perform.

In addition to a sub-solver for linear equations, the SRADAU solver also needs two sub-solvers for nonlinear algebraic equations. One of these is used for the initialisation of the dynamic simulation and the other one for re-initialisation following discontinuities. In the above example, we are specifying that the SPARSE solver should be used for both of these tasks. SPARSE is one of the nonlinear algebraic equation solvers provided as standard within gPROMS.

In all cases, note that the value of a solver-type algorithmic parameter (i.e. the name of the sub-solver to be used) needs to be enclosed in double quotes. Of course, a sub-solver is itself a solver and may have its own algorithmic parameters that the user may specify. In the above example, we may wish to specify a tight convergence tolerance for the initialisation solver and a slightly less tight one for re-initialisation. This can be done using the syntax:

```
DASolver := "SRADAU" [ "OutputLevel"      := 2;
                        "AbsoluteTolerance" := 1E-8;
                        "Diag"              := TRUE;
                        "LASolver"          := "MA28";
                        "InitialisationNLSolver" := "SPARSE"
```

```
[ "ConvergenceTolerance" := 1E-8];
"ReinitialisationNLSolver" := "SPARSE"
[ "ConvergenceTolerance" := 1E-7 ]
```

In fact, some of the sub-solvers may themselves have solver-type parameters. For example, nonlinear equation solvers, such as SPARSE, often need to solve sub-problems that involve sets of linear algebraic equations. Again, this can be accommodated within the general syntax presented above. For example:

```
DASolver := "SRADAU" [ "OutputLevel"           := 2;
                        "AbsoluteTolerance"   := 1E-8;
                        "Diag"                := TRUE;
                        "LASolver"             := "MA28";
                        "InitialisationNLSolver" := "SPARSE"
                                         [ "ConvergenceTolerance" := 1E-8;
                                         "LASolver"              := "MA48" ];
                        "ReinitialisationNLSolver" := "SPARSE"
                                         [ "ConvergenceTolerance" := 1E-7;
                                         "LASolver"              := "MA28" ]
```

specifies that the SPARSE solver used for initialisation should make use of the MA48 linear algebra solver, while that used for re-initialisation should employ the MA28 solver. Moreover, MA28 will be used by SRADAU to solve any linear equations systems arising outside the initialisation and re-initialisation stages of its operation. The above syntax for specifying and configuring sub-solvers within solvers is recursive and can be used to define solver hierarchies with any number of levels. For example, a dynamic optimisation solver can use a differential-algebraic equation solver, which in turn can make use of a nonlinear equation solver, which can employ a linear equation solver.

Specifying default linear and nonlinear equation solvers

Most mathematical solvers for simulation, optimisation and parameter estimation need to make use of sub-solvers for the solution of sets of linear and nonlinear algebraic equations. In order to avoid having to specify and configure these low level solvers repeatedly within the same SOLUTION PARAMETERS section, gPROMS provides two solution parameters that can be used to specify and configure *default* linear and nonlinear algebraic equation solvers. Thus, in addition to the four main solver parameters DASolver, DOSolver , EDSolver and PESolver described in section on DAE solvers, gPROMS recognises the following two parameters:

- LASolver specifies the default sub-solver for sets of linear algebraic equations;
- NLSolver specifies the default sub-solver for sets of nonlinear algebraic equations.

Consider, for example, the specification:

```
# default linear algebraic equation solver configuration
LASolver := "MA28" [ "PivotStabilityFactor"      := 0.2;
                      "ExpansionFactor"        := 3;
                      "MaxStructures"          := 4] ;

# default nonlinear algebraic equation solver configuration
NLSolver := "SPARSE" [ "OutputLevel"            := 3;
                       "MaxFuncs"              := 1000;
                       "MaxIterNoImprove"      := 5;
                       "NStepReductions"       := 10;
                       "MaxIterations"          := 1000;
                       "ConvergenceTolerance"  := 1E-8] ;

DASolver := "DASOLV" [ "OutputLevel"           := 1;
```

```
"AbsoluteTolerance"      := 1E-8] ;  
  
DOSolver := "CVP_MS" ;
```

This specifies that, whenever the DASOLV solver needs to solve sets of linear or nonlinear algebraic equations, it should use, respectively, the MA28 and SPARSE solvers configured as shown above. Also, whenever SPARSE itself requires the solution of a set of linear equations, it should also use MA28 in the same configuration. The above also specifies that the CVP_MS solver should be used for the execution of dynamic optimisation activities. This solver will also make use of the specified sub-solver choices and configurations for linear and nonlinear algebraic equations. Interestingly, CVP_MS also requires a differential-algebraic equation solver for its operation. This could be achieved by specifying the value of a solver-type algorithmic parameter called DASolver, e.g. DOSolver := "CVP_MS" ["DASolver" := "SuperDAE"] ; where SuperDAE is a (hypothetical) third-party solver for differential-algebraic equations. However, since no such explicit specification is made above, CVP_MS will actually use the DASolver choice and configuration shown above for this purpose. In conclusion, specifying the DASolver parameter in Solutionparameters fulfils a dual function as it defines:

- the mathematical solver to be used for simulation activities;
- the default sub-solver to be used by the optimisation and parameter estimation activity solvers whenever they need to solve sets of differential and algebraic equations.

Standard solvers for linear algebraic equations

There are two standard mathematical solvers for the solution of sets of linear algebraic equations in gPROMS, namely MA28 and MA48. Both of these employ direct LU-factorisation algorithms, designed for large, sparse, asymmetric systems of linear equations. MA48 is the newer of the two codes. The LASolver solution parameter may be used to change and/or configure the default linear algebra sub-solver used by all higher-level solvers. If this parameter is not specified, then the MA48 solver is used, with the default configuration shown at the start of section below.

The MA28 solver

The algorithmic parameters used by MA28 along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"MA28" [ "OutputLevel"      := 0;  
          "PivotStabilityFactor" := 0.1;  
          "ExpansionFactor"     := 4;  
          "MaxStructures"       := 6;  
          "MaxStructuresMemory" := 100000 ] ;
```

- OutputLevel: An integer in the range [-1, 3].

The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

-1	(None)
0	Errors and important warnings. Workspace increases.
1	Structure analysis messages
2	Location of singularities
3	Informative messages. Creation and deletion of systems. Usage statistics on deletion.

- PivotStabilityFactor: A real number in the range [0.0, 1.0].

Controls the balance between minimising the creation of new non-zero elements during the matrix factorisation⁵(PivotStabilityFactor = 0) and numerical stability (PivotStabilityFactor = 1).

- ExpansionFactor: An integer of value 1 or higher.

The amount of space that gPROMS allocates for the matrix factorisation at the start of a computation is given by:

$$\text{ExpansionFactor} \times (\text{Number of Nonzero Elements in Matrix})$$

gPROMS will automatically expand this storage at a later stage during the computation if the original allocation is found to be insufficient. However, if the amount of storage needed by a particular computation is known *a priori*⁶, it will usually be more efficient to allocate it from the start by specifying an appropriate value for ExpansionFactor.

- MaxStructures: An integer of value 0 or higher.

The execution of a model-based activity in gPROMS typically involves the factorisation of a number of matrices of several different structures. The gPROMS implementation of MA28 allows the option of storing information on one or more structures encountered for possible re-use at a later stage of the execution if it is required again to factorise a matrix with one of those structures. This may significantly improve the efficiency of handling discontinuities at the expense of higher memory requirements. The parameter MaxStructures is an upper limit on the number of distinct structures that may be stored during any one simulation.

- MaxStructureMemory: An integer of value 0 or higher.

This is an upper bound on the number of integer variable locations that may be used as part of the structure storage scheme described above.

The MA48 solver

The algorithmic parameters used by MA48 along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"MA48" [ "OutputLevel"           := 0;
            "PivotStabilityFactor" := 0.1;
            "ExpansionFactor"      := 5;
            "FullSwitchFactor"     := 0.5;
            "PivotSearchDepth"    := 3;
            "BLASLevel"             := 32;
            "MinBlock"              := 1 ] ;
```

- OutputLevel: An integer in the range [-1, 4].

The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

0	(None)
1	Creation and deletion of systems, usage statistics including CPU, workspace increases, numerical singularity
2	Warning messages, e.g. for duplicate entries, which can be ignored
3	Information from the internal Fortran calls: a few entries of the matrix to be factorised and the result

⁵And consequently, the amount of storage required by the factorisation.

⁶For example, from experience from earlier similar computations.

4

More information, including all entries in the factorised matrices, and the right-hand-side and solutions vectors.

- PivotStabilityFactor: A real number in the range [0.0, 1.0].

Controls the balance between minimising the creation of new non-zero elements during the matrix factorisation⁷(PivotStabilityFactor = 0) and numerical stability (PivotStabilityFactor = 1).

- ExpansionFactor: An integer of value 1 or higher.

The amount of space that gPROMS allocates for the matrix factorisation at the start of a computation is given by:

$$\text{ExpansionFactor} \times (\text{Number of Nonzero Elements in Matrix})$$

gPROMS will automatically expand this storage at a later stage during the computation if the original allocation is found to be insufficient. However, if the amount of storage needed by a particular computation is known *a priori*⁸, it will usually be more efficient to allocate it from the start by specifying an appropriate value for ExpansionFactor.

- FullSwitchFactor: A real number in the range [0.0, 1.0].

The MA48 linear solver has an option of switching to full-matrix linear algebra computations at any stage during the matrix factorisation process if the proportion of non-zero elements in the matrix remaining to be factorised exceeds a specified threshold. The latter can be adjusted by the parameter FullSwitchFactor.

- PivotSearchDepth: An integer of value 0 or higher.

The number of columns within which the search for an appropriate pivot element during a factorisation is limited. Generally, a higher number will result in a more numerically stable pivot selection, at the expense of higher computation time. If PivotSearchDepth is set to zero, MA48 will use a special technique for finding the best pivot. Although this may result in reduced fill-in, pivot search in this case is usually slower and occasionally very slow.

- BLASLevel: An integer of value 0 or more.

MA48 makes use of the Basic Linear Algebra System (BLAS) for vector and matrix operations. BLAS is organised in three different levels, in ascending order of sophistication of the services offered. The BLASLevel parameter specifies that BLAS level BLASlevel+1 should be used by MA48. Additionally, if the value is 2 or more, it is used to set the block column size, a parameter only applicable to level 3. For this reason, the default is 32.

- MinBlock: An integer of value 1 or higher.

MA48 makes use of block triangularisation as a means of accelerating the factorisation and solution of linear systems. This parameter specifies the minimum block size to be considered in this context.

Standard solvers for nonlinear algebraic equations

There are two standard mathematical solvers for the solution of sets of nonlinear algebraic equations in gPROMS, namely BDNLSOL and SPARSE:

- BDNLSOL stands for 'Block Decomposition NonLinear SOLver'. It is a new implementation of a general solver for solving sets of nonlinear equations rearranged to block triangular form, and employs a novel algorithm for the handling of equations with reversible symmetric discontinuities (IF equations). As a modular solver component, BDNLSOL can in principle make use of any other nonlinear solver component to solve its individual blocks.

⁷And consequently, minimising the amount of storage required by the factorisation.

⁸For example, from experience from earlier similar computations.

- SPARSE is a true solver component for solution of nonlinear algebraic systems without block decomposition. It provides a sophisticated implementation of a Newton-type method.

The above solvers are designed to deal with large, sparse systems of equations in which the variable values are restricted to lie within specified lower and upper bounds. Moreover, they can handle situations in which some of the partial derivatives of the equations with respect to the variables are available analytically while the rest have to be approximated. In gPROMS models, almost all partial derivatives are computed analytically from expressions derived using symbolic manipulations. The main exception is partial derivatives of equations involving any Foreign Object methods that are not capable of returning partial derivatives.

An efficient combination of finite difference approximations and least-change secant updates is used for the latter purpose.

The NLSolver solution parameter may be used to change and/or configure the default nonlinear algebra sub-solver used by all higher-level solvers. If this parameter is not specified, then all activities make use of the BDNLSOL solver with the default configuration shown in the corresponding section

- simulation;
- optimisation and parameter estimation activities make use of the BDNLSOL solver with the default configuration shown in the corresponding section.

Note that NLSOL is no longer available as its functionality has been entirely been replaced by BDNLSOL.

The BDNLSOL solver

The algorithmic parameters used by BDNLSOL along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"BDNLSOL" [ "BlockSolver"           := "SPARSE" ;
             "LASolver"            := "MA48" ;
             "OutputLevel"          := 0 ;
             "MaxStructureSwitches" := 100 ;
             "UseIFSuperstructure"  := FALSE ] ;
```

- BlockSolver: A quoted string specifying a nonlinear algebraic equation solver.

The solver to be used for the solution of the nonlinear systems representing each block. This can be either SPARSE or a third-party nonlinear algebraic equation solver (see the gPROMS System Programmer Guide). This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- LASolver: A quoted string specifying a linear algebraic equation solver.

The solver to be used for the solution of linear algebraic equations. This can be either one of the standard gPROMS linear algebraic equation solvers or a third-party linear algebraic equation solver (see the gPROMS System Programmer Guide). The default is MA48. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- OutputLevel: An integer in the range [-1, 5].

The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

0	(None)
1	Numbers of equations in each block in the main block decomposition Failures to solve linear blocks
2	Result of the block decomposition: equation and variable numbers in each block 'Solving block <i>n</i> ' message

3	Changed/unchanged variables due to solving single linear equations Final variable values after solving nontrivial blocks
5	Table of equation names necessary to interpret information from main block decomposition step

- MaxStructureSwitches: An integer in the range [0, 1000000]

The maximum number of successive switches of conditional equations before the solution iterations will stop.

- UseIFSuperstructure. A boolean value.

If set to TRUE, the solver will attempt to take account of the occurrence of variables in both branches of IF conditions when performing block decomposition, which will allow it to proceed through the blocks even when the need to change IF branches is detected after solution of a given block. For problems with a large number of IF conditions this can improve solution time considerably.

The SPARSE solver

The algorithmic parameters used by SPARSE along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"SPARSE" [ "LASolver" : = "MA48" ;
  "BoundsTightening" : = 0 ;
  "ConvergenceTolerance" : = 1E-5 ;
  "EffectiveZero" : = 1E-5 ;
  "FDPerturbation" : = 1E-5 ;
  "IterationsWithoutNewJacobian" : = 0 ;
  "MaxFuncs" : = 1000000 ;
  "MaxIterations" : = 1000 ;
  "MaxIterNoImprove" : = 10 ;
  "MaxStructureSwitches" : = 100 ;
  "NStepReductions" : = 10 ;
  "OutputLevel" : = 0 ;
  "SingPertFactor" : = 1E-2 ;
  "SLRFactor" : = 50 ; ] ;
```

- LASolver: A quoted string specifying a linear algebraic equation solver.

The solver to be used for the solution of linear algebraic equations at every iteration. This can be either one of the standard gPROMS linear algebraic equation solvers or a third-party linear algebraic equation solver (see the gPROMS System Programmer Guide). The default is MA48. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- BoundsTightening: A real number in the range [0.0, 1.0].

If this parameter is set to a non-zero value, then at each iteration, after applying its usual logic to impose the true variable bounds on the step taken, SPARSE will impose "tightened bounds". The exact value of the bounds used is dependent on the previous guess for each variable: if the i th variable has true lower bound x_{il} , and previous guess $x_i^{(k)}$, the tightened lower bound will be $x_{il} + p(x_i^{(k)} - x_{il})$, where p is the value of this parameter. Similar logic is applied to the tightened upper bound.

- ConvergenceTolerance: A real number in the range $[10^{-20}, 10^{10}]$.

The tolerance used in testing for convergence of the nonlinear system $f(x)=0$ being solved. A system of n equations $f(x)$ in n unknowns x is assumed to have converged when the norm of the equations:

$$\|f(x)\| \equiv \max_{i \in [1, n]} |f_i(x)|$$

falls below the ConvergenceTolerance. This is equivalent to the absolute value of the difference between the left and right hand sides of each and every equation in the system being below this tolerance. Note that no automatic scaling is applied by the solver.

- EffectiveZero: A real number in the range $[10^{-20}, 10^{10}]$.

The magnitude of a variable below which absolute rather than relative perturbations are used -- see parameters FDPPerturbation, SingPertFactor and SLRFactor below.

- FDPPerturbation: A real number in the range $[10^{-20}, 10^{10}]$.

Finite difference perturbation factor. If finite difference calculation of partial derivatives with respect to a variable x is required, x is perturbed by:

$$\text{FDPPerturbation} \times |x|$$

unless FDPPerturbation $\times |x|$ is less than EffectiveZero (see above), in which case it is perturbed by FDPPerturbation.

- IterationsWithoutNewJacobian: An integer in the range $[0, 1000000]$.

If set to 0 SPARSE computes the Jacobian at every iteration. Otherwise, SPARSE will use a simple form of Modified Newton keeping the Jacobian for a set number of iterations. In some cases this can be used to speed up the solution.

- MaxIterations: An integer in the range $[1, 1000000]$.

The maximum number of iterations that the solver is allowed to take. Note that, unlike MaxFuncs (see above), this does not include any evaluations of the equations for the purpose of estimating elements of the Jacobian matrix using finite difference perturbations.

- MaxFuncs: An integer in the range $[1, 1000000]$.

The maximum number of evaluations of the vector of equations $f(x)$ that is permitted during solution. This includes the equation evaluations required for approximating any elements of the Jacobian matrix $\partial f / \partial x$ that are not available analytically, using finite difference perturbations.

- MaxIterNoImprove: An integer in the range $[1, 1000000]$.

The maximum number of iterations without a reduction in the norm of the equation vector (see above) before the solver takes corrective action. For convergence to be achieved, this norm must eventually decrease to below the ConvergenceTolerance. However, it may actually increase between two consecutive iterations.

