Aspen Technology, Inc.

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Introduction to Aspen Dynamics™

Based on Aspen Dynamics™ 10

February 1999

Contact Information

- Phone: 888-996-7001 or 617-949-1021
- Email: support@aspentech.com
- Internet: http://www.aspentech.com
  - Technical Support Hotline
  - Training
    (Contact: Pat Sylvia or Faith Norton)
  - Customized Support Services
    (Contact: Desmond Jacas or Andrea Orchanian)

Course Agenda - Day 1

1. Overview of Aspen Dynamics

    Example - Applying Aspen Dynamics

    Workshop - Deethanizer Tower

2. Creating a Dynamic Simulation

    Workshop - Adding Dynamic Data

3. Running the Dynamic Simulation

    Workshop - Dynamic Simulation

4. Capabilities and Key Modeling Features

    Workshop - RPlug Thermal Inertia

    Workshop - Overfilled Vessel

Course Agenda - Day 2

5. Scripts

    Workshop - Scripts

6. Tasks

    Workshop - Tasks

9. Pressure Driven simulations

    Example - Water-Ethanol Simulation

    Workshop - Pressure Driven Simulation

10. Process Control

    Workshop - PID Controller Tuning

    Workshop - Cascade Control

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Overview of Aspen Dynamics

Objective:

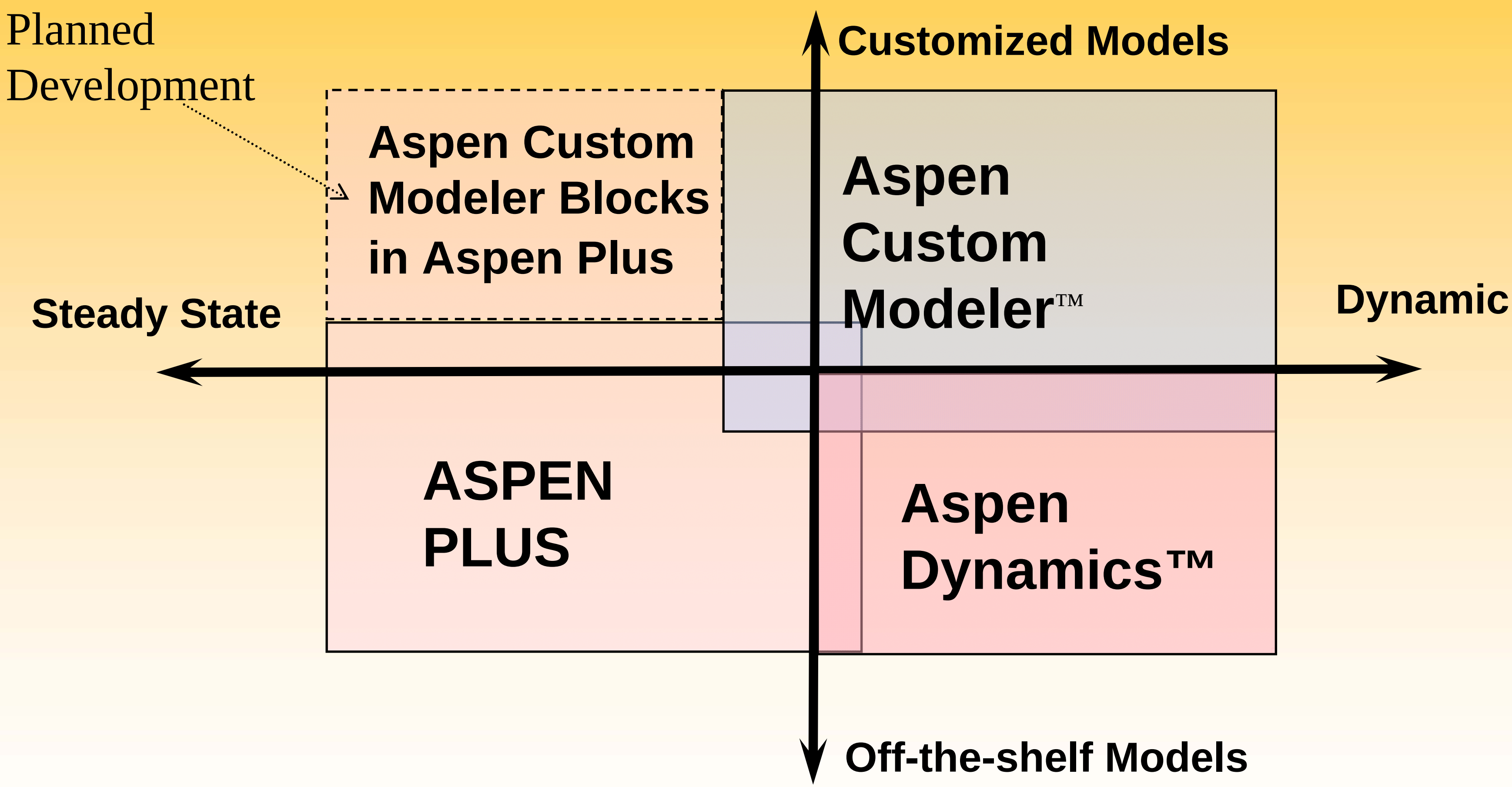
Obtain an overview of the features of Aspen Dynamics

Overview of Aspen Dynamics

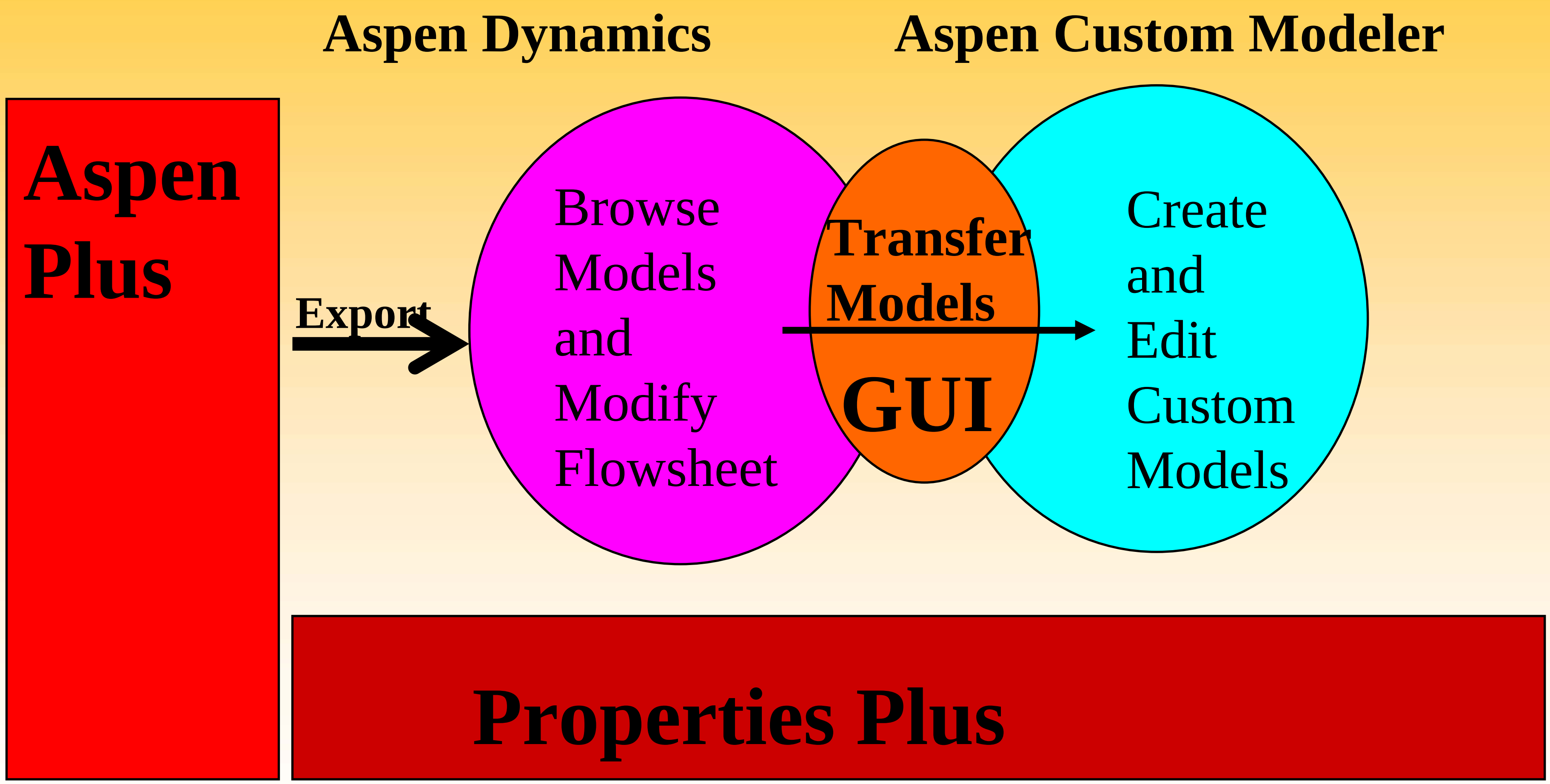
This section overviews the following

- What is Aspen Dynamics?
  - A tool for “off-the-shelf” simulations of dynamic processes
  - System requirements
- Example - Applying Aspen Dynamics
- The Aspen Dynamics Graphical User Interface (GUI)

What is Aspen Dynamics?



What is Aspen Dynamics?



What is Aspen Dynamics?