The solver monitors the norm at each iteration. It also keeps a record of the best (i.e. lowest) norm obtained so far in the solution, the values of the unknowns x^{best} at this point, and the step Δx^{best} taken from this point x^{best} . If no improvement over this best norm is observed within MaxIterNoImprove consecutive iterations, then the solver attempts to take corrective action, as follows:

- the unknowns are reset to $x^{best} + \Delta x^{best}/2$;
- the Jacobian matrix is recomputed, using finite differences for any elements not available analytically.
- MaxStructureSwitches: An integer in the range $[0, 1000000]$

The maximum number of successive switches of conditional equations before the solution iterations will stop.

- NStepReductions: An integer in the range $[1, 1000000]$.

The maximum number of consecutive corrective actions that the solver is allowed to attempt. As explained in the context of parameter MaxIterNoImprove above, the solver attempts to take certain corrective actions if no improvement in the equation norm is achieved within a certain number of consecutive iterations. If such

corrective action is attempted more than NStepReductions times in a row (i.e. having to return to the same x^{best} in all cases), then the solver terminates its operation unsuccessfully.

- OutputLevel: An integer in the range [-1, 10].

The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

-1	(None)
0	Halving of step due to unsatisfactory progress, initial point out of bounds
1	Solution parameters on first use, variables hitting bounds
2	Method and scaling information, residual and call number on convergence, failure to improve in MaxIterNoImprove iterations, residual and worst equation number at each call to driver, variables stuck on bounds, number of variables reset to bounds
3	Variable and equation names of each nonlinear system, call number and condition on each call to driver, step reduction factors, various measures of the largest steps taken at each iteration
4	Residuals at every evaluation, variables at each iteration, lists of variables being perturbed
5	Variable values before solution, workspace information, solutions of linear systems (i.e. steps)
6	Complete Jacobian at each factorisation
10	Solution parameters on every use

- SingPertFactor: A real number in the range $[10^{-20}, 10^{10}]$.

The perturbation factor used for escaping from local singularities. If, at a certain iteration, the Jacobian matrix is found to be singular (with a rank r that is less than the size of the system n), the solver attempts to escape from such a point by applying a perturbation to $n-r$ of the system variables. For a variable x , the size of this perturbation is:

$$\text{SingPertFactor} \times |x|$$

unless $|x|$ is less than EffectiveZero (see above), in which case it is perturbed by SingPertFactor.

- SLRFactor: A real number in the range $[10^{-20}, 10^{10}]$.

The step length restriction factor, $\#$. In the interests of improving convergence from poor initial guesses, the solver automatically limits the step taken in any iteration by a fraction $\# \in (0,1]$ so that the magnitude of the change in any variable x does not exceed:

- $\#|x|$ if x is equal to, or exceeds the EffectiveZero (see above);
- $\#$ otherwise.

Standard solvers for differential-algebraic equations

There are two standard mathematical solvers for the solution of mixed sets of differential and algebraic equations in gPROMS, namely DASOLV and SRADAU:

- DASOLV is based on variable time step/variable order Backward Differentiation Formulae (BDF). This has been proved to be efficient for a wide range of problems. However, BDF solvers suffer from loss of stability for certain types of problems (e.g. highly oscillatory ones) and they are not very efficient for problems with frequent discontinuities.
- SRADAU implements a variable time step, fully-implicit Runge-Kutta method. It has been proved to be efficient for the solution of problems arising from the discretisation of PDAEs with strongly advective terms (in general, highly oscillatory ODEs), and models with frequent discontinuities.

Both of the above solvers are designed to deal with large, sparse systems of equations in which the variable values are restricted to lie within specified lower and upper bounds. Moreover, they can handle situations in which some of the partial derivatives of the equations with respect to the variables are available analytically while the rest have to be approximated⁹. Efficient finite difference approximations are used for the latter purpose. Both solvers automatically adjust each time step taken so that the following criterion is satisfied:

$$\sqrt{\frac{1}{n_d} \sum_{i=1}^{n_d} \left(\frac{\epsilon_i}{a+r|x_i|} \right)^2} \leq 1$$

where:

- n_d is the number of differential variables in the problem (i.e. those that appear as \$x in the gPROMS model);
- ϵ_i is the solver's estimate for the local error in the i^{th} differential variable;
- x_i is the current value of the i^{th} differential variable;
- a is an absolute error tolerance;
- r is a relative error tolerance.

In rough terms, this means that the error ϵ_i incurred in a particular variable x_i over a single time step is not allowed to exceed $a + r|x_i|$. The default values for a and r (10^{-5} in both cases) are usually adequate since:

- they control the error in variables x_i of size 0.01 or higher to within acceptable ranges;
- smaller variable values are often not important from an engineering point of view¹⁰.

However, for problems in which small variable values may have an important effect on system behaviour, it is advisable to specify a smaller absolute tolerance¹¹.

At the end of each simulation, if an estimate of the error committed in any variable at any time step exceeds a threshold, this is reported. See the Large residual warnings section for details.

The DASolver solution parameter may be used to change and/or configure the solver used for simulation activities, as well as the default DAE sub-solver used by all higher-level solvers. If this parameter is not specified, then the DASOLV solver is used, with the default configuration shown at the start of the section below.

The DASOLV solver

The algorithmic parameters used by DASOLV along with their default values are shown below. This is followed by a detailed description of each parameter.

```
"DASOLV" [ "InitialisationNL Solver" ] := "BDNLSOL" ;
```

⁹In gPROMS models, almost all partial derivatives are computed analytically from expressions derived using symbolic manipulations. The main exception is partial derivatives of equations involving any Foreign Object methods that are not capable of returning partial derivatives.

¹⁰For example, a liquid level in a processing vessel of 10^{-4} m is practically indistinguishable from one of 10^{-5} m.

¹¹For example, in a problem involving free radicals or ions, it may be important to distinguish between mole fraction of 10^{-6} and 10^{-7} .

```

"LASolver" : = "MA48";
"ReinitialisationNLSSolver" : = "BDNLSOL";
"Absolute1stTimeDerivativeThreshold" : = 0.0;
"AbsolutePerturbationFactor" : = 1.0E-7;
"AbsoluteTolerance" : = 1E-5;
"Diag" : = FALSE;
"EffectiveZero" : = 1E-5;
"EventTolerance" : = 1E-5;
"FDPPerturbation" : = 1E-6;
"FiniteDifferences" : = FALSE;
"HigherOrderBiasFactor" : = 1;
"MaxCorrectorIterations" : = 5;
"MaxSuccessiveCorrectorFailures" : = 12;
"MinimumRatioForOrderDecrease" : = 1000;
"OutputLevel" : = 0;
"Relative1stTimeDerivativeThreshold" : = 0.0;
"Relative2ndTimeDerivativeThreshold" : = 0.0;
"RelativePerturbationFactor" : = 1E-4;
"RelativeTolerance" : = 1E-5;
"SenErr" : = FALSE;
"VariablesWithLargestCorrectorSteps" : = 0]

```

However, BDNLSOL is used as the default InitialisationNLSSolver and ReinitialisationNLSSolver when DASOLV is used for *simulation* activities.

- InitialisationNLSSolver: A quoted string specifying a nonlinear algebraic equation solver.

The solver to be used for the solution of nonlinear algebraic equations occurring at the initialisation stage of the integration. This can be either one of the standard gPROMS nonlinear algebraic equation solvers or a third-party nonlinear algebraic equation solver (see the gPROMS System Programmer Guide). The default is BDNLSOL. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- LASolver: A quoted string specifying a linear algebraic equation solver.

The solver to be used for the solution of linear algebraic equations at each step of the integration. This can be either one of the standard gPROMS linear algebraic equation solvers or a third-party linear algebraic equation solver (see the gPROMS System Programmer Guide). The default is MA48. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- ReinitialisationNLSSolver: A quoted string specifying a nonlinear algebraic equation solver.

The solver to be used for the solution of nonlinear algebraic equations that is necessary for re-initialisation following discontinuities. This can be either one of the standard gPROMS nonlinear algebraic equation solvers or a third-party nonlinear algebraic equation solver (see the gPROMS System Programmer Guide). The default is BDNLSOL. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- Absolute1stTimeDerivativeThreshold: A real number in the range [0, 10¹⁰].

Unless this parameter has the value zero, it represents the value θ_A in the condition used to determine reporting of potential 'runaway' derivatives.

If it is zero (the default), no runaway derivatives will be reported.

- AbsolutePerturbationFactor: A real number in the range [10⁻²⁰, 10¹⁰]; default = 10⁻⁷.

Absolute perturbation factor for varied trajectories and second-order sensitivities.

- AbsoluteTolerance: A real number in the range $[10^{-20}, 10^{10}]$.

The absolute integration tolerance. Together with the parameter RelativeTolerance (see below), they determine whether or not a time step taken by the solver is sufficiently accurate.

- Diag: A boolean value.

Specifies whether very detailed diagnostic information is to be generated during integration.

- EffectiveZero: A real number in the range $[10^{-20}, 10^{10}]$.

The magnitude of a variable below which absolute rather than relative finite difference perturbation is used -- see parameter FD_Perturbation below.

- EventTolerance: A real number in the range $[10^{-20}, 10^{10}]$.

The event tolerance, i.e. the maximum time interval within which discontinuities during integration are located.

- FD_Perturbation: A real number in the range $[10^{-20}, 10^{10}]$.

Finite difference perturbation factor. If finite difference calculation of partial derivatives with respect to a variable X is required, X is perturbed by:

$$\text{FD_Perturbation} \times |X|$$

unless $|X|$ is less than EffectiveZero, in which case it is perturbed by FD_Perturbation.

- FiniteDifferences: A boolean value; default = FALSE.

Controls whether second-order sensitivities are calculated via finite differences (TRUE) or within the BDF code (FALSE).

- HigherOrderBiasFactor: A real number in the range [0.001, 1000].

The factor B used in the tests which the integrator makes periodically to determine whether to change the order of integration within DASOLV. Giving this factor a value greater than 1 will "bias" the integrator towards using higher order steps. This has been found to result in quicker solution for many problems (see also MinimumRatioForOrderDecrease).

This test is of the form

```
IF r_up*B > r_sm AND r_up*B > r_dn THEN
    Raise integration order
END
```

Where:

- r_{up} is the ratio which DASOLV will apply to the step if it increases the order by 1,
- r_{sm} is the ratio which DASOLV will apply to the step if it keeps the order the same,
- r_{dn} is the ratio which DASOLV will apply to the step if it decreases the order by 1.
- MaxCorrectorIterations: An integer number in the range [1,50].

The maximum number of corrector iterations to allow on a single attempt to solve the system (i.e. before cutting the step).

- MaxSuccessiveCorrectorFailures: An integer number in the range [1,100].

The maximum number of successive corrector failures to allow before declaring an integration failure.

- MinimumRatioForOrderDecrease: A real number in the range [0.0, 10⁹].

The factor F used in the tests which the integrator makes periodically to determine whether to reduce the order of integration within DASOLV. Giving this factor a value greater than zero will "bias" the integrator against reducing the step. This has been found to result in quicker solution for many problems (see also HigherOrderBiasFactor) - in particular, setting the value to 1.0 will ensure that the order is not reduced unless the step itself is being reduced, which often proves beneficial.

This test is of the form

```
IF r_dn > r_sm AND r_dn > r_up AND r_sm > F THEN
    Reduce integration order
END
```

Where:

- r_up is the ratio which DASOLV will apply to the step if it increases the order by 1,
- r_sm is the ratio which DASOLV will apply to the step if it keeps the order the same,
- r_dn is the ratio which DASOLV will apply to the step if it decreases the order by 1.
- OutputLevel: An integer in the range [-1, 7].

The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

0	(None)
1	(Re-)initialisation times, projection of predictor onto bounds, variables hitting bounds
2	Successful initialisation, change of branch in IF conditional equations, location of discontinuities, step failures, repeated convergence failures, predictor outside bounds, predictor step reduction, variables stuck on bounds
3	Detail of convergence failures, values of derivatives on commencing integration, number of perturbation groups, step length reduction due to bounds violation
4	Variable causing discontinuity, detail of perturbation groups
5	Entry to main integrator routines, all error test values, nonfatal singularities during integration, greatest changes in variables at each corrector iteration
6	Convergence values at every corrector iteration, step change factors
7	Time, step, variables, derivatives and residuals at every corrector iteration

When OutputLevel is 3 or more, gPROMS reports the norms for differential and algebraic Variables, as shown in the example below.

Norm values

```
... differential and algebraic variables: 2.19219E-005
... algebraic variables only: 2.19607E-005
```

These norms are calculated using the following equations.

$$norm = C(n_q) \sqrt{\frac{1}{N} \sum_{i=1}^N \left(\frac{x_i}{a+r x_i} \right)^2},$$

where:

- $C(n_q)$ are constants depending on the on the order of the step
- N is the number of equations
- x_i are the current values of the variables
- a and r are the absolute and relative tolerances

For algebraic Variables only, the norm is calculated by:

$$norm_{alg} = C(n_q) \sqrt{\frac{1}{N_{alg}} \sum'_i \left(\frac{x_i}{a+r x_i} \right)^2},$$

where N_{alg} is the number of algebraic variables and the summation is performed over only the N_{alg} algebraic variables.

- Relative1stTimeDerivativeThreshold: A real number in the range $[0, 10^{10}]$.

Represents the value θ_R in the condition used to determine reporting of potential ``runaway'' derivatives.

- Relative2ndTimeDerivativeThreshold: A real number in the range $[0, 10^{10}]$.

Represents the value θ_2 in the conditions used to determine reporting of potential ``runaway'' derivatives.

- RelativePerturbationFactor: A real number in the range $[10^{-20}, 10^{10}]$; default = 10^{-4} .

Relative perturbation factor for varied trajectories and second-order sensitivities.

- RelativeTolerance: A real number in the range $[10^{-20}, 10^{10}]$; default = 10^{-5} .

The relative integration tolerance. Together with the parameter AbsoluteTolerance (see above), they determine whether or not a time step taken by the solver is sufficiently accurate.

- SenErr: A boolean value.

For optimisation type activities: specifies whether the sensitivity error test is to be applied at each step of the integration.

- VariablesWithLargestCorrectorSteps: An integer between 0 and 1000; default = 0.

On rare occasions, DASOLV fails with a "corrector step failure" message. This indicates that the code is unable to establish a set of variable values that satisfy the system equations at a particular point. It is often caused by errors or bad scaling in some modelling equations which results in the corrector iterations taking excessively large steps in some of the variables. To help with the diagnosis of such problems, DASOLV can report the variables with the largest relative change at each corrector iteration. The relative change for a variable X is defined as:

$$\frac{\delta X}{a+r|X|}$$

where:

- δX is the step in the variable at this corrector iteration;
- a is the absolute tolerance;
- r is the relative tolerance.

The parameter `VariablesWithLargestCorrectorSteps` specifies the number of variables to be reported in this manner. Note that such reporting takes place only if the parameter `OutputLevel` is set to a value of 0 or higher.

An example of the output is shown below:

```
variables with largest (weighted) corrector steps follow...
```

```
Differential and algebraic variables (norm = 227.542):
```

Variable	Name	Current Value	Corrector Step	Weight
1	Plant.Reactor.STR.rho_L	12126	548.071	
2	Plant.Reactor.STR.c(5)	12126	548.071	
3	Plant.Reactor.STR.vol_L	0.000824675	-3.72737E-05	
4	Plant.Reactor.STR.q_Loss	0.00692394	-6.05969E-06	
5	Plant.Reactor.STR.ThermoHL.hli(2)	-5.12137E-10	-1.41695E-06	

```
Algebraic variables only (norm = 250.308):
```

Variable	Name	Current Value	Corrector Step	Weight
1	Plant.Reactor.STR.rho_L	12126	548.071	
2	Plant.Reactor.STR.c(5)	12126	548.071	
3	Plant.Reactor.STR.vol_L	0.000824675	-3.72737E-05	
4	Plant.Reactor.STR.q_Loss	0.00692394	-6.05969E-06	
5	Plant.Reactor.STR.ThermoHL.hli(2)	-5.12137E-10	-1.41695E-06	

The output is grouped in terms of differential and algebraic Variables and only algebraic Variables. In each case, a norm value is also reported. For differential and algebraic variables, this is defined by:

$$norm = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(\frac{X_i}{a+rX_i} \right)^2},$$

where N is the number of equations. Subsequent lines list the largest `VariablesWithLargestCorrectorSteps` Variables and their relative changes.

For algebraic Variables only, then norm is similarly defined:

$$norm_{alg} = \sqrt{\frac{1}{N_{alg}} \sum'_i \left(\frac{X_i}{a+rX_i} \right)^2},$$

where N_{alg} is the number of algebraic Variables and the summation is over only the algebraic Variables. Again, a list of the algebraic variables with the largest corrector steps then follows.

If a subset of the system being solved by DASOLV becomes unstable, then DASOLV may fail, issuing a "repeated error test failure" message. This indicates that the code is no longer able to control the error of integration. The variables associated with such instabilities often exhibit excessively large values of their first and second time

derivatives immediately preceding the instability. DASOLV exploits this fact to help in the diagnosis of such problems. More specifically, DASOLV will report any variable X which satisfies **all three** of the following tests:

1. Minimum magnitude: The value of $|X|$ must be greater than 10^{-5}

2. First derivative:

- EITHER

$$|\dot{X}| > \theta_A$$

(specified with the AbsoluteDerivativeThreshold parameter)

- OR

$$\frac{|\dot{X}|}{|X|} > \theta_R$$

(specified with the RelativeDerivativeThreshold parameter)

3. Second derivative:

$$\frac{|\ddot{X}|}{|\dot{X}|} > \theta_2$$

(specified with the RelativeSecondDerivativeThreshold parameter)

Large residual warnings

At the end of every time step, DASOLV examines the equation which has the largest residual in magnitude, and records an estimate of the error committed in each variable x_i in this equation. To do this it uses the value of the Jacobian element with respect to that variable (i.e. the partial derivative of the equation w.r.t. x_i), to estimate the change δ_i that would be needed in that variable in isolation to bring the residual to zero. The specific measure used is $|\delta_i|/\max(|x_i|, |x_i + \delta_i|)$, i.e. the size of the change relative to either the actual value or the value which would remove the residual, whichever is greater. This is referred to as the error measure for that variable.

The most important consideration for a given equation is then the *smallest* error measure. The reason for this is that if the residual can be brought to zero by a very small change in any variable, a larger error measure for another variable is relatively meaningless.

At the end of the integration, when the smallest error measure in the equation with the largest residual on any single time step exceeds the threshold $\text{convtol} * 10$, this single equation is reported¹². All such residuals are reported as follows:

- First the residual and time are indicated.
- The smallest error measure and the variable concerned are displayed in parentheses.
- The equation itself is then displayed.
- This is followed by a table containing a row for each variable in the equation, indicating its name, value at the time, Jacobian element value at the time, the value of δ_i as described above, and the error measure in the form of a percentage.

Note that if one or more singular Jacobians were observed during the solution, all equations where the smallest error measure exceeds $\text{convtol}/10$ (i.e. 100 times more sensitive than the normal case) are reported, since this situation has been found to lead to problems with variable values.

¹²Note that the tolerance used in the test, convtol , is taken from DASOLV's ReinitialisationNLSolver. This is done in order to relate the error acceptable at an integration step to the error that might be committed when reinitialising the system at a discontinuity.

Also, if the DASOLV solution parameter Diag is set to true, the threshold used for this test is 10^{-8}

In these cases where more than one residual is reported, the list is displayed in descending order of error measure, so that the first entries are likely to be the most significant.

The SRADAU solver

The algorithmic parameters used by SRADAU along with their default values are shown below. This is followed by a detailed description of each parameter.

```

"SRADAU" [ "InitialisationNLSolver"           := "BDNLSOL";
            "LASolver"                   := "MA48";
            "ReinitialisationNLSolver"   := "BDNLSOL";
            "AbsoluteTolerance"          := 1E-5;
            "Diag"                      := FALSE;
            "MaxStepSize"                := 1.0E10;
            "EventTolerance"             := 1E-5;
            "OutputLevel"                := 0;
            "RelativeTolerance"          := 1E-5;
            "VariablesWithLargestCorrectorSteps" := 0 ]

```

- InitialisationNLSolver: A quoted string specifying a nonlinear algebraic equation solver.

The solver to be used for the solution of nonlinear algebraic equations occurring at the initialisation stage of the integration. This can be either one of the standard gPROMS nonlinear algebraic equation solver or a third-party nonlinear algebraic equation solver (see the gPROMS System Programmer Guide). The default is BDNLSOL. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- LASolver: A quoted string specifying a linear algebraic equation solver.

The solver to be used for the solution of linear algebraic equations at each step of the integration. This can be either one of the standard gPROMS linear algebraic equation solvers or a third-party linear algebraic equation solver (see the gPROMS System Programmer Guide). The default is MA48. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- ReinitialisationNLSolver: A quoted string specifying a nonlinear algebraic equation solver.

The solver to be used for the solution of nonlinear algebraic equations that is necessary for re-initialisation following discontinuities. This can be either one of the standard gPROMS nonlinear algebraic equation solvers or a third-party nonlinear algebraic equation solver (see the gPROMS System Programmer Guide). The default is SPARSE. This parameter can be followed by further specifications aimed at configuring the particular solver by setting values to its own algorithmic parameters.

- AbsoluteTolerance: A real number in the range $[10^{-20}, 10^{10}]$.

The absolute integration tolerance. Together with the parameter RelativeTolerance (see below), they determine whether or not a time step taken by the solver is sufficiently accurate.

- Diag: A boolean value.

Specifies whether very detailed diagnostic information is to be generated during integration.

- EventTolerance: A real number in the range $[10^{-20}, 10^{10}]$.

The event tolerance, i.e. the maximum time interval within which discontinuities during integration are located.

- MaxStepSize: A real number in the range $[10^{-20}, 10^{100}]$; default = 10^{10} .

This Solution Parameter sets the maximum step size used by the integrator when advancing in time.

- OutputLevel: An integer in the range [0, 4].

The amount of information generated by the solver. The following table indicates the lowest level at which different types of information are produced:

0	(None)
1	(Re-)initialisation times, projection of predictor onto bounds, variables hitting bounds
2	Successful initialisation, change of branch in IF conditional equations, location of discontinuities, step failures, repeated convergence failures, predictor outside bounds, predictor step reduction, variables stuck on bounds
3	Detail of convergence failures, values of derivatives on commencing integration, number of perturbation groups, step length reduction due to bounds violation
4	Variable causing discontinuity, detail of perturbation groups

- RelativeTolerance: A real number in the range $[10^{-20}, 10^{10}]$.

The relative integration tolerance. Together with the parameter AbsoluteTolerance (see above), they determine whether or not a time step taken by the solver is sufficiently accurate.

- VariablesWithLargestCorrectorSteps: An integer between 0 and 1000; default = 0.

On rare occasions, SRADAU fails with a "corrector step failure" message. This indicates that the code is unable to establish a set of variable values that satisfy the system equations at a particular point. It is often caused by errors or bad scaling in some modelling equations which results in the corrector iterations taking excessively large steps in some of the variables. To help with the diagnosis of such problems, SRADAU can report the variables with the largest relative change at each corrector iteration. The relative change for a variable X is defined as:

$$\frac{\delta X}{a + r|X|}$$

where:

- δX is the step in the variable at this corrector iteration;
- a is the absolute tolerance;
- r is the relative tolerance.

The parameter VariablesWithLargestCorrectorSteps specifies the number of variables to be reported in this manner. Note that such reporting takes place only if the parameter OutputLevel is set to a value of 0 or higher.

An example of the output is shown below:

```
Variables with largest (weighted) corrector steps follow...
```

```
Differential and algebraic variables (norm = 227.542):
```

Variable	Name	Current Value	Corrector Step	Weight
----------	------	---------------	----------------	--------

Controlling the Execution
of Model-based Activities

1	Plant.Reactor.STR.rho_L	12126	548.071
2	Plant.Reactor.STR.c(5)	12126	548.071
3	Plant.Reactor.STR.vol_L	0.000824675	-3.72737E-05
4	Plant.Reactor.STR.q_Loss	0.00692394	-6.05969E-06
5	Plant.Reactor.STR.ThermoHL.hli(2)	-5.12137E-10	-1.41695E-06

Algebraic variables only (norm = 250.308):

Variable	Name	Current Value	Corrector Step	Weight
1	Plant.Reactor.STR.rho_L	12126	548.071	
2	Plant.Reactor.STR.c(5)	12126	548.071	
3	Plant.Reactor.STR.vol_L	0.000824675	-3.72737E-05	
4	Plant.Reactor.STR.q_Loss	0.00692394	-6.05969E-06	
5	Plant.Reactor.STR.ThermoHL.hli(2)	-5.12137E-10	-1.41695E-06	

The output is grouped in terms of differential and algebraic Variables and only algebraic Variables. In each case, a norm value is also reported. For differential and algebraic variables, this is defined by:

$$norm = \sqrt{\frac{1}{N} \sum_{i=1}^N \left(\frac{X_i}{a+rX_i} \right)^2},$$

where N is the number of equations. Subsequent lines list the largest VariablesWithLargestCorrectorSteps Variables and their relative changes.

For algebraic Variables only, then norm is similarly defined:

$$norm_{alg} = \sqrt{\frac{1}{N_{alg}} \sum'_i \left(\frac{X_i}{a+rX_i} \right)^2},$$

where N_{alg} is the number of algebraic Variables and the summation is over only the algebraic Variables. Again, a list of the algebraic variables with the largest corrector steps then follows.

Chapter 15. Model Analysis and Diagnosis

At the start of each simulation, gPROMS analyses the mathematical model so as to assist the user in identifying structural problems and errors in the modelling and/or the problem specification. In particular, gPROMS attempts to determine:

- if the model is well-posed and whether alternative specifications are required for the degrees-of-freedom;
- if the underlying set of differential and algebraic equations is of index exceeding 1; and
- if the initial conditions are inconsistent.

These structural problems are considered in more detail in this section.

Well-posed models and degrees-of-freedom

In order for gPROMS to solve the underlying equation system associated with a given simulation, the model must be well-posed and all degrees-of-freedom must be specified correctly. If there are too many or too few assignments for the degrees-of-freedom then gPROMS will issue an error upon instantiation and state that the equations system is over-specified or under-specified respectively. As a user you should then analyse the suggestions regarding specifications and take the necessary action to ensure the equation system is correctly specified.

Case I: over-specified systems

An over-specified system is one which either itself consists of more equations than unknown variables, or involves an over-specified sub-set of equations and unknowns. Mathematically, it can be shown that *any* over-specified system will contain at least one sub-system involving k equations in only $(k-1)$ distinct unknowns. gPROMS identifies this sub-system and, where appropriate, offers informed suggestions on which Assignments may be responsible for the over-specification. As a simple example of this, consider the gPROMS input shown in the gPROMS code below:

Example 15.1. Illustrative example: over-specified system

```
#=====
#MODEL mod1

VARIABLE
  x1, x2, y1, y2 AS NoType

EQUATION
  $x1 = x1*y1 ;
  $x2 = x1 + x2*y1 + y2 ;
  x1^2 = y2 ;
  0 = y1 - y2 ;

#=====
#PROCESS proc

UNIT
  mymod      AS mod1

ASSIGN
  WITHIN mymod DO
    y2 := 3 ;
  END #within

INITIAL
  WITHIN mymod DO
    x1 = 0 ;
    x2 = 0 ;
  END #within

SOLUTIONPARAMETERS
  ReportingInterval := 1 ;

SCHEDULE
  CONTINUE FOR 10
```

It is easy to see that MODEL mod1 consists of 4 equations in 4 variables, one of which, y2, is Assigned in the PROCESS proc. Execution of the PROCESS proc leads to the following diagnostic message:

```
Executing process PROC...
All 4 variables will be monitored during this simulation!
Building mathematical problem description took 0.014 seconds.
Loaded MA48 library
Execution begins....
Variables
  Known          :      1
  Unknown        :      3
  Differential   :      2
  Algebraic      :      1
```

```
Model equations      :      4
Initial conditions :      2
```

Checking consistency of model equations and ASSIGN specifications...

```
ERROR: Part of your problem is over-specified.
The following 3 equation(s) involve only 2 unknown variable(s).
    Model Equation      1: MYMOD.$X1 = MYMOD.X1 * MYMOD.Y1 ;
    Model Equation      3: MYMOD.X1^2 = MYMOD.Y2 ;
    Model Equation      4: 0 = MYMOD.Y1 - MYMOD.Y2 ;
```

The 2 unknown(s) occurring in these 3 equations are:

```
MYMOD.Y1 (ALGEBRAIC)
MYMOD.X1 (STATE)
```

The problem may have been caused because you ASSIGNED the
following variable(s):

```
    MYMOD.Y2 (INPUT)
```

Initialisation calculation failed.

Execution of PROC fails prematurely.

gPROMS identifies the over-specified sub-system of 3 equations in 2 unknown variables and suggests that the Assignment of the variable y2 is causing the problem. UnAssigning this variable leads to a working simulation.

Case II: under-specified systems

An under-specified system has more unknown variables than equations. In this case, gPROMS diagnoses the problem and provides a list of candidate variables for Assignment (while advising against Assigning differential variables). This is illustrated by the gPROMS code below:

Example 15.2. Illustrative example: under-specified system

```
#=====
#MODEL mod1

VARIABLE
  x1, x2, y1, y2, y3           AS NoType

EQUATION
  $x1 = x1*y1 ;
  $x2 = x1 + x2*y1 + y2 + 3*y3 ;
  x1^2 = y2 ;
  0 = y1 - y2 ;

#=====
#PROCESS proc

UNIT
  mymod    AS mod1

INITIAL
  WITHIN mymod DO
    x1 = 0 ;
    x2 = 0 ;
  END #within

SOLUTIONPARAMETERS
  OutputLevel := 2 ;
  gRMS := OFF ;
  ReportingInterval := 1 ;

SCHEDULE
  CONTINUE FOR 10
```

gPROMS issues the following message upon execution of the PROCESS proc:

Executing process PROC...

All 5 variables will be monitored during this simulation!

Building mathematical problem description took 0.001 seconds.

Loaded MA48 library
Execution begins....

Variables
 Known : 0
 Unknown : 5
 Differential : 2
 Algebraic : 3

 Model equations : 4
 Initial conditions : 2

Checking consistency of model equations and ASSIGN specifications...

```
ERROR: Your problem is underspecified.  
You need to ASSIGN 1 of the following unknown variables:  
      MYMOD.X2 *** Not recommended ***  
      MYMOD.Y3
```

Initialisation calculation failed.

Execution of PROC fails prematurely.

Assigning the algebraic variable y3 leads to a well-posed system.

High-index DAE systems

Consistent initialisation of DAE systems is often related to their *index*. The index of a DAE system is defined as the minimum number of differentiations with respect to time that are necessary in order to obtain the time derivatives of *all* variables, i.e. to reduce the system to a set of ordinary differential equations (ODEs). Index-1 systems are generally very similar to ODEs in that the number of initial conditions that can be specified arbitrarily is equal to the number of differential variables in the system, all the differential variables may be given arbitrary initial values, and similar numerical methods can be used for the solution of the system. On the other hand, in "high-index" DAEs (index > 1), the number of initial conditions that can be specified arbitrarily may be *less than* the number of differential variables, the differential variables are not independent and ODE-type numerical methods may fail.

This section comprises:

- an overview of the cause of indices higher than 1 and their potential complications;
- the diagnostics, structural analysis and model manipulation performed by gPROMS to identify, report and rectify problems with high index; and
- a more detailed explanation of high index, with examples.

Origin of index and the initialisation of DAEs

Most DAE systems follow the rule that the number of initial conditions specified must be equal to the number of differential variables in the system. This is true for ODEs as well. Although the initial conditions do not need to be specified directly in terms of the differential variables (e.g. the internal energy may be a differential variable in an energy balance but the initial condition may be a temperature specification), they must be specified *consistently* (more details on specifying initial conditions can be found in the Initial section and how to ensure they are specified consistently).

However, for certain "high index" DAE systems, this is not the case. For example, if one or more algebraic equations only include differential variables, this will reduce the number of degrees of freedom in the initial conditions, since all of the initial values of the differential variables cannot be specified independently. Not only does this make initialisation difficult, but it also causes problems for the DAE solver.

These high-index DAE systems can arise in a number of process-engineering applications. Some typical examples are:

- Constant-volume mixer
- Heater
- Chemical equilibrium

A more thorough description of these is given here.

To date, the only way around these problems has been to identify the algebraic equations that cause the complications, differentiate them with respect to time to generate additional constraints on the initial conditions and then specify a reduced number of initial conditions consistent with these constraints. The DAE system is augmented with these additional differential equations and solved.

gPROMS performs the following analysis automatically:

- determine the index of the set of equations
- identify the causes (if any) of high index
- identify remedial modifications to the equations
- identify constraints on the initial conditions

These automatic index-reduction procedures are described next.

For the interested reader, more details on the causes of high index, its implications on the solution of the DAE system and how it can be avoided or rectified are given here. However, it is not essential to read this section.

Constant-volume mixer example

This is an example where a simplification to an index-1 system results in a high-index system. The following is the EQUATION section of a gPROMS Model of a constant-volume mixing tank.

```
EQUATION
  FOR i := 1 TO NoComp DO
    $M(i) = SIGMA( F_in*x_in(i,) ) - F_out*x(i) ;
  END
  M_total = SIGMA(M) ;
  rho*V = M_total ;
  rho = PhysProp.Density(T, P, x) ;
  x = M/M_total ;
  F_out = alpha*(P - P_out) ;
```

where $M(i)$ is the molar holdup of component i ; M_{total} the total molar holdup; $F_{in}(j)$ is the flowrate of inlet j ; F_{out} the outlet flowrate; $x(i)$ and $x_{in}(i,j)$ are the mole fractions in the mixer and inlet j , respectively; ρ is the density of fluid in the tank; V the volume of the tank (specified); $PhysProp.Density(T, P, x)$ is a physical-property foreign-object method returning the density of a mixture given its temperature, T , pressure, P , and mole fractions x ; P_{out} is the exit pressure (specified); and finally α is a constant.

The above model is a fairly straightforward index-1 system that can easily be solved. If, however, we were to simplify the model by considering only liquid feeds and using a different physical property: $LiquidDensity(T,x)$, we would find that the model could no longer be solved using standard codes.

Heater example

This example illustrates how a very simple model can still become high index, given the wrong input specification. This is a model of a well-stirred tank used to heat a single-component stream.

```
EQUATION
  rho*V*$u = F*(h_in - h) + Q ;
  u = PhysProp.InternalEnergy(T) ;
  h = PhysProp.Enthalpy(T) ;
```

here, F is the flowrate of material through the heater; ρ is the density of the fluid; V the volume of the tank; u and h are the internal energy and enthalpy, respectively, of the material in the tank; h_{in} is the inlet enthalpy; $PhysProp.InternalEnergy(T)$ and $PhysProp.Enthalpy(T)$ are physical-property foreign-object

methods returning the internal energy and enthalpy of a single component given its temperature, T ; and finally Q is rate of heating. ρ , V , F and h_{in} are all given.

To complete the model, the variable Q must be specified. If the heating was being provided by a steam jacket, then Q can be determined using a suitable heat-transfer law. Alternatively, electric heating can be modelled simply by specifying the value of Q over time, e.g. $Q = Q(t)$. In either of these cases, the model can be solved easily. Since there is one differential variable, u , we can provide an initial condition for it, $u(0)$. We can now calculate $T(0)$ from the second equation and $h(0)$ from the third. Now the first equation can be used, along with the initial value of Q , to calculate $u(0)$, completing the initialisation problem.

However, what if we wanted to know what heating profile would provide a given temperature profile? We may, then, choose to release the specification on Q and provide one for T . Given the same initial specification, $u(0)$, we can still calculate $T(0)$ from the second equation and $h(0)$ from the third. Immediately, we can see that there is a problem, because our calculated $T(0)$ may not be the same as the $T(0)$ specified. Another problem is that there is only one equation left, in the two unknowns, $u(0)$ and Q . There is no way to solve the problem!