- Graphical User Interface (GUI)
- Automatic generation of dynamic simulation input specifications
  - Modify flowsheets with GUI as required
- Automatic initialization of dynamic simulations
  - Uses Aspen Plus results
- Automatic insertion of inventory controllers
  - Configure own control scheme with GUI
- Ability to import existing flowsheet blocks

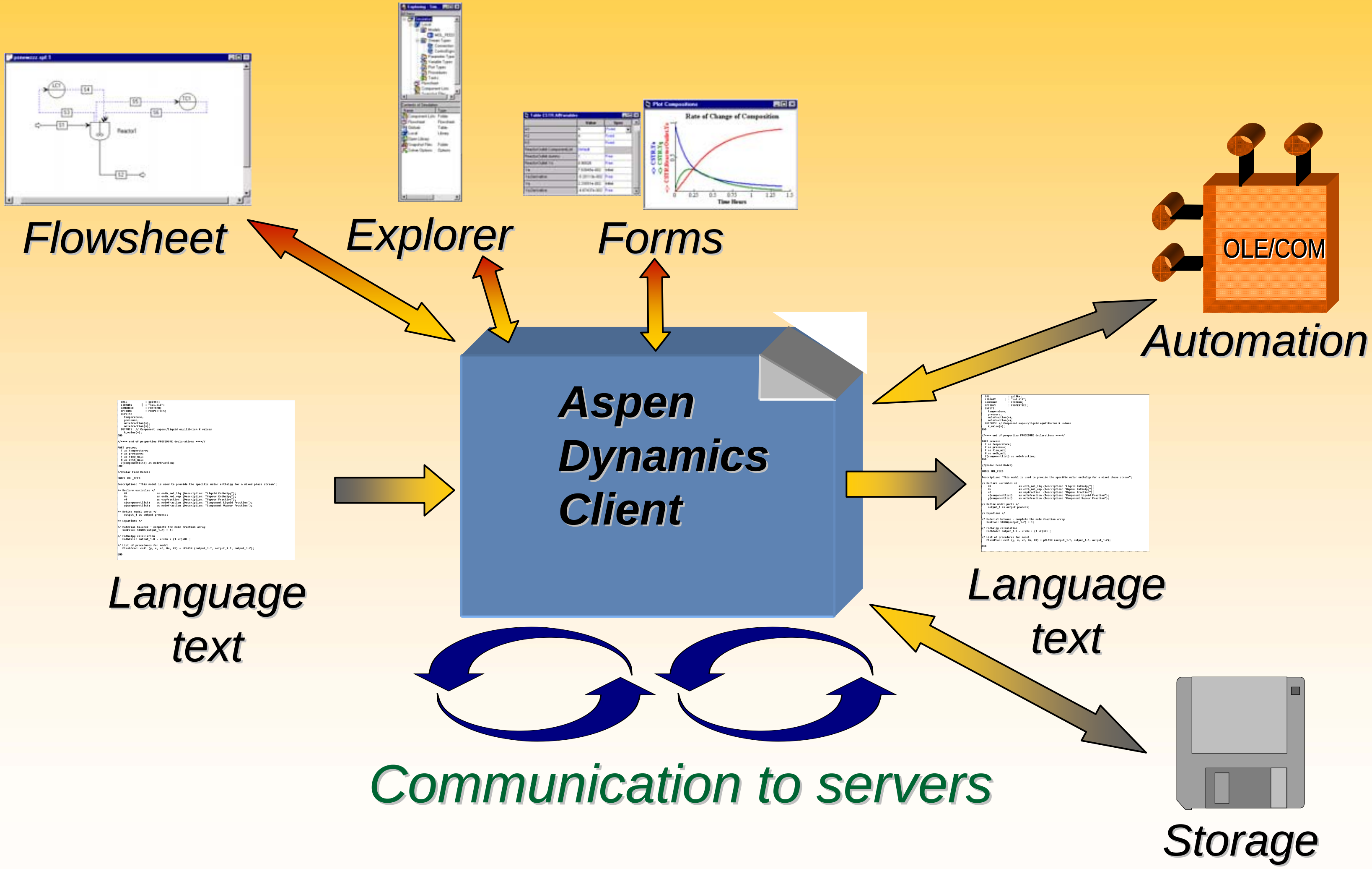
What is Aspen Dynamics?

- Supported Simulation Run Modes
  - Steady State
  - Initialization
  - Dynamic
  - Optimization
  - Estimation
- Pressure Driven Simulations

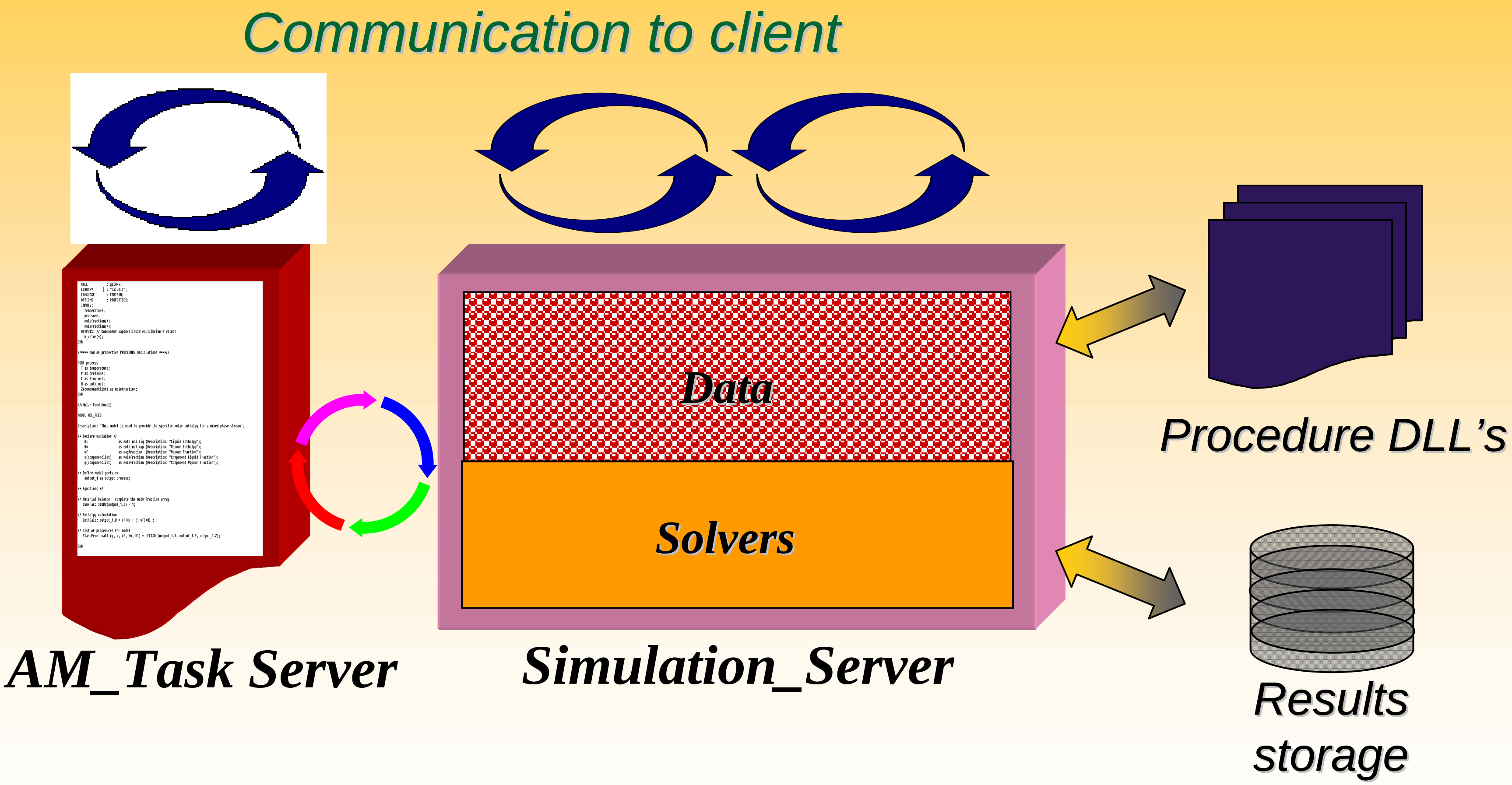
What is Aspen Dynamics?

- Access to equations for dynamic models
- Three-phase & electrolyte modeling capability
- US or Metric units of measure (UOM)
- Windows OLE Automation
- Client / Server architecture
  - Run the graphical user interface (the client) on a PC
  - Run the simulation engine (the server) on the same PC or on a separate workstation
    - Workstation servers available at version 10.1

Client Architecture



Server Architecture



System Requirements

- PCs running Windows NT (with Service Pack 3) or Windows 95
  - Intel Pentium processor with a recommended minimum speed of 166 MHz
  - 64MB RAM of memory (128 MB RAM of memory is recommended)
- Aspen Plus server MUST run on the same hardware platform

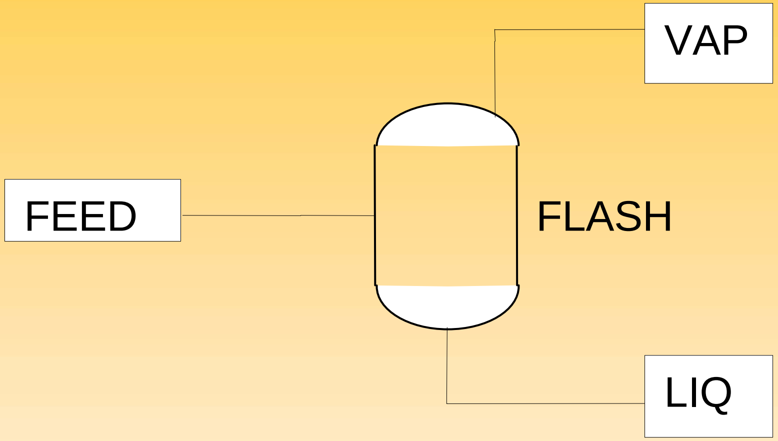
Example: Applying Aspen Dynamics

Objective:

Show how to apply Aspen Dynamics, including the key features of the graphical user interface.

Example: Applying Aspen Dynamics

Water-Methanol Flash



Vapor fraction 0.5
Pressure drop 0.0 atm
Vertical Vessel
Length 3.0 m
Diameter 2.0 m
Constant duty heat transfer
Initial liquid fillage fraction 0.5

Flowrate 100 Kmol/hr
Temperature 50 C
Pressure 2 Bar
Mass-Fractions:
Water 0.5
Methanol 0.5

Example: Applying Aspen Dynamics

- Start with a converged flowsheet: *Start-FlashExample.bkp*

- Use Aspen Plus to add dynamic data
  - Use the dynamic button to access the dynamic data folder
    - Dynamic data forms requires data for;
      - Vessel geometry
      - Heat transfer method
      - Initial liquid holdup

- Export the dynamic problem files for Aspen Dynamics

Example: Applying Aspen Dynamics

- Load the problem in Aspen Dynamics
- Use the user interface features
  - Process Flowsheet window
  - Simulation Explorer
    - All Items pane
    - Contents pane
  - Simulation Messages window
  - Menu bar
  - Tools buttons
  - Status Bar

Example: Applying Aspen Dynamics

- Initialize the dynamic simulation
  - Use (rewind) current snapshots
  - Use archived snapshots
- Run the simulation and view results from predefined tables and plots
- Produce customized tables and plots
- Modify the flowsheet control scheme by adding new controller controller elements.