Chemical-equilibrium example

In this example, we have a batch-reactor model with reversible reactions at equilibrium. The general material balance for this problem is:

```
FOR i := 1 TO NoComp DO
  $M(i) = V*SIGMA( r*nu(i,) ) ;
END
```

where, $M(i)$ is the molar holdup of component i , V is the volume of the reaction mixture, $r(j)$ is the rate of reaction j and $nu(i,j)$ is the stoichiometric coefficient of component i in reaction j .

There is no difficulty in solving this problem (with appropriate definitions of the new variables introduced) if the rates of reaction are specified using an equation similar to the following:

```
FOR j := 1 TO NoReac DO
  r(j) = k(j)*PRODUCT( C^ReactionPartialOrder(,j) ) ;
END
```

where $k(j)$ is the rate constant for reaction j , $C(i)$ is the molar concentration of component j and $ReactionPartialOrder(i,j)$ is the partial order of component i in reaction j .

This model can be used for irreversible and reversible reactions where the rate expressions are known. E.g., for reversible reactions, simply treat the forward and reverse reactions as entirely separate reactions, with their own rate constants.

However, it is often not possible (nor useful) to measure the rates of fast reversible reactions; usually only an equilibrium constant is known, and so we may have *instead of a rate expression* a relationship similar to the following:

```
EqmConst(1) = C(2)/C(1)^2 ;
```

where the equilibrium constant, $EqmConst$, is given. It is clear now that we have a problem, because some of the $r(j)$ variables only appear in the differential equation for the material balance. There is no way to calculate the $r(j)$ associated with the reactions at equilibrium and so the problem cannot be solved. This is a typical cause of high index: algebraic variables only occurring in differential equations.

Also of note is that the equation above introduces a relationship between the concentrations of some of the species in the problem, and therefore also the molar holdups. So it is clear that we cannot specify arbitrary initial conditions for all of the components, as they are not all independent.

Automatic index reduction in gPROMS

gPROMS is able to reduce the index of problems automatically. However, it initially reports problems of high index and informs the user how to turn on index reduction. Index reduction is off by default because it is usually

better to develop index-1 models rather than rely on gPROMS to reduce the index automatically, since the index reduction techniques can be quite computationally intensive.

To illustrate automatic index reduction, consider the following model of a heater.

```
EQUATION
$HoldUp = Fin - Fout ;
$U = Fin*hin - Fout*h + Q ;
U = Holdup*h - P*TotalVolume ;
P * TotalVolume = Holdup * R * T ;
Fout = alpha * Holdup ;
h = hr + Cp*(T - Tr) ;
hin = hr + Cp*(Tin - Tr) ;
```

When the following process is executed, gPROMS can solve the problem with no difficulty.

```
UNIT
T101 AS Heater

SET
WITHIN T101 DO
Cp      := 1.121 * 28.013 ;
hr      := 0.0          ;
Tr      := 298.15       ;
R       := 0.082        ;
alpha   := 1           ;
END

ASSIGN
WITHIN T101 DO
Fin    := 10          ;
Tin    := 600         ;
P      := 5           ;
Q      := 10          ;
END

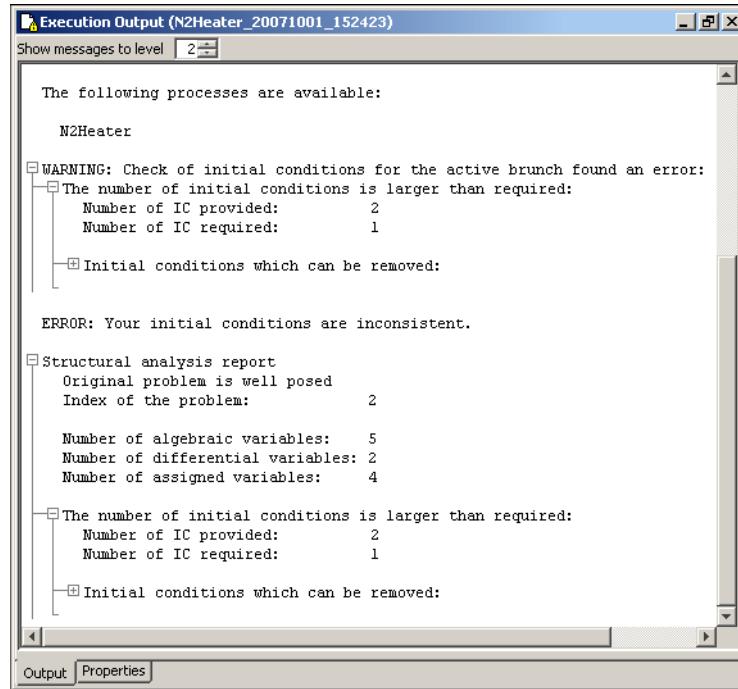
INITIAL
WITHIN T101 DO
HoldUp     = 0.5 ;
TotalVolume = 4    ;
END
```

However, if we replace the Assignment of Q with one on T:

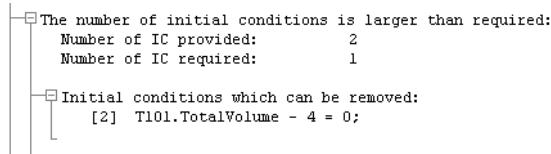
```
ASSIGN
WITHIN T101 DO
Fin    := 10          ;
Tin    := 600         ;
P      := 5           ;
T      := 487.8049   ;
END

INITIAL
WITHIN T101 DO
HoldUp = 0.5 ;
TotalVolume = 4 ;
END
```

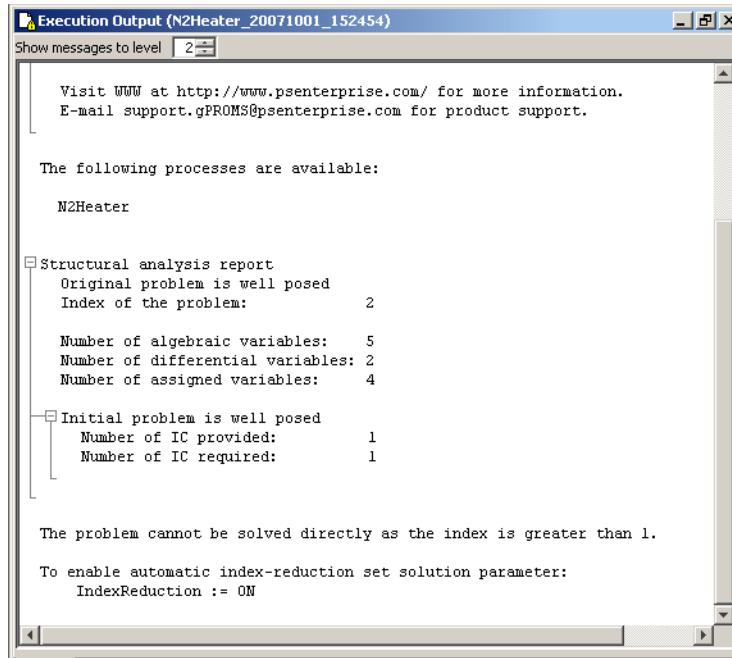
we will get a high-index problem (see the Heater Example) and gPROMS will give the following output.

Figure 15.1. gPROMS diagnostics for a high-index problem

Click on the "+" symbol to see which initial condition should be removed:

Figure 15.2. The initial condition that needs to be removed

Now, by removing this initial condition, gPROMS reports that the correct number of conditions are specified but that the index of the system is 2 and cannot be solved directly.

Figure 15.3. gPROMS diagnostics for a high-index problem

To enable the automatic index reduction, copy the suggested Solution Parameter into the Process as below.

```
ASSIGN
WITHIN T101 DO
    Fin := 10      ;
    Tin := 600     ;
    P    := 5       ;
    T   := 487.8049 ;
END

INITIAL
WITHIN T101 DO
    HoldUp      = 0.5 ;
END

SOLUTIONPARAMETERS
IndexReduction := ON ;
```

Now, with index reduction enabled, gPROMS is able to reduce the problem to index 1 and solve it. The replacements made during the reduction are shown in the output:

Figure 15.4. gPROMS output after automatic index reduction

The screenshot shows the 'Execution Output' window for the model 'N2Heater_20071001_152507'. The output details the structural analysis report, initial problem status, index reduction process, system of equations, and variables after reduction.

```

Structural analysis report
Original problem is well posed
Index of the problem: 2

Number of algebraic variables: 5
Number of differential variables: 2
Number of assigned variables: 4

Initial problem is well posed
Number of IC provided: 1
Number of IC required: 1

Index reduction performed successfully
Index of the problem: 1

Number of algebraic variables: 9
Number of differential variables: 1
Number of assigned variables: 4

System of equation to solve after index reduction:
Derived from No diff.
Eqn original eqn over time Full form of the equation
=====
[1] [1] 0 T101.HoldUp' - (T101.Fin - T101.Fout) =
[2] [2] 0 $(T101.U) - (T101.Fin * T101.hin - T101.
[3] [3] 0 T101.U - (T101.HoldUp * T101.h - T101.I
[4] [4] 0 T101.P * T101.TotalVolume - T101.HoldUp
[5] [5] 0 T101.Fout - T101.HoldUp = 0;
[6] [6] 0 T101.h - 31.4026 * (T101.T - 298.15) =
[7] [7] 0 T101.hin - 31.4026 * (T101.Tin - 298.15
[8] [3] 1 $(T101.U) + ((0 - (T101.h)) * T101.Ho
[9] [4] 1 T101.P * T101.TotalVolume' + ((0 - (0.0
[10] [6] 1 T101.h' = 0;

Variables after index reduction:
Var Original Diff Name Type
=====
[1] [1] 0 T101.Fin I(input)
[2] [2] 0 T101.Fout A(algebraic)
[3] [3] 0 T101.HoldUp A
[4] [4] 0 T101.TotalVolume A
[5] [5] 0 T101.P I
[6] [6] 0 T101.T I
[7] [7] 0 T101.Tin I
[8] [8] 0 T101.h A
[9] [9] 0 T101.hin A
[10] [10] 0 T101.U Differential
[11] [11] 0 T101.Q A
[12] [3] 1 T101.HoldUp' A
[13] [4] 1 T101.TotalVolume' A
[14] [8] 1 T101.h' A

```

After giving the above output, gPROMS continues to integrate the model as normal, since the index has now been reduced to 1.

The above example can be found in the gPROMS Project `highindex_N2_heater.gPJ` in the examples subdirectory. Please note that in the Project two Processes are present: one which specifies the temperature T as in the explanation above. In the other Process, `Specify_Q`, the heat load is specified rather than the temperature. This specification has been chose to demonstrate that the index does not only depend on the equations but also on the chosen degrees of freedom. A more detailed explanation is given in the mathematical analysis of the heater model.

Limitations

Currently, the following limitations exist for Models and Processes to which automatic index reduction can be applied

- When the Index-Reduction code detects that an equation inside an IF or CASE block needs to be differentiated to reduce the index, gPROMS will issue an error message and stop executing the simulation shortly after system construction. Supporting such models in index reduction may be added in future releases.

- The index may change during the execution of an activity when an IF or CASE branch switches. This is currently not supported. When running a problem with `IndexReduction := ON`, this change (following any type of switch) will be detected and will terminate the activity with an error message indicating the reason for the termination.

Please note that it is possible to use solver settings for which the index analysis is ignored. In this case the gPROMS solver may proceed with simulating a high-index problem without error messages but the results may be incorrect.

High-index DAEs, initialisation and integration

This section is aimed at the interested reader who would like a more detailed mathematical analysis of the causes of high index and how it may be avoided or remedied. None of the content here is required for an understanding of how gPROMS reports and rectifies high-index problems, so it is safe to ignore this section. However, a thorough understanding of index is likely to be beneficial for any modeller of chemical (or of many other) processes. Furthermore, although gPROMS can reformulate most high-index problems automatically, this can be quite computationally intensive, so it is preferable to reduce any high-index models to index 1 by hand.

The following are considered:

- A simple example of an index-1 DAE system
- Simple examples of high-index DAE systems
- Index classification of DAE systems
- Integration of high-index DAE systems
- High-index DAEs in process-engineering applications

A simple example of an index-1 DAE system

It can be shown that most DAE systems of the form:

$$f(x, \dot{x}, y, u) = 0 \quad (1a)$$

$$g(x, y, u) = 0 \quad (1b)$$

are similar to ODEs in several ways. In particular, one can specify as many arbitrary initial conditions as there are differential variables x in the system. Moreover, give values for x , we can solve 1b for y (usually numerically), then substitute y in 1a, essentially converting 1a to a set of ODEs in x .

These points can be illustrated with a simple example:

$$\dot{x}_1 = x_1 + 2x_2 - y \quad (2a)$$

$$\dot{x}_2 = x_1 - x_2 + 2y \quad (2b)$$

$$0 = x_1 + x_2 - y \quad (2c)$$

Here we have two differential variables and one algebraic variable. We can clearly specify two arbitrary initial conditions, e.g.:

$$x_1(0) = 1; x_2(0) = 1 \quad (3)$$

from which we can calculate:

$$y(0) = 2; \dot{x}_1(0) = 1; \dot{x}_2(0) = 4 \quad (4)$$

In fact, we can use 2c to eliminate y from 2a and 2b, yielding:

$$y = x_1 + x_2 \Rightarrow \begin{cases} \dot{x}_1 = x_2 \\ \dot{x}_2 = 3x_1 + x_2 \end{cases} \quad (5)$$

which is simply a set of two ODEs in x_1 and x_2 . Overall, then, the DAE system 2 behaves very similarly to an ODE one.

Simple examples of high-index DAE systems

In this section, two examples of high-index systems are described.

Consider, for this first example, a slightly modified version of the index-1 system (2) described previously:

$$\dot{x}_1 = x_1 + 2x_2 - y \quad (6a)$$

$$\dot{x}_2 = x_1 - x_2 + 2y \quad (6b)$$

$$0 = x_1 + x_2 \quad (6c)$$

the only difference being between 2c and 6c.

We immediately note that we can no longer specify arbitrary initial values for the differential variables $x_1(0)$ and $x_2(0)$ since they have to satisfy 6c. Furthermore, we cannot convert 6 to a set of ODEs in x_1 and x_2 by using 6c to eliminate y from 6a and 6b since y does not even occur in 6c!

It can be shown that initial conditions for DAE systems (1) do not necessarily have to be specified in terms of the differential variables x . This might seem to imply that, although we cannot specify both $x_1(0)$ and $x_2(0)$, perhaps we could specify some other combination of two variables, for instance:

$$x_1(0) = 1; y(0) = 0 \quad (7)$$

Then from 6c, we would get $x_2(0) = -1$ and from 6a and 6b:

$$\dot{x}_1(0) = -1; \dot{x}_2(0) = 2 \quad (8)$$

This, however, is not correct. We note, in particular, that 6c is valid at all times $t \geq 0$. We can therefore derive a valid equation by differentiating 6c with respect to time:

$$0 = \dot{x}_1 + \dot{x}_2 \quad (9)$$

Now, 9 is valid at all times $t \geq 0$, so, in particular, it should hold at $t = 0$:

$$0 = \dot{x}_1(0) + \dot{x}_2(0) \quad (10)$$

which is *not* satisfied by our initial condition 8. Thus the latter is, in fact, inconsistent.

In fact, 6 and 9 form a set of 4 independent consistency relations that the initial variable values must satisfy:

$$\begin{aligned} \dot{x}_1(0) &= x_1(0) + 2x_2(0) + y(0) \\ \dot{x}_2(0) &= x_1(0) - x_2(0) + 2y(0) \\ 0 &= x_1(0) + x_2(0) \\ 0 &= \dot{x}_1(0) + \dot{x}_2(0) \end{aligned} \quad (11)$$

Since these involve 5 variables, we can specify only 1 (=5-4) arbitrary initial condition, which is less than the number of differential variables (2) in the system 6.

Now, for the second example, consider a slight modification of 6:

$$\dot{x}_1 = x_1 + 2x_2 - y \quad (12a)$$

$$\dot{x}_2 = x_1 - x_2 + 2y \quad (12b)$$

$$0 = 2x_1 + x_2 \quad (12c)$$

By differentiating 12c with respect to time, we get:

$$0 = 2\dot{x}_1 + \dot{x}_2 \quad (13)$$

which, together with system 12 yields 4 consistency relations that the initial variable values must satisfy. So, once again, it appears that we can specify 1 ($= 5 - 4$) arbitrary initial condition. However, if we combine 13 with 12a and 12b, we obtain:

$$0 = 3x_1 + 3x_2 \quad (14)$$

which is also valid at all times. We can therefore differentiate this with respect to time to obtain:

$$0 = \dot{x}_1 + \dot{x}_2 \quad (15)$$

We now have 5 consistency relations 12, 13 and 14 that the 5 initial variable values must satisfy — in fact, there is no freedom left with respect to the specification of initial conditions. The *only* possible initial condition for the system is:

$$x_1(0) = x_2(0) = y(0) = \dot{x}_1(0) = \dot{x}_2(0) = 0 \quad (16)$$

Overall, what we have seen is that the three example systems 2, 6 and 12, albeit ostensibly very similar, are, in fact, quite different. Perhaps a natural question to ask at this point is:

Are there some further consistency relations also hidden within 2?

Of course, we can easily obtain a valid relation by differentiating 2c with respect to time:

$$0 = \dot{x}_1 + \dot{x}_2 - \dot{y} \quad (17)$$

However, this does not impose any further restrictions on both $\dot{x}_1(0)$ and $\dot{x}_2(0)$ since it also involves a new variable $\dot{y}(0)$.

Similarly, in the case of system 6, we could combine 9 with 6a and 6b to yield:

$$0 = 2x_1 + x_2 + y \quad (18)$$

and then differentiate this with respect to time to obtain:

$$0 = 2\dot{x}_1 + \dot{x}_2 + \dot{y} \quad (19)$$

but, once again, this does not actually restrict $\dot{x}_1(0)$ and $\dot{x}_2(0)$.

Overall, our original conclusions regarding the initial conditions of 2 and 6 were correct.

We can summarise what we have seen so far with reference to the general DAE system 1, as follows:

- A set of initial values $\{x(0), \dot{x}(0), y(0)\}$ must always satisfy:

$$f(x(0), \dot{x}(0), y(0), u(0)) = 0$$

$$g(x(0), y(0), u(0)) = 0$$

- For some systems, the values $\{x(0), \dot{x}(0), y(0)\}$ may also have to satisfy additional relations obtained by differentiating 1 one or more times with respect to time.

Index classification of DAE systems

The issue of consistent initialisation of DAE systems is closely related to their classification according to their *index*. The index of 1 can be defined as the minimum number of differentiations with respect to time that are necessary to obtain the time derivative of *all* variables (*i.e.* both \dot{x} and \dot{y}) in terms of x and y — *i.e.* to reduce the system to a set of ODEs.

We can apply this definition to 2: to obtain \dot{y} , we differentiate 2c with respect to time; this yields 17 which, together with 2a and 2b, leads to:

$$\dot{y} = 2x_1 + x_2 + y \quad (20)$$

We note that 2a, 2b and 20 form a set of 3 ODEs in x_1 , x_2 and y . Since one differentiation was sufficient to reduce 2 to an ODE system, we conclude that 2 is an index-1 system.

In the case of system 6, differentiating 6c with respect to time led to 9 which, combined with 6a and 6b, yielded 18. A second differentiation led to 19 which, when combined with 6a and 6b yields:

$$\dot{y} = -3(x_1 + x_2) \quad (21)$$

This, together with 6a and 6b, form a set of ODEs in x_1 , x_2 and y . Since two differentiations were needed to reduce 6 to an ODE system, we conclude that 6 is an index-2 system.

Finally, in the case of system 12, two differentiations with respect to time yielded 15. To obtain \dot{y} , we need to combine 15 with 12a and 12b and differentiate the result with respect to time to get:

$$\dot{y} = -2\dot{x}_1 - \dot{x}_2 = -3(x_1 + x_2) \quad (22)$$

Since three differentiations were necessary, 12 is an index-3 system.

By the definition of index, ODE systems are classified as "index-0". Usually, index-1 systems are very similar to ODEs with respect to the number of initial conditions that can be specified arbitrarily and the behaviour of numerical solution methods.

On the other hand, DAE systems of index 2 or higher are different. We have already seen the fact that their consistent initialisation requires taking into account additional "hidden" relations that can be obtained from the original equations via differentiation — and hence the number of arbitrary initial conditions is reduced accordingly.

Integration of high-index DAE systems

A further complication with DAE systems of high index is that the usual numerical algorithms are generally incapable of controlling the error of integration, and this very often leads to failure, or, even worse, spurious solutions!

For these reasons, DAE systems of index higher than 1 are usually solved by reducing their index to 1 via differentiation with respect to time. For instance, the index-2 system 6 can be reduced to the index-1 system:

$$\dot{x}_1 = x_1 + 2x_2 - y \quad (23a)$$

$$\dot{x}_2 = x_1 - x_2 + 2y \quad (23b)$$

$$0 = \dot{x}_1 + \dot{x}_2 \quad (23c)$$

by differentiating 6c with respect to time. Note that it is not necessary to combine 23c with 23a and 23b to obtain a purely algebraic equation. System 23 can then be solved using standard algorithms and codes.

Of course, one immediate question is: "Will the solution of 23 be the same as the solution of 6? More specifically, will the solution of 23 satisfy equation 6c, which has now been replaced by its time differential 23c?". The answer is: "Yes, provided the initial conditions satisfy the consistency relations 11."; in this case,

- the initial value of the quantity $x_1 + x_2$ is zero
- the time gradient of $x_1(t) + x_2(t)$ is zero for all times $t \geq 0$ (*cf.* equation 23c)

and, therefore, $x_1(t) + x_2(t) = 0$ for all $t \geq 0$ — hence 6c is satisfied — at least in the exact mathematical sense.

A complication arises from the fact that, if system 23 is solved *numerically* (rather than exactly), then equation 23c will be satisfied only within a certain specified accuracy and not exactly. Over long time horizons, this may allow $x_1(t) + x_2(t)$ to deviate significantly from its correct value of 0. A way of avoiding this "drift" is to include both 6c and 23c in the set of equations being integrated, thereby making sure that both of them are satisfied to the required accuracy. However, this leads to redundancy since now we have 4 equations in the 3 unknowns $x_1(t)$, $x_2(t)$ and $y(t)$. One way of resolving this redundancy is to treat \dot{x}_1 and x_1 as completely distinct variables — effectively introducing an extra variable in the system:

$$\bar{x}_1 = x_1 + 2x_2 - y \quad (24a)$$

$$\dot{x}_2 = x_1 - x_2 + 2y \quad (24b)$$

$$0 = x_1 + x_2 \quad (24c)$$

$$0 = \bar{x}_1 + \dot{x}_2 \quad (24d)$$

Here \bar{x}_1 is a new variable bearing no relation to x_1 as far as the numerical solution is concerned. This is now an index-1 system that can be solved to arbitrary accuracy using standard codes.

High-index DAEs in process-engineering applications

This section is concerned with a detailed mathematical analysis of the following three examples of high-index DAEs in process-engineering applications.

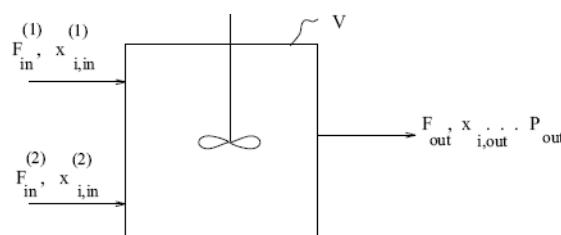
- Fixed Volume Mixing Tank
- Heater Tank
- Chemical Equilibrium

Some conclusions of the analysis are given here.

Fixed-volume mixing tank

We consider the well-stirred tank, shown in the figure below, used to mix two streams under isothermal conditions.

Figure 15.5. Constant-volume mixer tank



The mathematical model of the system is:

$$\frac{dM_i}{dt} = F_{in}^{(1)}x_{i,in}^{(1)} + F_{in}^{(2)}x_{i,in}^{(2)} - F_{out}x_i, \quad i = 1, \dots, c \quad (25)$$

$$M_T = \sum_{i=1}^c M_i \quad (26)$$

$$\rho V = M_T \quad (27)$$

$$\rho = \rho(T, P, x) \quad (28)$$

$$x_i = \frac{M_i}{M_T}, \quad i = 1, \dots, c \quad (29)$$

$$F_{out} = f(P - P_{out}) \quad (30)$$

This is a set of $(2c + 4)$ equations in the $(2c + 4)$ variables $M_i, x_i, i = 1, \dots, c; M_T, F_{out}, \rho, P$. The system contains c differential equations (25) and c differential variables, $M_i, i = 1, \dots, c$.

We note that with this model, we can give $M_i(0)$ arbitrary values: given $M_i(0)$, we can calculate $M_T(0)$ from 26, $x_i(0)$ from 29, $\rho(0)$ from 27, $P(0)$ from 28; $F_{out}(0)$ from 30; and finally $M_i(0)$ from 25. Hence, this is an index-1 system.

The above equations are valid for both gas and liquid systems. Of course, a reasonable simplification for liquids is to assume that they are incompressible. Therefore, equation 28 is simplified to:

$$\rho = \rho^L(T, x) \quad (28')$$

Once again, if we specify $M_i(0), i = 1, \dots, c$, we can calculate $M_T(0)$ from 26, $x_i(0)$ from 29 and $\rho(0)$ from 27. At this point, however, we hit a problem: both sides of equation 28' are already known! Effectively, we *cannot* specify $M_i(0), i = 1, \dots, c$ independently. Therefore we have a high-index problem.

To see more clearly how the problem arises, consider combining 26, 27, 28' and 29 into a single equation:

$$\sum_{i=1}^c M_i = V \rho^L \left(\frac{M_i}{\sum_{j=1}^c M_j}, T \right) \quad (31)$$

It is obvious that 31 only involves the differential variables M_i , and, therefore, not all of them can be given arbitrary initial values. For instance, for an ideal liquid mixture, 28 is of the form:

$$\frac{1}{\rho} = \sum_{i=1}^c \frac{x_i}{\rho_i^0} \quad (32)$$

and 31 becomes:

$$V = \sum_{i=1}^c \frac{M_i}{\rho_i^0} \quad (33)$$

where ρ_i^0 is the (constant) density of pure component i . Thus, 33 is a total volume constraint. Differentiating 33 with respect to time, we obtain:

$$0 = \sum_{i=1}^c \frac{1}{\rho_i^0} \frac{dM_i}{dt} \quad (34)$$

which, together with 25, lead to:

$$F_{\text{in}}^{(1)} \sum_{i=1}^c \frac{x_{i,\text{in}}^{(1)}}{\rho_i^0} + F_{\text{in}}^{(2)} \sum_{i=1}^c \frac{x_{i,\text{in}}^{(2)}}{\rho_i^0} = F_{\text{out}} \sum_{i=1}^c \frac{x_i}{\rho_i^0} \quad (35)$$

which is equivalent to:

$$\frac{F_{\text{in}}^{(1)}}{\rho_{\text{in}}^{(1)}} + \frac{F_{\text{in}}^{(2)}}{\rho_{\text{in}}^{(2)}} = \frac{F_{\text{out}}}{\rho} \quad (36)$$

i.e. a relationship between the volumetric flowrates of the input and output streams. Note that this is true for ideal liquid mixtures only (*i.e.* those obeying 32), but in any case a similar restriction could be obtained from the more general equation 31 with respect to time.

In any case, 33 is an additional constraint that must be satisfied by the initial condition of the system. We can therefore give arbitrary initial values to only $c - 1$ variables. For instance, if we specify $M_i(0), i = 1, \dots, c - 1$, we can calculate $M_c(0)$ from 33, then $M_T(0)$ from 26, $\rho(0)$ from 27, $x_i(0), i = 1, \dots, c$ from 29, $F_{\text{out}}(0)$ from 36, $P(0)$ from 30 and finally $\dot{M}_i(0), i = 1, \dots, c$ from 25.

No further equation differentiations are necessary, and therefore this is an index-2 system.

Heater tank

Consider a well-stirred tank used to heat up a single-component stream:

$$\rho V \frac{du}{dt} = F(h_{\text{in}} - h) + Q \quad (37)$$

$$u = u(T) \quad (38)$$

$$h = h(T) \quad (39)$$

To define this system fully, we need an additional relation characterising the heating rate Q . For instance, Q could be described by a heat-transfer mechanism from a steam jacket at a given temperature T_s :

$$Q = UA(T_s - T) \quad (40)$$

Overall, equations 37 to 40 form a DAE system in the 4 variables u, h, Q and T . The system has one differential variable, namely u . If we specify $u(0)$, then we can calculate $T(0)$ from 38, $h(0)$ from 39, $Q(0)$ from 40 and finally $\dot{u}(0)$ from 37. This is clearly an index-1 DAE system.

Of course, 40 corresponds to only one permissible heat-transfer mechanism. If, for instance, we were using electrical heating, then we could vary Q directly, so instead of 40 we could have:

$$Q = Q^*(t) \quad (41)$$

where $Q^*(t)$ is a given function of time. Again, this does not change the nature (*i.e.* the index) of the DAE system.

On the other hand, we could well be interested in determining the variation of Q that would produce a certain desired variation in the exit temperature T . In this case, we would replace 40 (or 41) with:

$$T = T^*(t) \quad (42)$$

where $T^*(t)$ is a given function of time.

Of course, equations 37 to 39 are always true, so our DAE system now comprises 37, 38, 39, 42 and the same set of variables (*i.e.* u , h , Q and T) as before. It also still has differential variable u . If we specify $u(0)$, we can still calculate $T(0)$ from 38 and $h(0)$ from 39. However, when we come to consider 42, we encounter a problem since the $T(0)$ we calculated from 38 may not be the same as $T^*(0)$. In any case, we cannot calculate $Q(0)$ from any one of the existing equations!

Again, this is a high index problem. In fact, if we combine 38 and 42, we see that:

$$u = u(T^*(t)) \quad (43)$$

and, therefore, it is not possible to specify an arbitrary initial value for u . Furthermore, by differentiating 43 with respect to time, we get:

$$\frac{du}{dt} = c_V \frac{dT^*}{dt} \quad (44)$$

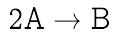
where $c_V \equiv (\partial u / \partial T)_V$, and this together with 37 yields:

$$\rho V c_V \frac{dT^*}{dt} = F(h_{\text{in}} - h) + Q \quad (45)$$

which is an additional restriction that the initial values of the variables must satisfy. Overall, we have 5 equations in 37 to 39, 42 and 45 in 5 initial values, *i.e.* $u(0), h(0), Q(0), T(0)$ and $\dot{u}(0)$ — therefore no arbitrary initial condition may be imposed on this system.

Systems of high-index DAEs in chemical equilibrium

Consider a constant-volume well-stirred reactor carrying out the gas-phase dimerisation reaction:



at a given temperature, T .

The mathematical model of this system comprises the equations:

$$\frac{dM_A}{dt} = F_{\text{in}}x_{\text{A,in}} - F_{\text{out}}x_{\text{A}} - 2rV \quad (46a)$$

$$\frac{dM_B}{dt} = F_{\text{in}}x_{\text{B,in}} - F_{\text{out}}x_{\text{B}} + rV \quad (46b)$$

$$M_T = M_A + M_B \quad (46c)$$

$$x_A = \frac{M_A}{M_T}; \quad x_B = \frac{M_B}{M_T} \quad (46d)$$

$$PV = M_T RT \quad (46e)$$

$$F_{\text{out}} = f(P - P_{\text{out}}) \quad (46f)$$

Here we have assumed perfect-gas behaviour (equation 46e) and that the exit flowrate is a function of the difference between the pressure in the reactor and the downstream pressure, P_{out} (equation 46f).

To complete the above model, we need to characterise the reaction rate, r . Assume first, that the reaction is irreversible with the rate given by:

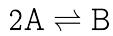
$$r = k \left(\frac{x_A P}{RT} \right)^2 \quad (47)$$

We note that equations 46 and 47 form a set of 8 DAEs in the 8 unknowns M_A , M_B , M_T , x_A , x_B , P , F_{out} and r . The system involves two differential variables (M_A and M_B). If we specify arbitrary values of $M_A(0)$ and $M_B(0)$, then:

From	Calculate
46c	$M_T(0)$
46d	$x_A(0), x_B(0)$
46e	$P(0)$
46f	$F_{\text{out}}(0)$
47	$r(0)$
46a, 46b	$\dot{M}_A(0), \dot{M}_B(0)$

Hence, this is an index-1 system, which can be solved without much difficulty.

Consider, however, what happens if the dimerisation reaction takes place under conditions of chemical equilibrium, *i.e.*:



For an ideal gas mixture, 47 will be replaced by an equilibrium relation of the form:

$$K = \frac{x_B}{x_A^2 P} \quad (47')$$

where K is the equilibrium constant. Since the temperature T is fixed, K also has a constant value.

Once again, the DAE system 46 and 47' comprises 8 equations in the same 8 unknowns as before. If we specify $M_A(0)$ and $M_B(0)$, we can again compute $M_T(0)$ from 46c; $x_A(0)$ and $x_B(0)$ from 46d; $P(0)$ from 46e and F_{out} from 46f. However, we now note that all variables in 47' have already been computed, and therefore this equation is either redundant or inconsistent. Moreover, we cannot get unique values for $r(0)$, $\dot{M}_A(0)$ and $\dot{M}_B(0)$ from the remaining two equations 46a and 46b.

As we have seen previously, the above are clear symptoms of a high-index DAE system. In fact, by combining 47' with 46c and 46e, we obtain:

$$\frac{KRT}{V} = \frac{M_B}{M_A^2} \quad (48)$$

The left hand side of 48 is just a constant. Therefore, $M_A(0)$ and $M_B(0)$ are related to each other and cannot be specified arbitrarily. This is the underlying cause of the high index.

Equation 48 also provides a way of determining $r(0)$. We can write is as:

$$\frac{KRT}{V} M_A^2 = M_B \quad (48')$$

which, upon differentiation with respect to time, yields:

$$\frac{2KRT}{V} M_A \frac{dM_A}{dt} = \frac{dM_B}{dt} \quad (49)$$

We can then use 46a and 46b to eliminate $\dot{M}_A(0)$ and $\dot{M}_B(0)$. Solving the resulting equation for r , we obtain:

$$r = \frac{2KRTM_A(F_{in}x_{A,in} - F_{out}x_A) - V(F_{in}x_{B,in} - F_{out}x_B)}{V(V + 4KRTM_A)} \quad (50)$$

A consistent set of initial variable values must satisfy 46, 47' and 48' at time $t = 0$. Thus we have 9 equations in the 10 unknowns $M_A(0)$, $M_B(0)$, $M_T(0)$, $x_A(0)$, $x_B(0)$, $P(0)$, $F_{out}(0)$, $r(0)$, $\dot{M}_A(0)$ and $\dot{M}_B(0)$, which leaves only one degree of freedom in the specification of the initial conditions.

Once we have a consistent set of initial values, we can solve the index-1 system 46 and 48' using standard algorithms.

Example of index reduction in chemical equilibrium

The handling of the high-index complications in the previous example was relatively straightforward. However, in general, things may be much more complicated, for instance, if we had non-ideal behaviour (with chemical equilibrium expressed in terms of fugacities rather than partial pressures, as in 47'); or if we had multiple reversible reactions at equilibrium. We also note that much of the effort in reformulating the prior system was expended in deriving a complex relation 50 for r — a quantity we need not know in the first place!