The User Interface

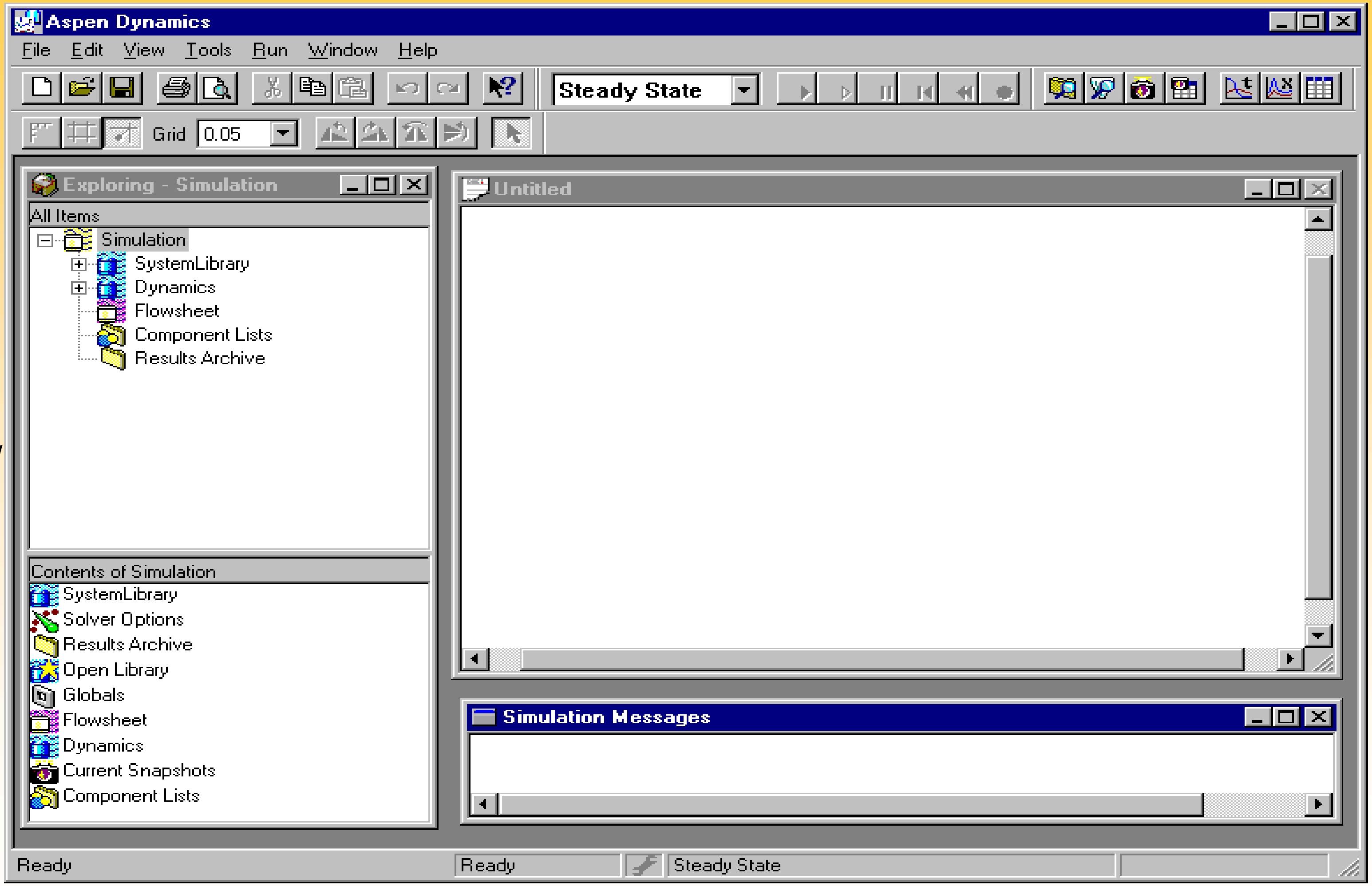
Title bar

Menu bar

Tool bars

Simulation Explorer

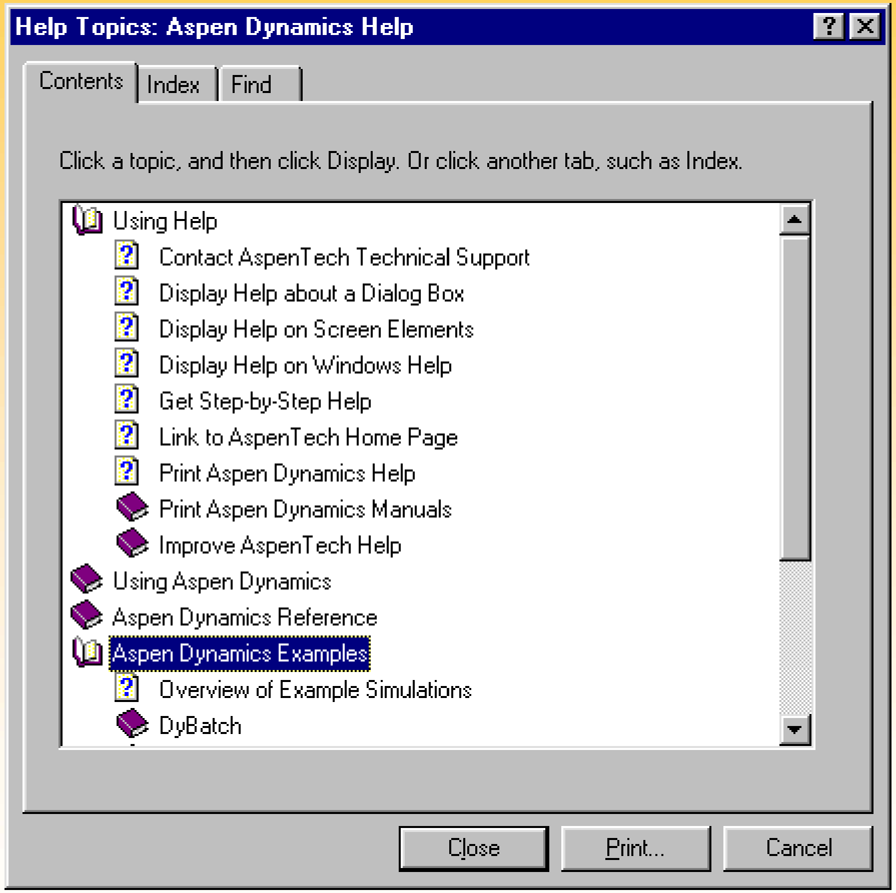
Status bar



The User Interface

- Windows 95/98 and Windows NT Client
  - Menu bar with common drop-down menus
    - Context-sensitive menus
  - Tool bars for quick access buttons to actions
    - Run, Pause (to stop), Rewind, Plot, Table, etc.
    - Includes online and context sensitive help
      - Help on using Help
      - Help on modeling assumptions and modeling philosophy
      - Help on Aspen Dynamics delivered examples

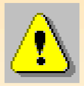
Help Window


Help Topics: Aspen Dynamics Help
Contents
Index
Find
Click a topic, and then click Display. Or click another tab, such as Index.
Using Help
Contact AspenTech Technical Support
Display Help about a Dialog Box
Display Help on Screen Elements
Display Help on Windows Help
Get Step-by-Step Help
Link to AspenTech Home Page
Print Aspen Dynamics Help
Print Aspen Dynamics Manuals
Improve AspenTech Help
Using Aspen Dynamics
Aspen Dynamics Reference
Aspen Dynamics Examples
Overview of Example Simulations
DyBatch
Close
Print...
Cancel

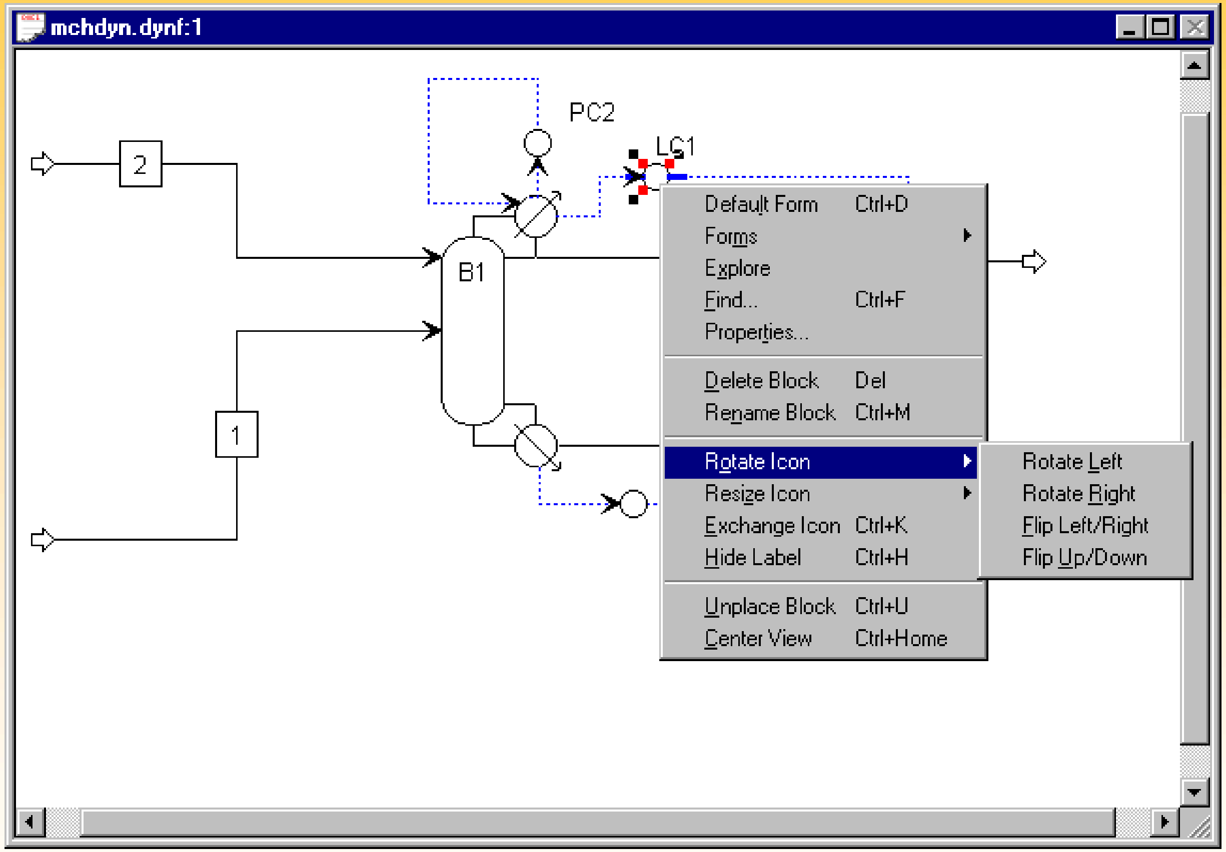
The User Interface

- Process Flowsheet Window: graphical view of block connectivity
  - Blocks are connected via streams
  - Streams are connected to ports
  - Ports are attached to blocks
- Simulation Explorer Window
  - All Items pane contains the “parent” of the objects displayed in the Contents pane
  - Contents pane displays the contents of the selected object from the All Items pane