One approach to overcoming these difficulties is to try to eliminate r from the model. In particular, since r occurs only in 46a and 46b, we can eliminate it by combining these two equations. In this case, we have to multiply 46b by 2 and add it to 46a, which yields:

$$\frac{dM_A}{dt} + 2\frac{dM_B}{dt} = F_{in}(x_{A,in} + 2x_A) - F_{out}(x_A + 2x_B) \quad (51)$$

If we now define a new variable:

$$\tilde{M} = M_A + 2M_B \quad (52)$$

51 can be written as:

$$\frac{d\tilde{M}}{dt} = F_{in}(x_{A,in} + 2x_A) - F_{out}(x_A + 2x_B) \quad (53)$$

Now consider the DAE system formed by 46c to 46f, 47', 52 and 53. This comprises 8 equations in the 8 unknowns \tilde{M} , M_A , M_B , M_T , x_A , x_B , P and F_{out} . There is only one differential variable: \tilde{M} . If we specify $\tilde{M}(0)$, we can:

- Calculate $M_A(0)$, $M_B(0)$, $M_T(0)$, $x_A(0)$, $x_B(0)$ and $P(0)$ by solving 52, 46c to 46e and 47' simultaneously. To understand this, remember that 46d, 46e and 47' can be combined to yield 48 which, together with 52 form a set of two simple equations in $M_A(0)$ and $M_B(0)$. Once we get these two values, we can calculate $M_T(0)$ from 46c; $x_A(0)$ and $x_B(0)$ from 46d; and $P(0)$ from 46e.
- Calculate F_{out} from 46f.
- Calculate $d\tilde{M}/dt(0)$ from 53.

This, then, is an index-1 system which again can be solved with standard algorithms. It is interesting to note that this has been obtained from the original index-2 problem without any differentiations. This would appear to contradict the definition of index (*cf.* index classification of DAEs). However, the reduction has been possible only because we did not insist on determining *all* the variables in the original system; in particular, we decided that r was of no interest and we eliminated it using purely algebraic manipulations (*i.e.* no differentiations).

In doing so, we have introduced the new variable \tilde{M} defined by equation 52. \tilde{M} has an interesting physical interpretation: it is a quantity that remains unchanged by the reaction $2A \rightarrow B$, a so called "reaction invariant". Equation 53 can be interpreted as a balance on this quantity; as might be expected this balance does not involve a reaction term.

The procedure described here can be generalised to systems that include multiple reversible reactions at equilibrium, including additional reversible reactions where the rates of the forward and reverse reactions are known, and additional irreversible reactions. However, this general treatment is beyond the scope of this document.

Some general conclusions

The three examples presented in this section allow us to draw certain more general conclusions:

1. High-index DAEs often arise in process-engineering applications due to "simplifications" that impose additional constraints on the differential variables (or quantities directly related to them — *cf.* mixing-tank example). For instance,
 - Incompressibility → Volume constraint.
 - Phase equilibrium → Vapour/liquid composition relation.
 - Reaction equilibrium → Relations between component concentrations.
2. High-index DAEs also arise from "perfect control" specifications on process outputs, *i.e.* specifying them as given explicit functions of time (*cf.* heater-tank example).
3. In all cases, a high-index DAE implies that the differential variables in the model are not independent and cannot all be assigned arbitrary initial values.
4. Another frequent symptom that can be useful in detecting high-index DAEs is that one or more algebraic variables occur in differential equations only (*cf.* Q in the heater-tank example).
5. If we have a high-index DAE model, in general we can either:
 - a. change our assumptions ("simplifications") or specifications to develop a different, index-1 model or,
 - b. reduce the index by differentiating some of the equations a sufficient number of times.

Inconsistent initial conditions

Once gPROMS has checked that the system is well-posed, square and of index 1, it checks the consistency of the initial conditions and identifies sub-systems that are over- or under-specified at $t = 0$. For example, consider the system shown in the gPROMS code below:

Example 15.3. Illustrative example: system with inconsistent initial conditions

```
#=====
#MODEL mod1

VARIABLE
  x1, x2, y1, y2, y3          AS NoType

EQUATION
  $x1 = x1*y1 ;
  $x2 = x1 + x2*y1 + y2 + 3*y3 ;
  x1^2 = y2 ;
  x2 = x1 + y1 + y2*y3 ;
#=====
#PROCESS proc

UNIT
  mymod      AS mod1

ASSIGN
  WITHIN mymod DO
    y3 := 1 ;
  END #within

INITIAL
  WITHIN mymod DO
    x1 = 0 ;
    y2 = 1 ;
  END #within

SOLUTIONPARAMETERS
  ReportingInterval := 1 ;

SCEDULE
  CONTINUE FOR 10
```

In this case, it is clear from inspection that the initial conditions, $x_1(0) = 0$ and $y_2(0) = 1$, are inconsistent due to the relationship $x_1^2 = y_2$. This is confirmed by the gPROMS output:

Executing process PROC...

All 5 variables will be monitored during this simulation!

Building mathematical problem description took 0.001 seconds.

Loaded MA48 library
Execution begins....

Variables
 Known : 1
 Unknown : 4
 Differential : 2
 Algebraic : 2

```
Model equations      :      4
Initial conditions :      2
```

Checking consistency of model equations and ASSIGN specifications... OK!

Checking index of differential-algebraic equations (DAEs)... OK!

Checking consistency of initial conditions...

ERROR: Your initial conditions are inconsistent.
At time t=0, the following 3 equation(s) involve only 2 unknown
variable(s).

Model Equation	3: MYMOD.X1^2 = MYMOD.Y2 ;
Initial Condition	1: MYMOD.X1 = 0 ;
Initial Condition	2: MYMOD.Y2 = 1 ;

The 2 unknown(s) occurring in these 3 equations are:

MYMOD.Y2 (ALGEBRAIC)
MYMOD.X1 (STATE)

Initialisation calculation failed.

Execution of PROC fails prematurely.

Note that using the initial conditions:

```
INITIAL
  WITHIN mymod DO
    $x1 = 0 ;
    y2 = 1 ;
  END #within
```

for example, rectifies the problem.

Chapter 16. Initialisation Procedures

Initialisation procedures are a way to control more precisely how gPROMS initialises models. For complex models, this can substantially reduce the time taken to initialise them and also increase the robustness of the models (i.e. initialisation can be performed successfully for a wider set of initial conditions, variable specifications and parameter values). As this is done transparently, the model user can concentrate on the physical problem being solved and need not be concerned with the mathematical and numerical issues of getting a complex model to initialise.

Initialisation procedures comprise a set of simplifications and changes to the model, which guarantee that the model will initialise. These changes can then be reverted in a specified order so that the original problem is solved. By moving from an easy problem to the complex, original problem in this sequence, the ease of initialisation of complex models can be increased significantly, which means faster and more reliable initialisation over a wider range of input specifications compared with trying to initialise the problem in one step.

This is a procedure that good modellers tend to use: they begin modelling a process by using simplified equations so that they have a working simple model. They then gradually add complexity until the model has the desired fidelity. This sometimes requires using the solution of a simpler model as an initial guess for a more detailed model. gPROMS Initialisation Procedures essentially mimic this process without the need to use Saved Variable Sets and by permitting more than one intermediate stage; hence complex models built in this way are more flexible and reusable.

Initialisation Procedures for Non-Composite Models

To specify and use Initialisation Procedures for non-composite Models (i.e. Models that contain no Model instances (UNITs)), you need to:

- Specify at least one Initialisation Procedure in the Model
- Specify which Initialisation Procedure to use in the Process

Specifying Initialisation Procedures in the Model

There are four basic techniques associated with Initialisation procedures. These are:

- Initialisation Procedures that change the value of a Parameter
- Initialisation Procedures that change the value of a Degree of Freedom (Specification)
- Initialisation Procedures that change the choice of a Degree of Freedom
- Initialisation Procedures that use simplified equations

All of the above can be combined into a single Initialisation Procedure. When more than one simplification is applied, the order in which the simplifications are reverted can be important. The way in which these reversions take place may also be important. These are described in:

- Specifying the order of reversions
- Specifying how the reversions are performed

Initialisation Procedures are defined using one or more INITIALISATION PROCEDURE sections following the PRESET section of the Model (if one exists — see gPROMS Language declaration for Models for more information). The syntax (for non-composite Models) is:

```
INITIALISATION PROCEDURE ipname DEFAULT
```

```
START
  # list of modifications to the Model or its specifications
END
NEXT # NEXT sections are optional, there may be more than one
  # list of Initialisation Procedure actions
END
```

An alternative spelling is INITIALIZATION_PROCEDURE.

The DEFAULT keyword defines the default Initialisation Procedure and makes specifying Initialisation Procedures in Processes more convenient (this will become clearer later).

If only one Initialisation Procedure is specified, then the DEFAULT keyword compulsory. If there are more than one Initialisation Procedures in a Model then exactly one must contain the DEFAULT keyword. If none or more than one contain the DEFAULT keyword, then an error will be reported when executing the Process.

The START section of an Initialisation Procedure specifies which modifications should be made to the Model in order to initialise it. Exactly how this is done is described in the sections on changing the value of a Parameter, changing the value of a Degree of Freedom, changing the choice of a Degree of Freedom and simplifying equations.

The (optional) NEXT sections then define a sequence of changes (that of course move the initialisation problem closer to the one specified in the Process) to the Parameters or Variables listed in the START section. Changes specified in the same NEXT section are performed simultaneously and each NEXT section is executed in sequence. For more details, see specifying the order of reversions.

The changes specified in each NEXT section must be contained within either a MOVE_TO or JUMP_TO section. There can be only one of each in any NEXT section. Any changes specified within a MOVE_TO section are performed gradually, using a continuation method; those within a JUMP_TO section are performed in a single step. These sections are described in more detail in: specifying how reversions are performed.

After the final NEXT section has been executed, any modifications that are still in place are automatically reverted to the original problem in a final step. This is also described in: specifying the order of reversions. Parameters and Variables can be reverted to their original values explicitly using the REVERT keyword. This is illustrated in the following sections on changing the value of a Parameter, changing the value of a Degree of Freedom, changing the choice of a Degree of Freedom and simplifying equations.

Changing the Value of a Parameter

gPROMS initialisation procedures allow the model developer to specify a set of Parameter values that will guarantee successful initialisation. From this solution of the simplified problem the Parameter values are replaced with the desired ones in such a way that the model will always initialise. As an example, consider a lumped model of a CSTR in which the following energy balance occurs.

$$\frac{dU}{dt} = F_{\text{in}}h_{\text{in}} - F_{\text{out}}h + V \sum_{j=1}^{N_{\text{R}}} r_j \Delta H_{\text{R},j} + Q$$

The heats of reaction, $\Delta H_{\text{R},j}$, are Parameters to be specified by the Model user. Users may want to model highly energetic reactions, so that some of these Parameters will take very large values and in some cases these can cause difficulty or even failure during initialisation.

gPROMS Initialisation Procedures allow the Model developer to specify a set of Parameter values that will be used to initialise the Model first and then to change these values back to the user-specified ones in a controlled manner so that the initialisation converges even for extreme values of the Parameters. In the above example, the first step of the Initialisation Procedure might be to set all values of $\Delta H_{\text{R},j}$ to zero and solve the initialisation problem. Upon successful initialisation, the $\Delta H_{\text{R},j}$ Parameters are gradually¹ returned to the user-specified values.

¹By default, gPROMS applies a continuation method when reverting Parameters (and any other changes in the Initialisation Procedure) to the values specified in the Process: that is, their values are changed continuously and smoothly rather than in one discrete jump. See section xxx for more details.

If the ΔH_{Rj} Parameter is defined in the gPROMS Model by:

```
PARAMETER
  ...
  EnthalpyOfReaction AS ARRAY(NoReac) OF REAL
  ...
```

Then the Initialisation Procedure would be defined by:

```
# end of EQUATION section

INITIALISATION PROCEDURE IP_NoHeatOfReaction
  START
    EnthalpyOfReaction := 0 ;
  END
  NEXT
    MOVE_TO
      REVERT EnthalpyOfReaction ;
    END
  END
```

In other words, first solve the initialisation with EnthalpyOfReaction set to zero; then, once successful, gradually change all of their values back to those specified in the Process.

Changing the Value of a Degree of Freedom

The previous section described how models can be made more robust during initialisation. The approach was to use a gPROMS Initialisation Procedure to specify a set of Parameter values that guarantees initialisation and how these can be replaced by the desired values in a way that ensures successful initialisation. A similar situation arises with the specification of degrees of freedom: that is, any degrees of freedom need to be taken up by specifying the values of some Variables in the ASSIGN section.

Consider, once again, the energy balance equation for a lumped CSTR model:

$$\frac{dU}{dt} = F_{in}h_{in} - F_{out}h + V \sum_{j=1}^{N_R} r_j \Delta H_{Rj} + Q$$

Here for example, the rate of heat input to the system, Q , may depend on a Variable representing the steam flowrate, F_{steam} , through the vessel jacket or a coil. For an open-loop simulation, this variable would be specified in the ASSIGN section of the gPROMS Process.

One possible initialisation procedure would then be to start the initialisation with F_{steam} set to zero (which would guarantee initialisation) and then move the value of F_{steam} to the desired value.

This would be defined in gPROMS using the following code.

```
# end of EQUATION section

INITIALISATION PROCEDURE IP_NoSteamFlow
  START
    F_steam := 0 ;
  END
  NEXT
    MOVE_TO
      REVERT F_steam ;
    END
  END
```

Note that REASSIGN or RESET tasks cannot be used to redefine the value of any ASSIGNED variables in the context of an Initialisation Procedure.

Changing the Choice of a Degree of Freedom

In some cases, simply changing the values of ASSIGNED variables may not be sufficient to guarantee successful initialisation. The Model user may have chosen a particular set of Variables to ASSIGN that could cause difficulty or failure during initialisation. To avoid such possibilities, initialisation procedures can define which degrees of freedom should be specified to guarantee initialisation. The initialisation procedure then also specifies how the choice of degrees of freedom can be reverted to the one specified in the Process by the user.

One possible use of this feature can be seen in the following example. Consider a model of a tubular reactor in which the length of the reaction is a variable, L , to be specified (a degree of freedom) and in which there is an equation that defines the fractional conversion ξ of one of the reactants. ξ might then be defined as follows.

$$\xi = \frac{P_{\text{feed}1}/(RT_{\text{feed}}) - C_1(L)}{P_{\text{feed}1}/(RT_{\text{feed}})},$$

where the perfect gas law has been used to calculate the inlet concentration of component 1, using the partial pressure of component 1 in the feed and the feed temperature ($P_{\text{feed}1}$ and T_{feed} , respectively) and $C_i(z)$ is the concentration of component i at axial position z in the reactor.

It is usual to specify the value of L and calculate the conversion ξ , but it is also possible to specify ξ as a degree of freedom, which would then determine the value of L . The latter specification may present problems during initialisation, however, so a suitable initialisation procedure for this model would be to replace any choice of degree of freedom with a specification on the length of the reactor, L . This (maybe combined with a suitable value for L) would then result in a more robust model.

This can be achieved in gPROMS using the following.

```

DISTRIBUTION_DOMAIN
    Axial           AS [0:1]
# normalised as ReactorLength is a Variable ( PARTIAL(,Axial)
# becomes 1/ReactorLength * PARTIAL(,Axial) etc. )

VARIABLE
    ...
    ReactorLength AS Length
    C             AS DISTRIBUTION(NoComp,Axial) OF MolarConcentration
    Conversion    AS NoType

EQUATION
    ...
    Conversion = (Pfeed(1) / (Rg * Tfeed) - C(1,1)) /
#               -----
#               (Pfeed(1) / (Rg * Tfeed)) ;

INITIALISATION PROCEDURE IP_ReplaceConversion
    START
        REPLACE
            Conversion
        WITH
            ReactorLength := 5 ;
            # this value of L guarantees successful initialisation
        END
    END
NEXT
MOVE_TO
    REVERT Conversion ;
END
END

```

In this example, the conversion must be specified in the Process as follows.

```
ASSIGN  
R101.Conversion := 0.95 ;
```

Simplifying Equations

When developing very detailed models, it is often better to start with a simple model and gradually add more complexity. This is because initialising the fully-detailed model may be too difficult without good initial guesses. With a much simpler model, one can obtain a solution from a poor initial guess and then use that as the initial guess for a more detailed model. This process is repeated until the final model, with the desired level of detail, can be solved.

gPROMS Initialisation Procedures enable the modeller to automate this process and are much more flexible and reusable than manually initialising a complex model. This is because using the manual approach requires that published models contain the saved variable set that is necessary to initialise the simulation. Apart from making the published model large in size (due to the size of the saved variable set), the saved variable set will be suitable for only a narrow range of problems: for example, if the model user wanted to change the number of chemical species in the simulation, then the existing saved variable set may be useless and it would be impossible to initialise the simulation. This might also happen even if only a few species were changed (the number of components remaining the same). Initialisation Procedures allow complex models to be initialised successfully without the use of saved variable sets and for a very much wider range of problems.

To see how the initialisation procedures are defined, consider again the energy balance equation for a lumped CSTR model:

$$\frac{dU}{dt} = F_{in}h_{in} - F_{out}h + V \sum_{j=1}^{N_R} r_j \Delta H_{Rj} + Q$$

One way to build up to the full energy balance from simplified ones would be to start with an isothermal model, then switch to an adiabatic model and finally to arrive at the full non-isothermal, non-adiabatic model (the equation above).

The problem would then first be initialised using

$$\frac{dT}{dt} = 0$$

for the energy balance.

The solution of this would then be used as the initial guess to solve the next initialisation, using

$$\frac{dU}{dt} = F_{in}h_{in} - F_{out}h + V \sum_{j=1}^{N_R} r_j \Delta H_{Rj}$$

for the energy balance. Finally, the solution of the last problem would be used to initialise the model with the desired energy balance:

$$\frac{dU}{dt} = F_{in}h_{in} - F_{out}h + V \sum_{j=1}^{N_R} r_j \Delta H_{Rj} + Q$$

(Of course, this example is quite simple and it is probably not necessary to go to these lengths in this case. However, much more complicated models would require this treatment.)

This initialisation procedure can be defined in gPROMS first by specifying all of the equations within a CASE statement and then using the Initialisation Procedure to SWITCH from the simplified equation(s) to the final one(s). All of the following must be specified in the Model.