The User Interface

- Simulation Messages Window
  - Displays messages from the solver, from the compilers, output from Scripts and Tasks, etc...
- Specification Status Bar
  - Color code informs user of specification status
  - Green for Go 
  - Double-click on status button to access the specification Status window

Process Flowsheet Window



Process Flowsheet Window with RMB Popup Menu

Process Flowsheet Window

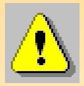
- Flowsheets are assembled using "Drag and Drop"
  - Use the left mouse button to drag an icon from the Simulation Explorer unto the Process Flowsheet window

- Pop-up menus are available with the right mouse button (RMB) on all objects
  - Flowsheet RMB actions include:
    - Zoom, Pan, Redraw, Print, etc…
  - Blocks and Streams also have RMB actions

Process Flowsheet Window

- Blocks & Streams Right Mouse Button (RMB) Pop-Up Menus
  - Move and delete blocks
  - Rotate and exchange icons
  - Rename blocks and streams
  - Reconnecting stream sources and destinations
  - Launch result tables, plots and other forms
  - Launch the Variable Find window

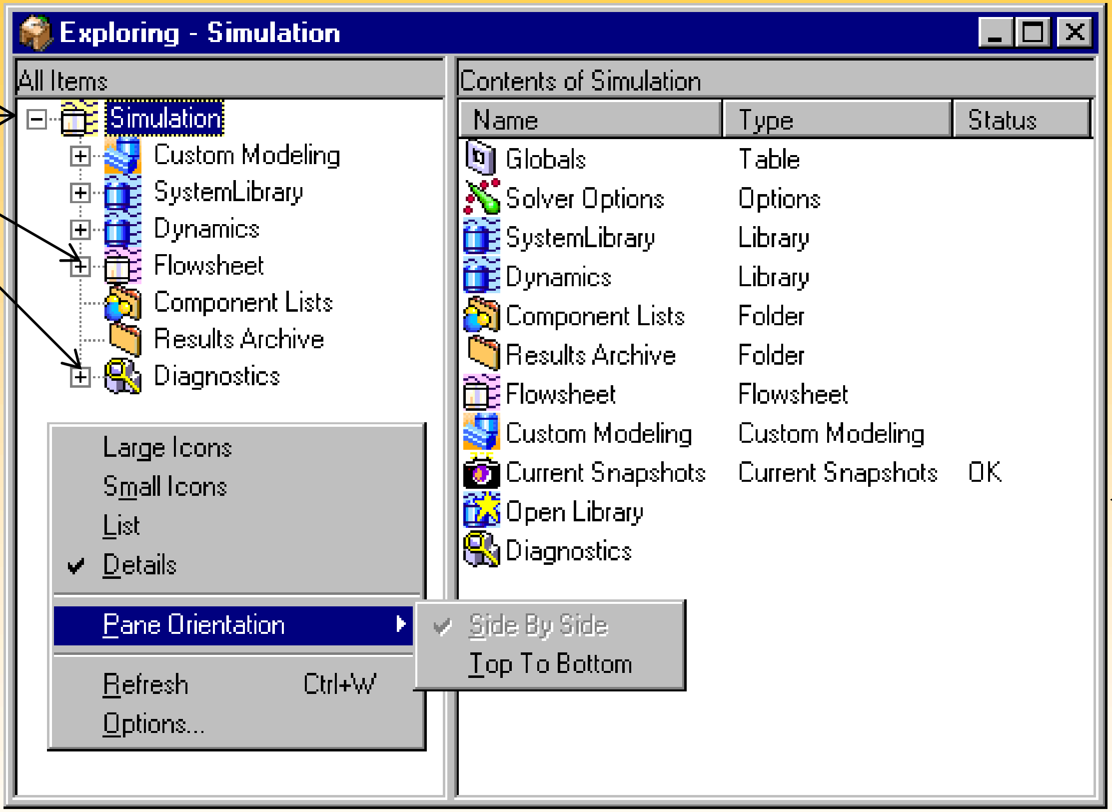
Process Flowsheet Window

- Ports
  - Connect blocks by connecting streams to ports on blocks
  - Re-position ports by dragging around icon
  - Red ports are mandatory 
  - Blue ports are optional
  - Multiple connections to single port allowed

Simulation Explorer Window

Expand/Collapse Contents

All Items Pane



Contents Pane

Simulation Explorer with RMB Popup Menu

Simulation Explorer Window

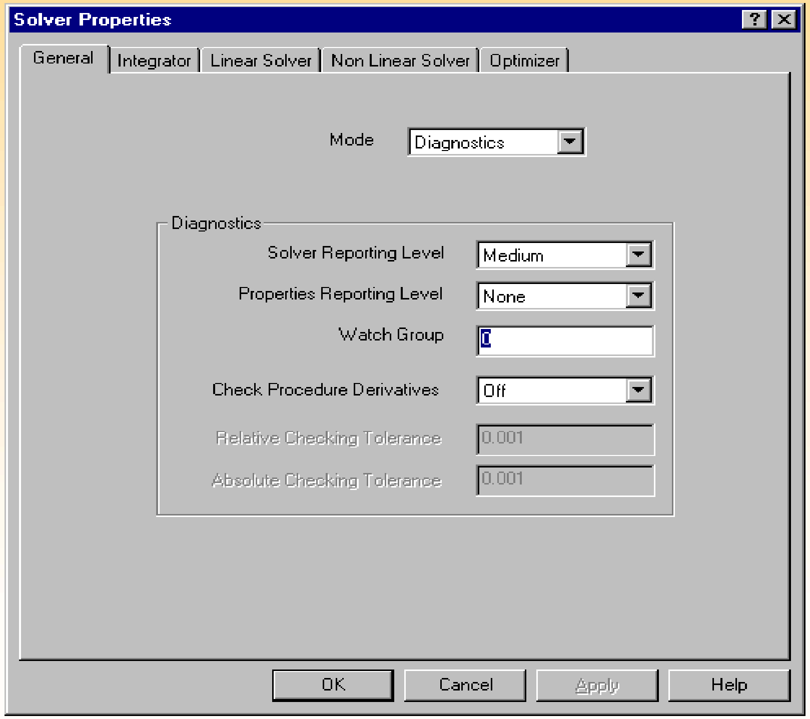
- Simulation folder contains:
  - Libraries
    - Dynamics library
      - For the Aspen Dynamics user. Folders include:
        - Models, Stream Types, Parameter Types, Variable Types, Port Types, Procedures, Tasks
    - Custom Modeling library
      - Available if enabled (and licensed)
    - Other libraries
      - Users can also create their own libraries

Simulation Explorer Window

- Simulation folder contains:
  - Flowsheet folder
    - Tree view of flowsheet blocks used in current simulation
    - Streams listed in the current simulation
    - Forms (custom and predefined)
      - Tables
      - Plots
      - Profile plots
      - LocalVariables Table
    - Tasks
    - Scripts

Simulation Explorer Window

- Simulation folder contains:
  - Solver Options forms
    - Selection of equation solvers, integrator, optimizer, diagnostic output, tolerance and other simulation options



Simulation Explorer Window

- Simulation folder contains:
  - Globals variables table
    - Details of variables global to the simulation

Table Globals

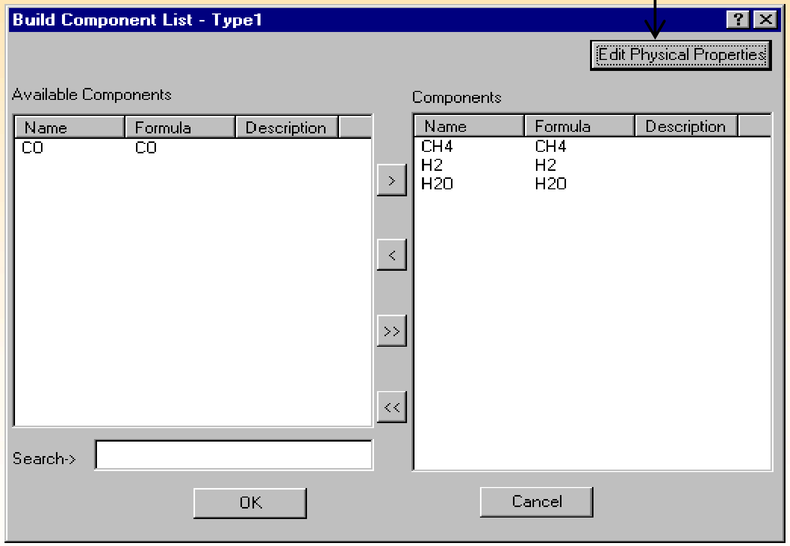
	Description	Value
global.GlobalPropMode	Global property mode	Local
global.GlobalPDriven	Simulation is pressure driven	False
global.F_max	Flow rate upper limit (kmol/hr)	1000000
global.P_max	Pressure upper limit (bar)	500
global.P_min	Pressure lower limit (bar)	0.0001
global.T_max	Temperature upper limit (C)	1995
global.T_min	Temperature lower limit (C)	-214