First the Selector Variable must be defined:

```
SELECTOR  
EnergyMode AS (Isothermal, Adiabatic, NINA) DEFAULT NINA
```

Then the equations can be defined using a CASE statement:

EQUATION

```
...
CASE EnergyMode OF
    WHEN Isothermal:
        $T = 0 ;
    WHEN Adiabatic:
        $U = F_in*h_in - F_out*h + V*SIGMA(rate()*DeltaH_R()) ;
    WHEN NINA:
        $U = F_in*h_in - F_out*h + V*SIGMA(rate()*DeltaH_R()) + Q ;
END
...
```

Finally, the initialisation procedure is defined by:

```
INITIALISATION PROCEDURE IP_SimpleEnergyBalance
    START
        EnergyMode := Isothermal ;
    END
    NEXT
        MOVE_TO
            EnergyMode := Adiabatic ;
        END
    END
    NEXT
        MOVE_TO
            EnergyMode := NINA ;
        END
    END
```

Behaviour of CASE branches during initialisation

When gPROMS performs a standard intialisation (i.e. without using any user-defined Initialisation Procedures) of a Model containing CASE statements, the active branches of *all* CASE statements are determined by the values of the Selector Variables specified in the INITIAL_SELECTOR section of the Process. These Selector Variables must remain fixed at these values throughout and at the end of the initialisation procedure (so that the CASE branches are locked) because their values are considered part of the initial state for the simulation.

In the case of Initialisation Procedures, all CASEs that contain SWITCH TO statements are free to switch during the Initialisation Procedure. The exception, of course, is when the Initialisation Procedure specifically changes the values of one or more Selector Variables. However, at the end of the Initialisation Procedure, all manipulated and implicitly-set Selector Variables are reverted back to their specified values, consistent with a standard initialisation. In other words, Initialisation Procedures must always result in the same initial state as a standard initialisation.

Specifying the sequence of Actions in Initilisations Procedures

Initialisation Procedures for non-composite Models must contain at least one START section and then optionally any number of NEXT sections.

The START section specifies which Parameters, Variables or Selector Variables are to be changed during initialisation. The START section may contain any number of simplifications (as described in the sections on changing the value of a Parameter, changing the value of a Degree of Freedom, changing the choice of a Degree of Freedom and simplifying equations) in any order: they are all performed in parallel and together form the first initialisation problem.

After the first initialisation is successful, gPROMS then needs to know in what order to relax the simplifications. This is specified by an optional sequence of NEXT sections, each of which contains a list of changes (either partial or complete relaxations of some of the simplifications in the START section) that are to be made in parallel. If no NEXT section is present, then gPROMS will relax all simplifications simultaneously and try to reinitialise the problem. If any NEXT sections are present, then each NEXT section is processed in sequence, reinitialising after

each one. Any simplifications that have not been completely relaxed after the final NEXT section are then relaxed simultaneously in an implicit final step.

Each NEXT section must contain a list of one or more changes to a Parameter or Variable listed in the START section: they may be assigned a new value or reverted to the value specified in the Process by use of the REVERT task. The syntax of the REVERT task is:

```
REVERT ParameterName ;
REVERT VariableName ;
REVERT SelectorName ;
```

All changes (including revertions) to a Parameter or a Variable must occur within either a MOVE_TO or JUMP_TO section.

The examples below illustrate these ideas more clearly.

The START section may contain any number of actions:

```
START
  aParameter := 0 ;
  aVariable   := 0 ;
  REPLACE
    anotherVariable
  WITH
    aThirdVariable := 0 ;
  END
  aSelector := Simple ;
END
```

In this example, all four actions are included: changing a Parameter value, changing a Variable value (degree of freedom), changing the choice of a degree of freedom and changing the value of a Selector variable (to change the equations being used).

Explicitly reverting changes:

```
INITIALISATION PROCEDURE IP_Example1
  START
    aParameter := 0 ;
    aVariable   := 0 ;
    REPLACE
      anotherVariable
    WITH
      aThirdVariable := 0 ;
    END
    aSelector := Simple ;
  END
  NEXT
    MOVE_TO
      REVERT aParameter ;
      REVERT aVariable ;
      REVERT anotherVariable ;
      REVERT aSelector ;
  END
END
```

Here, the NEXT section reverts all actions simultaneously and smoothly.

The implicit final step when no NEXT section is specified:

```
INITIALISATION PROCEDURE IP_Example1
```

```
START
aParameter := 0 ;
aVariable := 0 ;
REPLACE
    anotherVariable
WITH
    aThirdVariable := 0 ;
END
aSelector := Simple ;
END
```

Here, no NEXT sections are present, so all actions are reverted simultaneously after the first initialisation is successful. This example is identical to the previous one, where all actions were reverted explicitly in a NEXT section.

Making more than one change to a Variable/Parameter before reverting it:

```
INITIALISATION PROCEDURE IP_Example2
START
aParameter := 0 ;
aVariable := 0 ;
REPLACE
    anotherVariable
WITH
    aThirdVariable := 0 ;
END
aSelector := Simple ;
END
NEXT
MOVE_TO
    aParameter := 1 ;
END
END
```

In this example, the value of aParameter is changed continuously from 0 to 1 (with aVariable and aThirdVariable still equal to 0, and aSelector still equal to Simple). The implicit final step then will revert aParameter, the Variables and Selector Variable to their values specified in the Process. Implicit final steps always revert the changes smoothly (in an implicit MOVE_TO section).

Reverting some simplifications in parallel and some in sequence:

```
INITIALISATION PROCEDURE IP_Example3
START
aParameter := 0 ;
aVariable := 0 ;
REPLACE
    anotherVariable
WITH
    aThirdVariable := 0 ;
END
aSelector := Simple ;
END
NEXT
MOVE_TO
    REVERT aParameter ;
    REVERT aVariable ;
END
END
NEXT
```

```
MOVE_TO
    REVERT anotherVariable ;
    REVERT aSelector ;
END
END
```

Here, the Parameter and aVariable are reverted simultaneously and the system is reinitialised. Then the other two Variables are reverted. (This second NEXT section could have been omitted, as the reversions would have taken place implicitly anyway.)

They can all be combined:

```
INITIALISATION PROCEDURE IP_Example4
START
    aParameter := 0 ;
    aVariable := 0 ;
    REPLACE
        anotherVariable
    WITH
        aThirdVariable := 0 ;
    END
    aSelector := Simple ;
END
NEXT
    MOVE_TO
        REVERT aParameter ;
        aVariable := 1 ;
    MOVE_TO
END
NEXT
    MOVE_TO
        REVERT aVariable ;
        aSelector := NotSoSimple ;
    END
END
NEXT
    MOVE_TO
        REVERT anotherVariable ;
        aSelector := QuiteComplex ;
    END
END
```

In this final example, the Parameter is reverted to its specified value at the same time as aVariable is changed to 1. After reinitialisation, aVariable is reverted simultaneously with the change of equations to the NotSoSimple CASE. In the final NEXT section, the specification on aThirdVariable is reverted to the original specification on anotherVariable (note that anotherVariable is specified in the REVERT task) while the equations are changed once more. Finally, the implicit final step reverts the equations to their full form (i.e. the value originally specified for the aSelector Variable)

Specifying how the reversions are performed

Earlier sections have described how to make changes to Parameters, Variables and Equations during initialisation and in which order these changes should be reverted back to the original specifications. How these reversions are performed has not yet been discussed fully.

There are two ways that changes specified in a NEXT section can take place: either by making discrete jumps or by changing the value smoothly from one state to the next. Discrete changes are trivial to perform: simply change the value and reinitialise. To make a smooth change, gPROMS employs a continuation algorithm. Clearly, if the difference between the values is large, then it will be harder to make a discrete jump and the continuation method

will be more robust; however, when it is safe to make discrete jumps, this method will usually result in faster initialisation. In some cases, it is a matter of experimentation to determine which method is more robust and faster.

The JUMP_TO and MOVE_TO sections are used to specify which transitions are to be discrete and smooth respectively. One MOVE_TO section and one JUMP_TO section can be placed in each NEXT section. The example below illustrates the use of both discrete and continuous transitions.

```
INITIALISATION PROCEDURE IP_Example3a
START
  aParameter := 0 ;
  aVariable := 0 ;
REPLACE
  anotherVariable
WITH
  aThirdVariable := 0 ;
END
  aSelector := Simple ;
END
NEXT
MOVE_TO
  REVERT aVariable ;
  REVERT anotherVariable ;
END
END
NEXT
JUMP_TO
  REVERT aParameter ;
END
MOVE_TO
  REVERT aSelector ;
END
END
```

In this example, the problem is first initialised with aParameter and aVariable equal to 0, aThirdVariable is also equal to 0 (replacing the specification of anotherVariable) and aSelector is set to Simple (specifying the use of simplified equations).

In the first NEXT section, the two variables simultaneously make smooth transitions to their final values.

Finally, aParameter is reverted in a discrete jump at the same time as the Selector Variable is reverted to its original value in a smooth transition.

In this case, there are no implicit reversions to be made. Should there be an implicit final step, then all reversions are performed in a smooth transition.

This example illustrates that even though changing a degree of freedom (REPLACE) or the equations that are being solved (SWITCHing from one CASE to another) is a discrete change, gPROMS can still perform this change smoothly.

Specifying which Initialisation Procedures to use in the Process

Once one or more Initialisation Procedures have been specified for a Model, one can be selected for use in a simulation by specifying it in the Process.

The syntax is very simple:

```
INITIALISATION PROCEDURE
```

```
USE
  unitname : ipname ;
END
```

where *unitname* is the name of the Model instance specified in the UNIT section and *ipname* is the name of the Initialisation Procedure to use. Alternatively, the keyword NONE can be used in place of ipname to specify that no Initialisation Procedure should be used, or DEFAULT can be used to specify that the default Initialisation Procedure must be used. An alternative spelling, INITIALIZATION_PROCEDURE, is also allowed.

Performing a simulation activity using Initialisation Procedures

One one or more Initialisation Procedures have been defined in the Models and a Process, as described previously, gPROMS can then use them when performing a simulation activity. In order to do this, simply execute the Process as usual and then when the Execution control dialog appears select one of:

- *Perform Initialisation Procedure only*: This method only performs the Initialisation Procedure to generate the initial guesses but does not continue to initialise the problem or execute the Schedule. This is useful if you only want to generate the initial guesses and save them in a *Saved Variable Set*. (The generation of the *Saved Variable Set* is specified as part of the Initialisation Procedure.)
- *Perform Initialisation Procedure as part of the main activity*: This method generates the initial guesses using the Initialisation Procedure, then immediately performs an initialisation using them. If a Schedule is present, and the *Ignore schedule* option is unchecked, then gPROMS will complete the simulation according to what is specified in the Schedule. If the Initialisation Procedure specifies that a *Saved Variable Set* should be generated, then this is done too.

See Executing Simulations for a full description of the Execution control dialog.

Initialisation Procedures for Composite Models

Specifying initialisation procedures for composite Models is very similar to that of non-composite Models but with two additional complications:

- the sub Models within the composite model may also contain Initialisation Procedures, and there needs to be some mechanism for choosing which of these to use in a particular Initialisation Procedure; and
- any Initialisation Procedures in the sub Models may contain a number of NEXT sections and some control needs to be applied to ensure that these NEXT sections are processed at the right time relative to the NEXT sections in the composite Model and the ones in the other sub Models.

In order to specify which sub Model Initialisation Procedures must be used, a USE section has to be included in the composite Model's Initialisation Procedure. The syntax for the Initialisation Procedure in a composite Model is as follows.

```
INITIALISATION_PROCEDURE ipname [DEFAULT]
  USE
    # list of Unit and Model specifications
  END
  START
    # list of modifications to the Model or its specifications
  END
  NEXT # NEXT sections are optional, there may be more than one
    # list of Initialisation Procedure actions
  END
```

See The USE Section for Composite Models for more details on the USE section.

The START section is treated identically to non-composite Models (see Specifying Initialisation Procedures in the Model).

The NEXT section is similar to that for non-composite Models, but with additional Initialisation Procedure Actions for Synchronising the Initialisation Procedures of sub Models.

The USE Section for Composite Models

The syntax of the USE section in composite Models is similar to that for Processes (see Specifying which Initialisation Procedures to use in the Process). There are some additional features needed for composite Models that contain more than one sub Model. In this case, the USE section may contain a list of specifications: one for each instance. That is:

```
USE
  unitname1 : ipname1 ;
  unitname2 : ipname2 ;
  unitname3 : ipname3 ;
  # etc.
END
```

If there are lots of Model instances (e.g. if there is an array), then there are some short cuts to save typing many lines of specifications.

First, if all Model instances are to use the default Initialisation Procedure, then the following specification can be made:

```
USE
  : DEFAULT ;
END
```

If all Model instances apart from a few are to use the default Initialisation Procedure, then it is usually more efficient to specify the above and then to override it with specific Unit specifications:

```
USE
  # Use default ip for all units
  : DEFAULT ;
  # Override ip for Unit U1: use no ip
  U1 : NONE ;
  # Override ip for Unit U2: use specified ip
  U2 : ipname ;
END
```

Second, arrays and slices of arrays can be used in place of single Unit names:

```
USE
  # Specification for the whole array of Units
  # (both lines are acceptable syntax)
  ArrayUnit1 : ipname1 ;
  ArrayUnit2() : ipname2 ;
  # Specification for a slice of an array of Units
  ArrayUnit3(2:3) : ipname3 ;
END
```

Another useful option is to specify the Initialisation Procedure to be used by all Model instances (Units) of the same Model. This is done by:

```
USE
  [modelname] : ipname ;
```

```
END
```

where *modelname* is the name of a *Model* and *ipname* is the name of one of its Initialisation Procedures (the brackets are part of the syntax and must be typed — this distinguishes between a Model specification and a Unit specification, since gPROMS allows the name of a Unit to be the same as a Model name). Just as with Unit specifications, the NONE and DEFAULT keywords can be used.

Finally, one might want to specify a particular Initialisation Procedure for all Units of the same Model type apart from a certain number of specific Units. This can be done by combining Model specifications with Unit specifications as follows.

```
USE
  unitname : ipname ;
  [modelname] : ipname ;
END
```

In this case, all Unit specifications override the Model specifications, regardless of the order in which they are made. As an example, consider a Model with 3 instances of Model Tank, called T101, T102 and T103. If T101 and T102 are to use the default Initialisation Procedure, and T103 is to use none, then this can be done as follows.

```
USE
  [Tank] : DEFAULT ;
  T103 : NONE ;
END
```

Even if the T103 specification appears before the [Tank] one, it will override the [Tank] specification for T103.

Lastly, gPROMS will issue a warning if there are duplicate Unit specifications but will continue with the simulations using the last specification in the list to override all previous ones.

Synchronising the Initialisation Procedures of sub Models

Synchronisation of the various Initialisations Procedures for non-composite Models is specified using NEXT sections, as has been described before (Specifying the sequence of Actions in Initialisations Procedures). For composite Models, the same procedures apply in addition to being able to control when a NEXT section of a sub Model is processed. This is done using the ADVANCE and COMPLETE actions. The syntax of the ADVANCE action is:

```
ADVANCE unitname ;
```

or

```
ADVANCE [modelname] ;
```

The first command causes the next unprocessed NEXT section within the Initialisation Procedure of the Unit *unitname* to be processed in parallel with the actions specified in the NEXT section within which it resides. *unitname* may also be an array of Units or a slice of an array of Units. The second command does the same, but for all Units of Model type *modelname* (note that the brackets are part of the syntax).

Since the ADVANCE keyword specifies that a subsequent NEXT section of a sub Model should be executed, and all changes specified in NEXT sections must be within a MOVE_TO or JUMP_TO section, there must be no ADVANCE commands placed inside a MOVE_TO or JUMP_TO section: doing so will result in an error.

The COMPLETE action is similar to ADVANCE but causes *all* of the Unit's NEXT sections to be executed in sequence (beginning with the first unexecuted NEXT section of the Unit). The syntax is:

```
COMPLETE unitname ;
```

or

```
COMPLETE [modelname] ;
```

When more than one COMPLETE action resides in the same NEXT section, then the first unprocessed NEXT section of each Unit is executed in parallel, followed by the second set of NEXT sections and so on until all explicit and implicit steps are complete.

To illustrate the ADVANCE action, suppose a composite Model contains instances of two sub-models, A and B:

```
UNIT
  A1 AS A
  B1 AS B
  ...
  . . .
```

Now, the Models A and B may have a number of Initialisation Procedures, such as:

# in Model A	# in Model B
INITIALISATION_PROCEDURE IP_A1	INITIALISATION_PROCEDURE IP_B1
...	...
INITIALISATION_PROCEDURE IP_A2 DEFAULT	INITIALISATION_PROCEDURE IP_B2 DEFAULT
...	...

The choice of Initialisation Procedure for the sub Models is made within the USE section of the Initialisation Procedure of the composite Model:

```
INITIALISATION_PROCEDURE IP_composite1
  USE
    A1 : IP_A1 ;
    B1 : IP_B1 ;
  END
```

Now the Initialisation Procedures of the two sub models are defined as:

# in Model A	# in Model B
INITIALISATIONPROCEDURE IP_A1	INITIALISATIONPROCEDURE IP_B1
START	START
P1 := P1_0 ;	P2 := P2_0 ;
END	END
NEXT	NEXT
MOVE_TO	MOVE_TO
P1 := P1_1 ;	P2 := P2_1 ;
END	END
END	END
NEXT	
JUMP_TO	
P1 := P1_2 ;	
END	
END	

Notice that Model B's Initialisation Procedure has one less NEXT section, each is defined in terms of changes to a Parameter (P1 for Model A and P2 for Model B) and each has an implicit final step that reverts the Parameter back to its original value.