Variables Global to All Simulations

Simulation Explorer Window

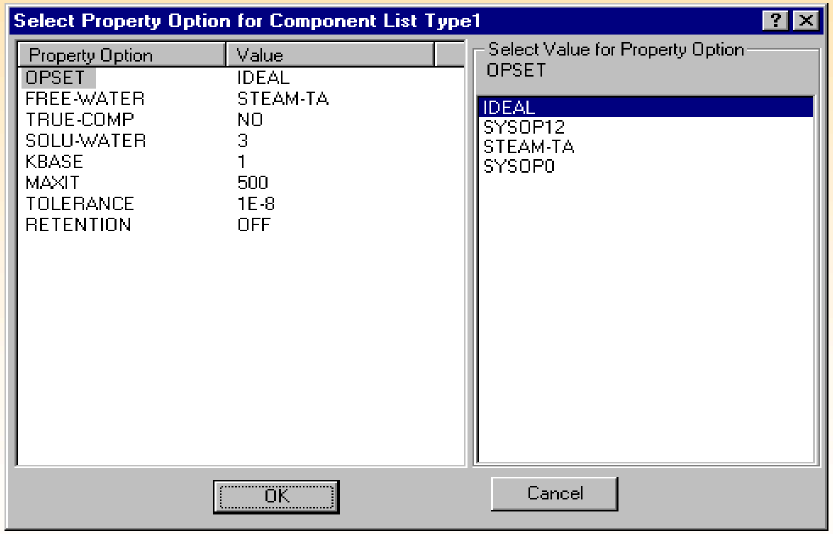
- Simulation folder contains:
  - Component Lists
    - Defines list of simulation component names and property methods used

Access to Physical Properties Options form



Component List

Physical Properties Options



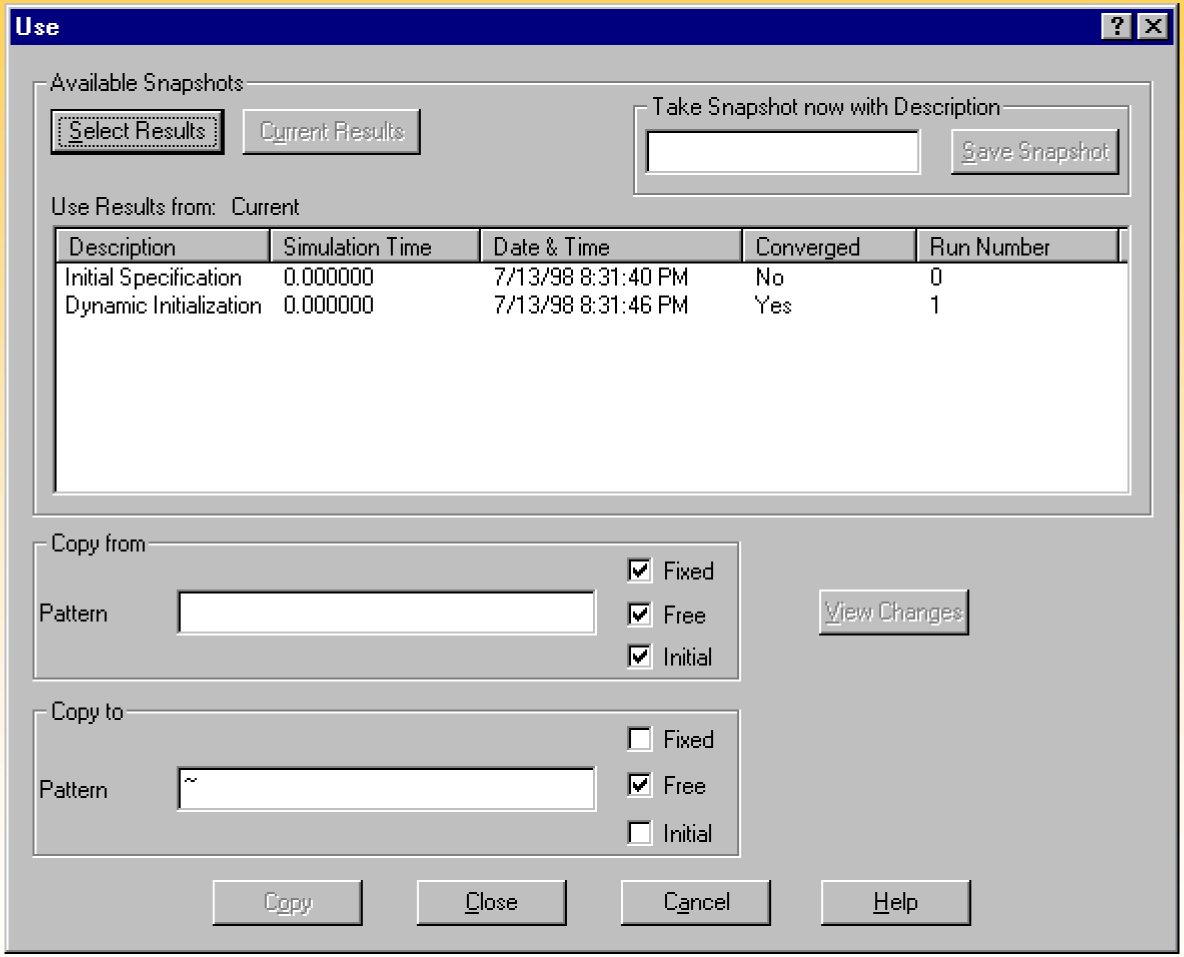
Simulation Explorer Window

- Simulation folder contains:
  - Current Snapshots (saved results applicable to current flowsheet)
    - Current snapshots are automatically (optionally) archived or removed when the flowsheet structure is modified
      - Accept option to save snapshot when prompted
  - Results Archive (stored binary format snapshots)
    - Snapshot files are stored in sub-directory with problem name under the working folder and have .snp extension.

Simulation Explorer Window

Select snapshot from archive to initialize simulation

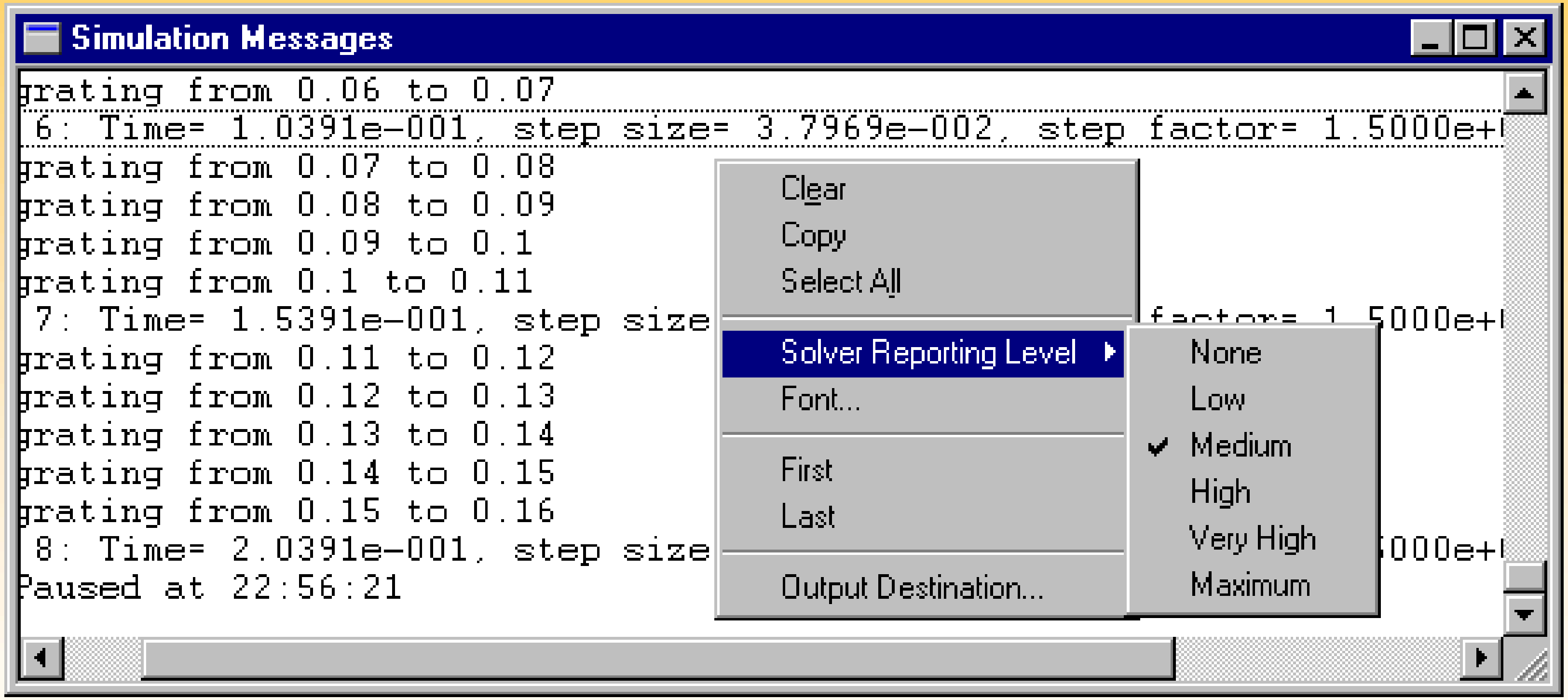
Select current snapshot to use to initialize simulation



Simulation Explorer Window

- Simulation folder contains:
  - Diagnostics
    - Information on the equations and variables pertaining to the progress of the simulation (available only during or after a run)

Simulation Messages Window



Simulation Messages Window

- Displays all messages including:
  - Errors messages
  - Compilation messages
  - Diagnostic output from solvers

- RMB Popup menu Actions:
  - Change print level
  - Change output destination
    - Screen
    - File
  - Clear contents

Workshop (15 min): Deethanizer Tower

Objective:

- Simulate a steady state deethanizer column with Aspen Plus.
- Perform a tray sizing calculation to determine the Radfrac column diameter