The Initialisation Procedure for the composite model is:

```
INITIALISATIONPROCEDURE composite_init_1
  USE
    A1 : IP_A1 ;
```

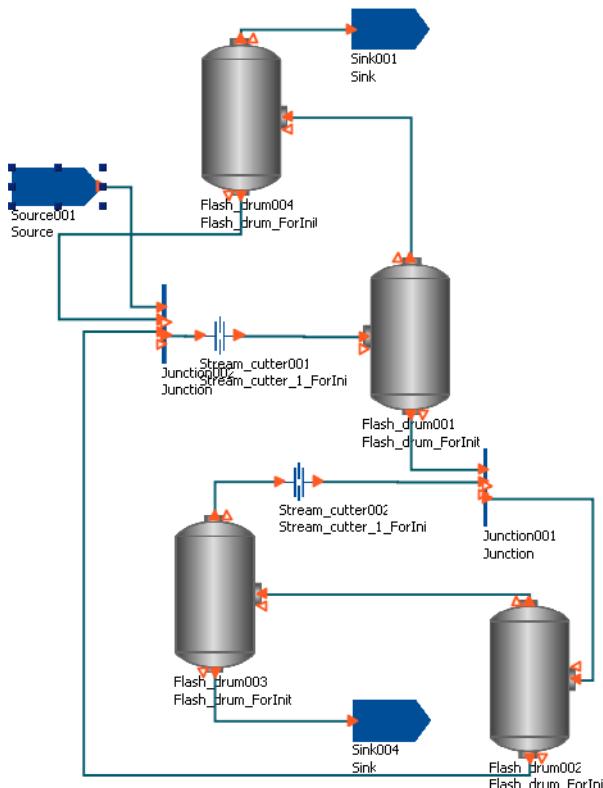
```
B1 : IP_B1 ;
END
START
    PP := PP_0 ;
END
# Step1
NEXT
    MOVE_TO
        PP := PP_1 ;
    END
END
# Step2
NEXT
    ADVANCE A1 ;
END
# Step3
NEXT
    ADVANCE A1 ;
    MOVE_TO
        PP := PP_2 ;
    END
END
# Step 4
NEXT
    ADVANCE B1 ;
END
# Step 5
NEXT
    ADVANCE A1 ;
    ADVANCE B1 ;
    MOVE_TO
        REVERT PP ;
    END
END
```

Now, during each step in the initialisation strategy of the composite Model, the following steps occur to each of the Models:

Step	PP	A1.P1	B1.P2	Comments
START	PP_0	P1_0	P2_0	The first, simplest initialisation.
1	PP_1	P1_0	P2_0	The first NEXT section only changes the value of PP.
2	PP_1	P1_1	P2_0	The second NEXT section advances the Initialisation Procedure for A1, which changes its value of P1 to P1_1.
3	PP_2	P1_2	P2_0	The third NEXT section changes the value of PP to PP_2 and at the same time advances the Initialisation Procedure for A1,

Step	PP	A1.P1	B1.P2	Comments
				which changes the value of P1 to P1_2.
4	PP_2	P1_2	P2_1	The fourth NEXT section only advances the Initialisation Procedure for B1, which changes its value of P2 to P2_1.
5	PP	P1	P2	The final NEXT section reverts PP to the value specified in the Process and simultaneously advances A1 and B1's Initialisation Procedures. This causes the implicit final steps to be called, which revert P1 and P2 to their values specified in the Process.

The example above is somewhat contrived, just to illustrate the processes occurring during initialisation. A more useful application of sequence control in composite-Model initialisation is the convergence of flowsheets with recycles. The figure below illustrates a composite Model containing 4 instances of a flash-drum Model, and various other connections and splitters. Of note are the two instances of a Stream-Cutter Model. These are models that perform stream tears but using equation simplifications: the full equations link the inlet of the Model to the outlet, effectively connecting the stream; the simplified equations set the outlet to some given condition, tearing the stream.



Now the Initialisation Procedures for the `Stream_Cutter` and `Flash_drum` Models are as follows.

<pre># in Model Stream_cutter INITIALISATION PROCEDURE Init START ConnectionEqns := Simple ; END NEXT MOVE_TO REVERT ConnectionEqns ; END END </pre>	<pre># in Model Flash_drum INITIALISATION PROCEDURE Init START REPLACE Pressure WITH VapourFraction := VapFracStart ; END END NEXT MOVE_TO REVERT Pressure ; END END </pre>
--	---

The Selector Variable `ConnectionEqns` represents the connection of the stream into and out of the unit; when `Simple`, the stream is torn. For the `Flash_drum` Model, one needs to specify the pressure, but it is difficult to initialise the Model with this specification, so the degree of freedom specified during initialisation is the vapour fraction: it is a much easier to determine the pressure from the vapour fraction than the reverse.

Finally, the flowsheet initialisation strategy is:

```
INITIALISATION PROCEDURE Init
  USE
    Flash_drum003 : Init;
    Flash_drum004 : Init;

    Stream_cutter001 : Init;
    Stream_cutter002 : Init;
  END
  NEXT
    ADVANCE Flash_drum003;
    ADVANCE Flash_drum004;
  END
  NEXT
    ADVANCE Stream_cutter001;
    ADVANCE Stream_cutter002;
  END
```

The overall Initialisation Procedure is as follows. The problem is first initialised with the simpler specification on the vapour fraction of two of the flash drums and both recycle streams torn. Switching back to the full Model in one step may still cause problems with convergence, so the next step is to revert the degree-of-freedom specifications back to the flash-drum pressures; the vapour fractions now being determined from these. Finally, both stream tears can be removed in parallel and the final solution is as desired: a fully converged flowsheet with both recycles in place and the vapour fraction of each flash drum determined by the specified pressures.

Reference

The following conventions are used in describing the syntax of Initialisation Procedures.

- gPROMS language keywords are shown coloured in CAPITALS, even though the language is case-insensitive
- Identifiers are shown in the italic font: *identifier*
- An optional language construct is enclosed in brackets, e.g.: [DEFAULT]
- A compulsory language construct is enclosed in angle brackets, e.g.: <USE section>

- Choices are indicated by pipes separating each option, e.g.: *identifier*|DEFAULT|NONE indicates the choice between an identifier or one of the keywords DEFAULT and NONE.
- When multiple language constructs are allowed, they are indicated by a following asterisk, e.g. [NEXT section]*

Specifying Initialisation Procedures in Models

The syntax for specifying an initialisation procedure in a Model is:

```
INITIALISATION PROCEDURE ipname [DEFAULT]
  [USE section]
  [START section]
  [NEXT section]*
```

A Model can have more than one initialisation procedure, each of which must have a uniquely defined name in the same Model. The following rules are imposed on the specification of an initialisation procedure in a Model:

- The alternative keyword INITIALIZATION PROCEDURE may be used.
- The Initialisation Procedure must not be completely empty; a syntax error will be reported if it is.
- The optional DEFAULT keyword following the name of the Initialisation Procedure is used to specify that an Initialisation Procedure is the default in a Model. Only one IP may be assigned as default. If a Model has only one IP specification, it is automatically assigned as the default (no keyword is required).
- The optional USE section defines which Initialisation Procedures are applied for any Units present in the Model. Only one USE section is allowed in an Initialisation Procedure and it must not be empty.
- The optional START section contains a list of IP actions to perform prior to initialisation. Only one START section is allowed in an Initialisation Procedure and it must not be empty.
- If there is a USE or START section in the IP, then one or more optional NEXT sections may be included. Each NEXT section must contain at least one Initialisation Procedure action; all IP actions in a NEXT section are performed simultaneously.
- All modifications must be declared explicitly in the START section of an Initialisation Procedure. Elementary IP tasks are only allowed for those Model elements which were modified in the START section. An error will be reported otherwise.
- A Unit can only be ADVANCED in a NEXT section if it is specified in the USE section; otherwise an error will be reported.

Specifying Initialisation Procedures in Processes

The syntax for specifying an initialisation procedure in a Process is:

```
INITIALISATION PROCEDURE ipname [DEFAULT]
  <USE section>
  [SAVE filename; ]
```

Only one IP specification is allowed in a Process. The SAVE task is optional and the USE section is compulsory.

The USE section

The USE section defines which Initialisation Procedures are applied for any Units present in the Model or Process. The USE section is compulsory for an IP in a Process but optional for IPs in a Model. The syntax of the USE section is:

```
USE
```

```
[ : DEFAULT ; ]
[ unitname : ipname|DEFAULT|NONE ; ]*
[ [ modelname ] : ipname|DEFAULT|NONE ; ]*
END
```

The USE section must contain at least one specification. Specifications can be made for any Unit present in the Model or Process, as indicated by the second line; for all Units in the Process, first line; or for all Units of the same Model type, third line.

Unit IP Specifications are made by entering the name of a Unit (or an array or slice of an array of Units) followed by a colon and then either a valid IP name for the Unit (i.e., the name of an IP in the Model of which the Unit is a type) or one of the keywords DEFAULT or NONE. The DEFAULT keyword indicates that the default IP for the Unit should be implemented; NONE indicates that no IP should be implemented (this is useful for overriding a previous specification for a Model or an array of Units). Lastly, if all Units in the Process are to use the default IP, then this can be done by omitting the *unitname* identifier and using the DEFAULT keyword, as in the first line above.

Model IP Specifications are made by entering the name of a Model enclosed in brackets (this is part of the syntax) followed by a colon and then either a valid IP name for the Model or one of the keywords DEFAULT or NONE. The DEFAULT keyword indicates that the default IP for all Units declared as *modelname* should be implemented; NONE indicates that no IP should be implemented.

Order and Precedence Rules

- A Unit specification can appear an arbitrary number of times, with each new specification overriding any previous one. Duplicated specifications of the same unit are reported as a warning
- An Initialisation Procedure specified explicitly for a Unit will override a setting arising from a Model specification.
 - The order of Model specifications and Unit specifications is insignificant: even if a Model specification is placed after a Unit specification, the Unit specification will always override the Model specification.

The START section

The START section may only appear in Models. There may only be one START section and it must contain at least one modification of the standard Initialisation Procedure. The syntax is:

```
START
  <modification of the standard IP>*
END
```

The modifications can be one of the following:

1. changes to the value of a Parameter
2. changes to the choice of a Degrees of Freedom (DoF) (i.e., changing the ASSIGNment of one Variable to an ASSIGNment of another)
3. changes to the value of a DoF (i.e., changing the value of an ASSIGNED Variable)
4. changes to the value of a Selector Variable

For modifications of a gIP that involve Variables (cf. items 2 and 3 above), the Variables must be already ASSIGNED, otherwise they will be reported as specification errors.

The syntax for modifications of a gIP involving Parameters, Variable values and Selectors respectively is:

```
ParameterPath := expression ;
VariablePath := expression ;
```

```
SelectorPath := value ;
```

The syntax for changing the choice of a DoF is:

```
REPLACE
  VariablePath1
WITH
  VariablePath2 := expression ;
END
```

where *VariablePath1* must be different to *VariablePath2*. *VariablePath* and *VariablePath1* must be ASSIGNED in the Process; *VariablePath2* must not have been ASSIGNED.

The modifications to the gIP are applied simultaneously *before* any initialisation takes place. The first initialisation problem that gPROMS solves is the one specified in the START section.

Behaviour of CASE statements duringin Initialisation Procedures

During an Initialisation Procedure, CASE statements are free to change branches based on the values of the Variables at each step of the Initialisation Procedure. However, the branches of any CASE specified in the START section can, of course, be changed explicitly in a NEXT section. The final implicit step of an Initialisation Procedure always reverts the values of Selector Variables to those specified in the INITIALSELECTOR section so that the correct initialisation is solved.

The NEXT section

After the first initialisation problem is solved (that specified by the modifications in the START section to the gIP), a sequence of actions may be performed in order to restore these modifications back to the initialisation problem specified in the SET, ASSIGN and INITIALSELECTOR sections of the Process. Each step in this sequence is specified in a NEXT section. There may be as many NEXT sections in the IP as required, including none (in which case, all modifications to the gIP are reverted in parallel). The syntax of the NEXT section is:

```
NEXT
  [MOVE_TO section]*
  [JUMP_TO section]*
  [ADVANCE statement]*
  [COMPLETE statement]*
END
```

Each NEXT section may comprise any combination of MOVE_TO, JUMP_TO, ADVANCE and COMPLETE statements (including multiple entries of each type). However, a NEXT section cannot be empty.

The syntax for the MOVE_TO and JUMP_TO sections are:

```
MOVE_TO
  <Unit Initialisation Procedure action>*
END

JUMP_TO
  <Unit Initialisation Procedure action>*
END
```

At least one Elementary UIP action must be specified in each MOVE_TO or JUMP_TO section; they must not contain any ADVANCE or COMPLETE actions.

All of the UIP actions specified in a NEXT section are executed in parallel. If COMPLETE actions are present along side MOVE_TO, JUMP_TO and/or ADVANCE actions, then the first NEXT sections of the Units being COMPLETED that need to be processed are executed in parallel with all of the other actions; the second NEXT sections in the Units that are being COMPLETED will then be executed in parallel, and so on until no more NEXT sections are left to be processed.

Elementary UIP actions

Elementary UIP tasks in a NEXT section declare the change of the UIP to be applied in the next step; they may be one of the following:

1. changes to the value of a Parameter
2. changes to the choice of a Degrees of Freedom (DoF) (i.e., changing the ASSIGNment of one Variable to an ASSIGNment of another)
3. changes to the value of a DoF (i.e., changing the value of an ASSIGNED Variable)
4. changes to the value of a Selector Variable
5. reversion of original value of a Parameter, DoF or Selector Variable.

Elementary UIP tasks are only allowed for those Model elements that were modified in the START section; otherwise a syntax error will occur. For changes to the choice of DoF, the Variables involved must be ASSIGNED ones, i.e. they were not REPLACED in an earlier step. Otherwise they will be reported as specification errors.

The syntax for items 1 to 4 above is identical to the START section. The syntax for reverting the original value of a Parameter, Variable or Selector Variable is, respectively:

```
REVERT ParameterPath ;  
REVERT VariablePath ;  
REVERT SelectorPath ;
```

Implicit Final Step

If, after the final NEXT section has been processed, one or more modifications of the gIP have not been REVERTed, a final implicit step will be performed where all remaining modifications are REVERTed to their original values in parallel.

Advancing Initialisation Procedures of Units

If a Model contains Units, then the Initialisation Procedure may control the advancing of steps for any of the Units' Initialisation Procedures. The ADVANCE task is used to do this within any of the NEXT sections:

```
NEXT  
    ADVANCE unitname ;  
    ADVANCE [modelname] ;  
END
```

The first line advances the IP of the Unit *unitname* by one step, where *unitname* may be the path of a single Unit, an array of Units or a slice of an array of Units. The IP of *unitname* can only be advanced if *unitname* was specified in the USE section.

The second line advances the IPs of all Units declared as *modelname* (the brackets [] are compulsory and are part of the syntax — *modelname* is not an optional argument in this case).

When more than one Unit is ADVANCED in a NEXT section, the appropriate NEXT sections within the Units' IPs are all processed in parallel. After the final NEXT section has been ADVANCED, the next ADVANCE task causes the implicit final step to be performed (if necessary). Any further ADVANCES have no effect on any Units that have completed their final step.

The COMPLETE task is used to advance all steps (in sequence) of a Unit or group of units and complete their initialisation procedures; its syntax is:

```
NEXT  
    COMPLETE unitname ;
```

```
COMPLETE [modelname] ;  
END
```

Using COMPLETE is equivalent to calling ADVANCE on a Unit (or group of Units of the same Model type) as many times as is necessary to complete the initialisation procedure. When more than one COMPLETE task is used in the same NEXT section, the first NEXT section of each Unit that has not yet been executed is processed in parallel, then the second and so on until all NEXT sections and explicit final steps have been completed. To illustrate this, the following two Initialisation Procedures are equivalent (Unit_1 has one step, Unit_2 has two and so on).

```
INITIALISATION PROCEDURE Initialise_flowsheet_using_complete DEFAULT  
USE  
    Stream_Cutter : DEFAULT  
    Unit_1 : DEFAULT;  
    Unit_2 : DEFAULT;  
    Unit_3 : DEFAULT;  
    Unit_4 : DEFAULT;  
END  
  
NEXT # just do the first steps in parallel  
    ADVANCE Unit_1;  
    ADVANCE Unit_2;  
    ADVANCE Unit_3;  
    ADVANCE Unit_4;  
END  
  
NEXT # finish them off (2nd steps in parallel, 3rd and so on)  
    COMPLETE Unit_1;  
    COMPLETE Unit_2;  
    COMPLETE Unit_3;  
    COMPLETE Unit_4;  
END  
  
NEXT  
    COMPLETE Stream_Cutter;  
END  
  
INITIALISATION PROCEDURE Initialise_flowsheet_with_advances DEFAULT  
USE  
    Stream_Cutter : DEFAULT  
    Unit_1 : DEFAULT;  
    Unit_2 : DEFAULT;  
    Unit_3 : DEFAULT;  
    Unit_4 : DEFAULT;  
END  
  
NEXT  
    ADVANCE Unit_1; # Step 1 of Unit_1  
    ADVANCE Unit_2; # Step 1 of Unit_2  
    ADVANCE Unit_3; # Step 1 of Unit_3  
    ADVANCE Unit_4; # Step 1 of Unit_4  
END  
  
NEXT  
    ADVANCE Unit_2; # Step 2 of Unit_2  
    ADVANCE Unit_3; # Step 2 of Unit_3  
    ADVANCE Unit_4; # Step 2 of Unit_4  
END
```

```
NEXT
    ADVANCE Unit_3; # Step 3 of Unit_3
    ADVANCE Unit_4; # Step 3 of Unit_4
END

NEXT
    ADVANCE Unit_4; # Step 4 of Unit_4
END

NEXT
    ADVANCE Stream_Cutter; # Step 1 of Stream_Cutter
END
```

UIP Algorithms

UIPs support discrete or continuous changes as advanced initialisation mechanisms. Algorithmically, discrete changes will be solved by conventional algorithms for the solution of non-linear algebraic systems. Continuous changes will be solved by a continuation method using DAE solvers.

In case of discrete changes, modifications are grouped via the following language construct:

```
JUMP_TO
    <elementary UIP task>*
END
```

In case of a continuous change, modifications are grouped via the following language construct:

```
MOVE_TO
    <elementary UIP task>*
END
```

The constructs above must contain at least one UIP task and cannot be nested. All UIP tasks must reside in either a MOVE_TO or a JUMP_TO section. The only exception is the ADVANCE task, which *must not* appear in a JUMP_TO or MOVE_TO section.