Getting Help on Using Aspen Plus

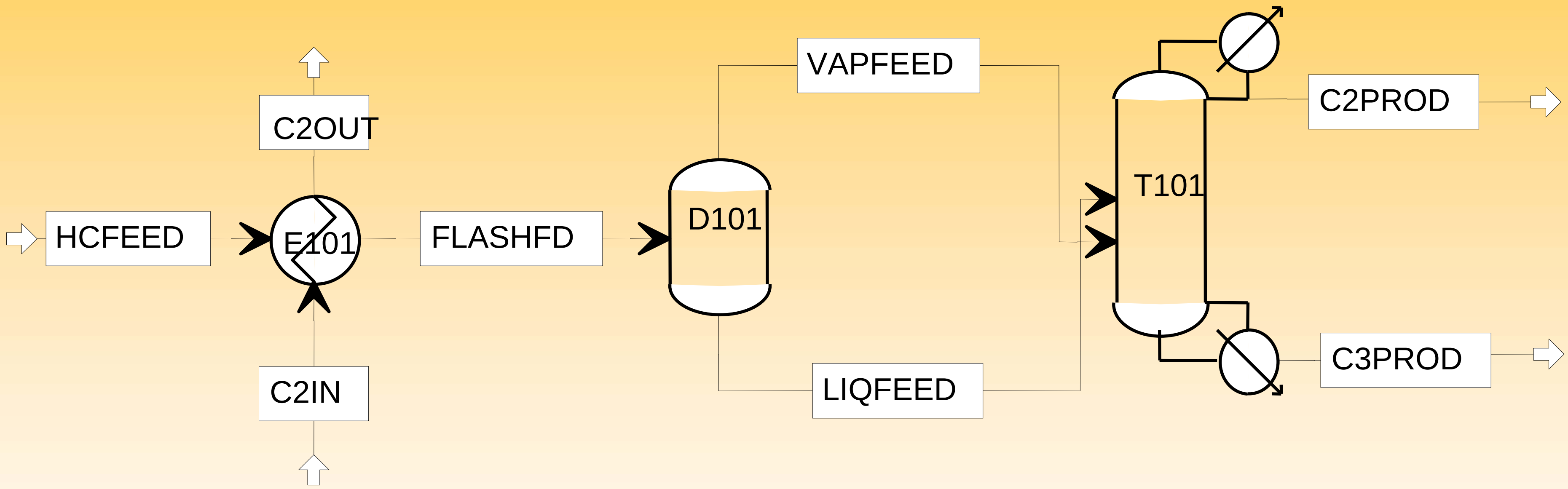
If you want help about	Do this
A particular topic	From the Help Topics dialog box, click the Index tab.
A form or field	On the Aspen Plus toolbar, click the What's This button then click the field or form.
A dialog box	Click the Help button on the dialog box.
The item the cursor or mouse pointer is on	Press F1

Workshop: Deethanizer Tower *(1)*

<u>Process Description</u>

This is a simulation of a de-ethanizer tower from an ethylene plant. The feed typically comes from a de-methanizer and is therefore colder than the deethanizer. The feed is preheated to better match the column conditions. C2 is used as the heating medium. Vapor and liquid are separated and sent to the most efficient locations in the tower. The reboiler is heated with quench water and the condenser uses C3 refrigerant. The control objective is to separate the C2s and C3s. The hard specification is the bottoms C2s concentration, although excessive C3s in the overhead can lead to operational problems in the C2-splitter downstream.

Workshop: Deethanizer Tower *(2)*



Workshop: Deethanizer Tower *(3)*

You are supplied with the backup file Start-Deethanizer.bkp. The process flowsheet and composition information have been specified. You are to add the remaining data required for the simulation, and the tray sizing (column diameter) calculations.

1. Load the file into Aspen Plus

2. Complete the information required to simulate the process described, using the data supplied - see following slides.

3. Additionally perform a tray sizing (TraySizing data sheet) for the de-ethanizer column.

4. Save your simulation as a backup file

What is the calculated column diameter?

Workshop: Deethanizer Tower *(4)*

Property Method: PSRK

Feed Streams

	HCFEED	C2IN
Mass Flowrate Kg/hr:	92,000	150,000
Temperature C:	-17	0
Pressure Bar :	21.0	25
Mole fractions:		
Methane:	0.003	
Ethane:	0.145	1.000
Propane:	0.032	
Ethylene:	0.615	
Propylene:	0.205	

Workshop: Deethanizer Tower *(5)*

Flash drum: FLASH2 block with adiabatic flash

Pressure drop = 0.1 Bar

Heat Duty = 0.0

Pre-heater: Shortcut HEATX block with cold-side outlet temperature specified.

Hot side inlet stream: C2IN

Cold side inlet stream : HCFEED

Specified cold stream outlet temperature = -12.8 C

Hot side pressure drop = -0.2 Bar

Cold side pressure drop = -0.2 Bar

Workshop: Deethanizer Tower *(6)*

De-ethanizer Column:

Number of stages = 21

Total condenser

Molar Reflux ratio = 0.6

Mass flow distillate product = 62541 Kg/hr

Feeds: Liquid to stage 13, ON-STAGE; Vapor to stage 17, ON-STAGE

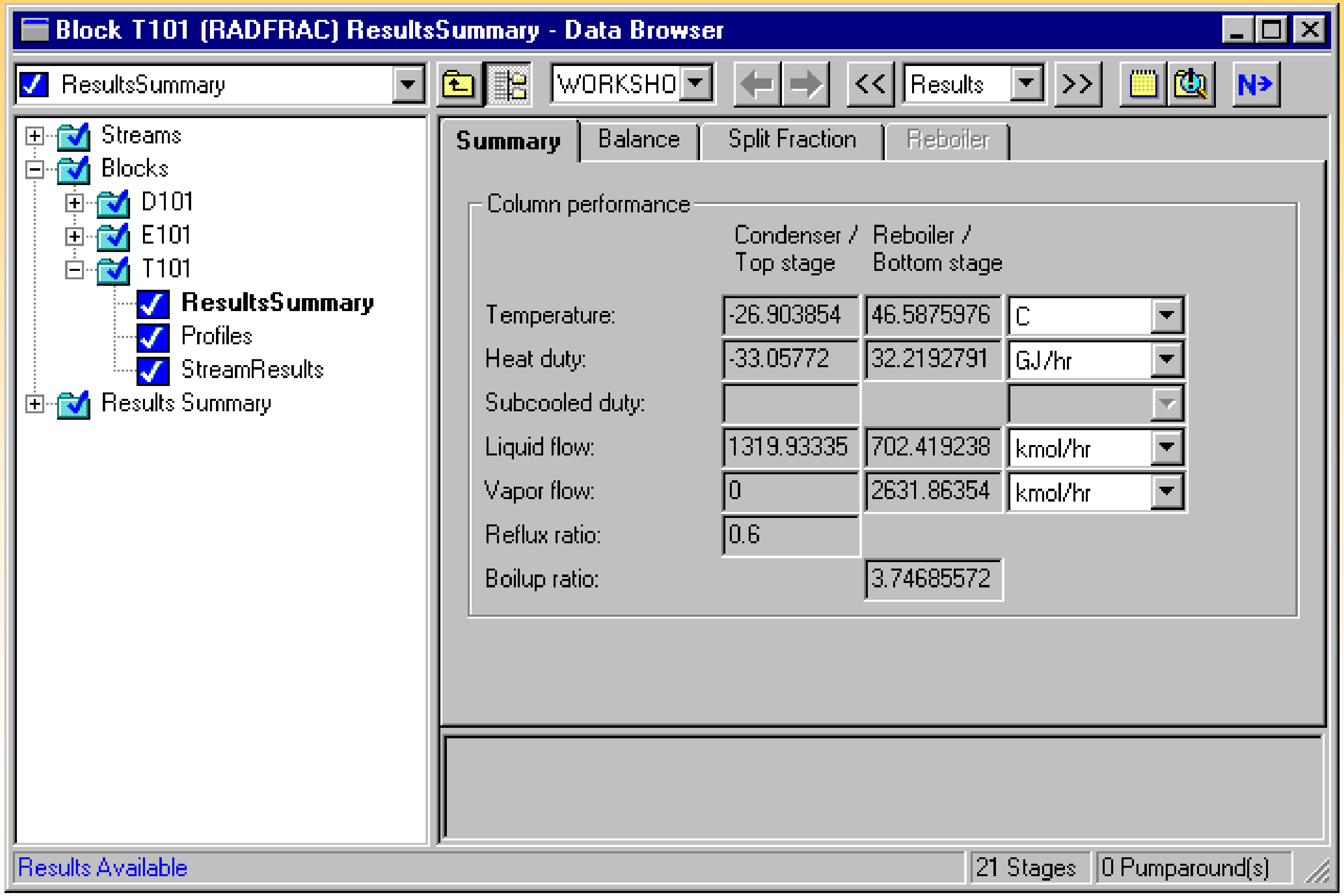
Pressures: Stage 1/Condenser = 20 bar; Stage 2 pressure = 20.1 bar

Stage pressure drop =0 .01 bar

Tray sizing calculations: Stages 2 to 20, Tray type = Sieve, Number of passes = 2

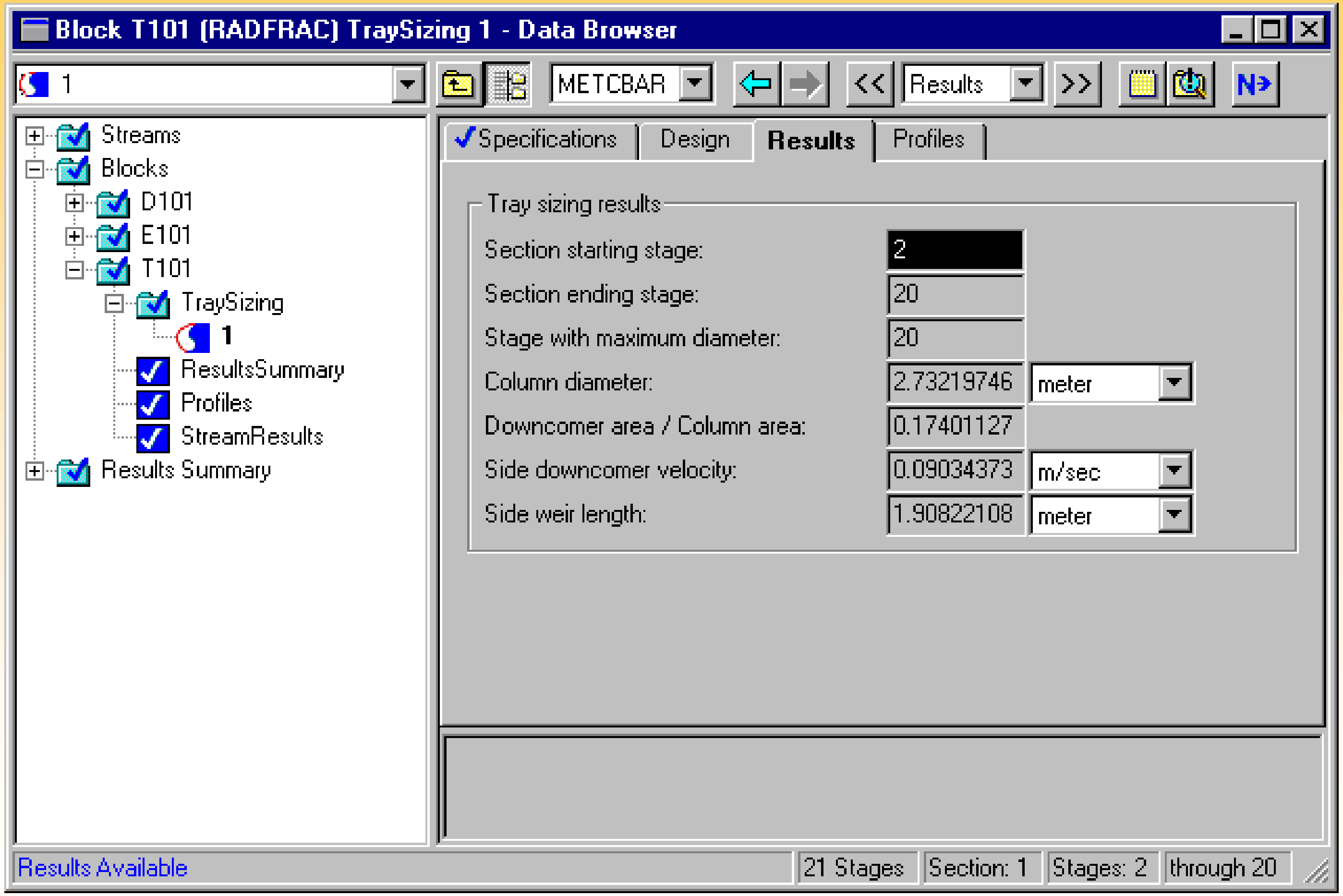
Workshop: Deethanizer Tower *(7)*

Column Results Summary



Workshop: Deethanizer Tower *(8/8)*

Tray Sizing Results Summary



Workshop: Deethanizer Tower

- Review

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Creating a Dynamic Simulation

Objective:

Describe and understand the data required for dynamic simulations and how to enter these data

Creating a Dynamic Simulation

The steps to create a dynamic simulation are:

- Start with a converged Aspen Plus steady state simulation
- Add the dynamic data required for the dynamic simulation
  - Dynamic data is not required for blocks operating in instantaneous mode by default
- Optionally convert the flowsheet to be fully pressure driven flowsheet
  - The Pressure Checker button will verify and advice on the status

Creating a Dynamic Simulation

- Run the Simulation
- Export the Simulation Problem Files
  - Flow Driven Dyn Simulation (*.dynf & *dyn.appdf)
  - P Driven Dyn Simulation (*.dynf & *dyn.appdf)

Note: You can only export simulations with status:

Results Available

Results with Warnings

Adding Dynamic Data

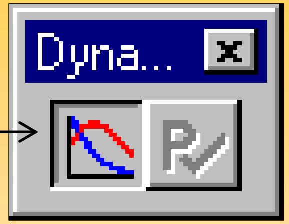
Dynamic data required includes:

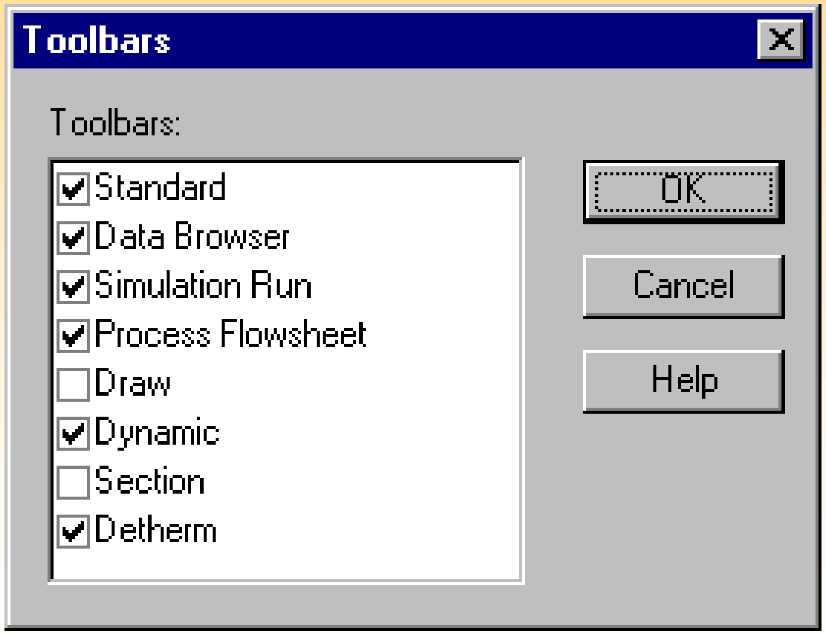
- Vessel geometry
  - Required to calculate material holdup
  - Vessels are assumed to be cylindrical
- Vessel initial fillage
  - Required to calculate the starting liquid Holdup
- Heat-transfer Method
- Hydraulics for Radfrac

Adding Dynamic Data

- Switch on access to dynamic data forms with Dynamic toolbar

Dynamic Toolbar



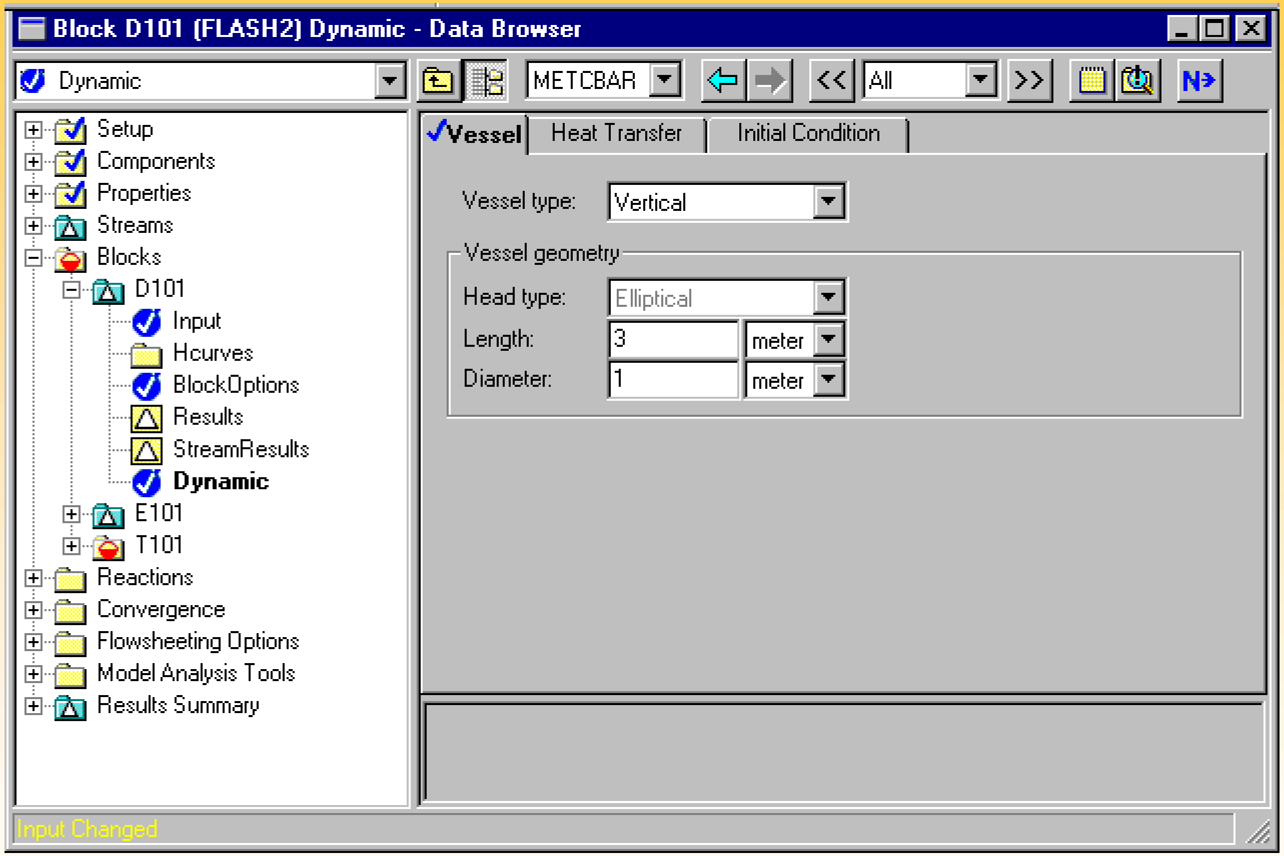


To view Dynamic Toolbar make sure Dynamic check box is selected from Toolbars dialogue box under View menu

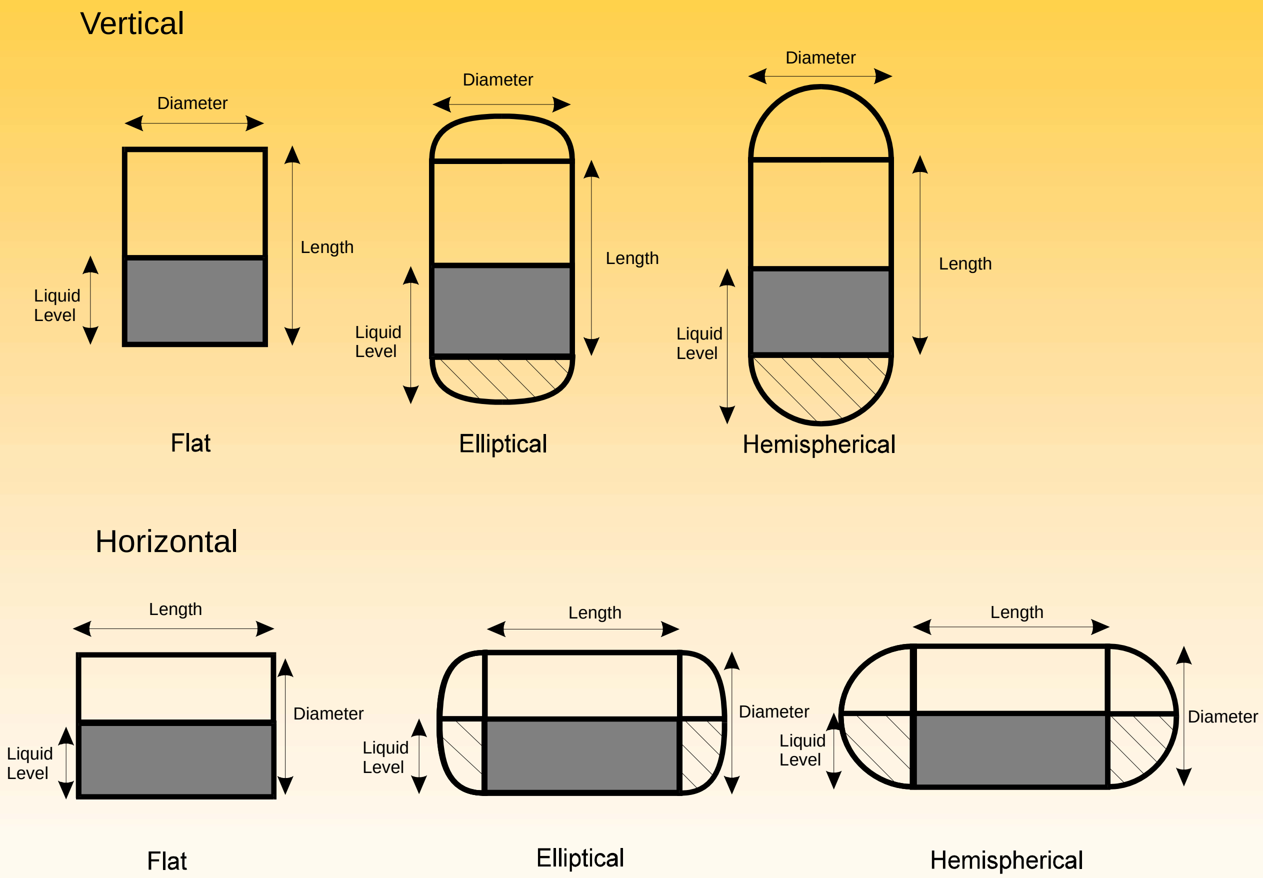
Adding Dynamic Data

- Dynamic Data Sheet
  - Vessel geometry and type
    - Orientation, Head type
    - Length, Diameter
  - Heat transfer option
    - Constant duty
    - Constant medium temperature
    - LMTD
  - Initial condition
  - Hydraulics for Radfrac Towers

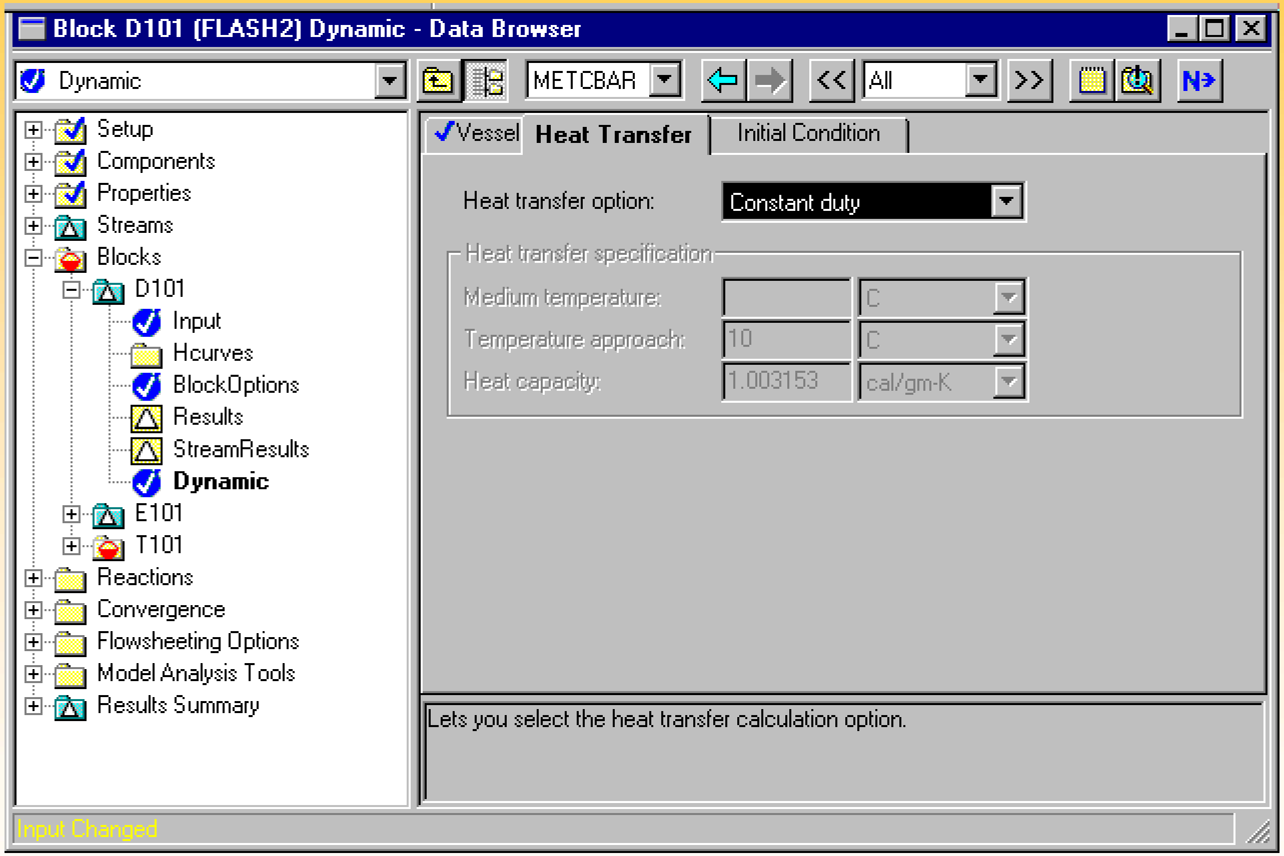
Vessel Geometry



Vessel Geometry



Heat Transfer Option



Heat Transfer Option

Method	Description
Constant Duty	Heat duty is set or directly manipulated.
Constant Medium Temperature	Heat duty is dependent on the temperature differential between the process fluid and the heating/cooling medium. The medium temperature is the same across the entire heat transfer area, and is set or directly manipulated.
LMTD	Heat duty is dependent on the log mean temperature differential between the process fluid and the heating/cooling medium. The medium inlet temperature is constant, and is set or directly manipulated.

Constant Duty Option

- Heat Duty
  - Value is fixed in the dynamic simulation initially at steady state Aspen Plus simulation results value
  - Can be manipulated in the dynamic simulation
    - Manipulate directly by manually changing the value
    - Manipulate with a PID controller

Constant Temperature Option

- Actual Duty: Q = UA . (T_process – T_medium)
  - Manipulate T_medium in dynamic simulation directly or with controller
  - Specify T_medium value on dynamic form

Variable	Description
UA	Product of the overall heat transfer coefficient (OHTC) and heat transfer area
T_process	Temperature of the process fluid
T_medium	Heating/cooling medium temperature

LMTD Option

- Actual Duty:

[1] Q = UA . LMTD

[2] Q = Fmmed . Cpmed . (Tmed_out – Tmed_in)

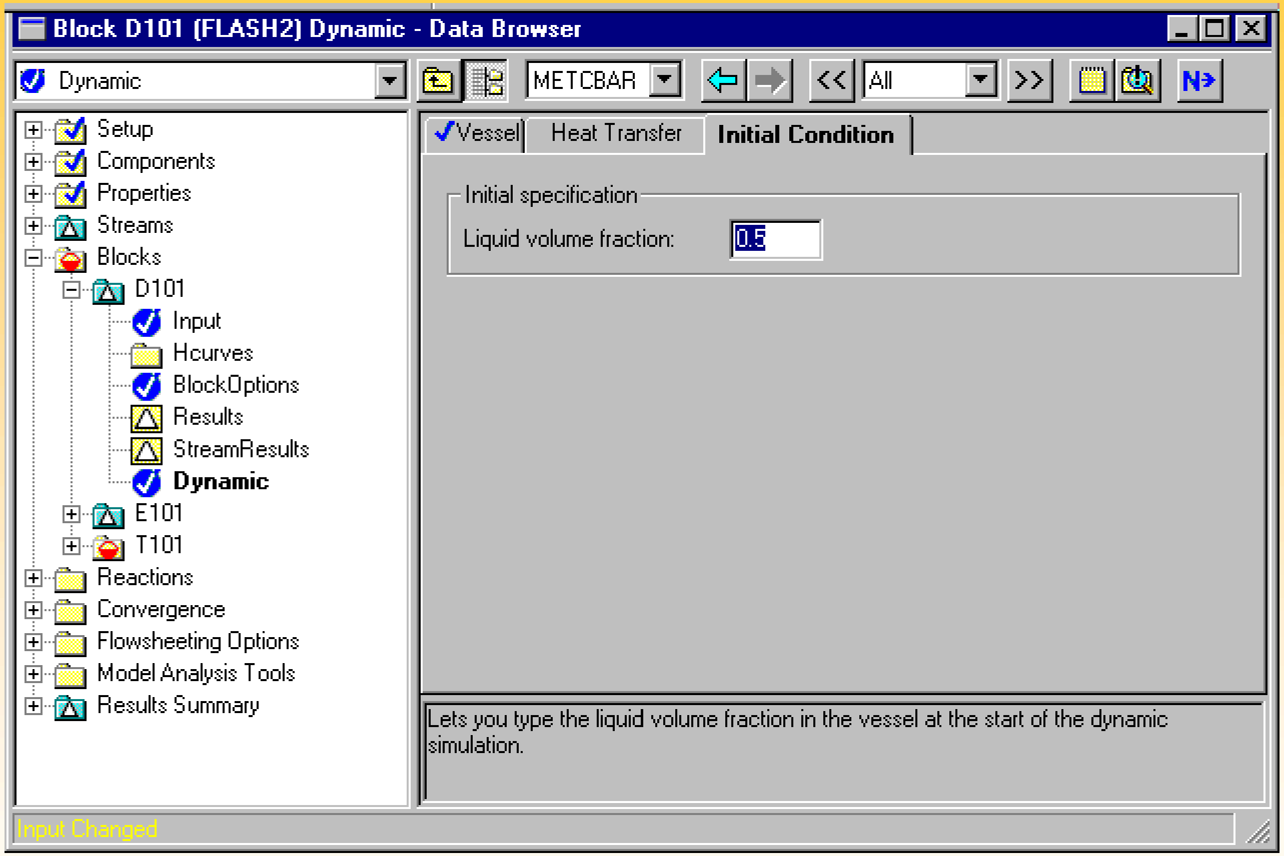
Variable	Description
LMTD	Log mean temperature difference
Fmmed	Mass flow rate of the heating/cooling medium
Tmed_in	Inlet temperature of heating/cooling medium
Tmed_out	Outlet temperature of the heating/cooling medium
Cpmed	Specific heat capacity of the heating/cooling medium
UA	Product of the OHTC and the heat transfer

LMTD Option

- Specify values for variables on the dynamic form

This variable	**Has a value that**
Tmed_in	Can be changed during a dynamic simulation
T_approach	Varies during a dynamic simulation
Cpmed	Is fixed during the dynamic simulation

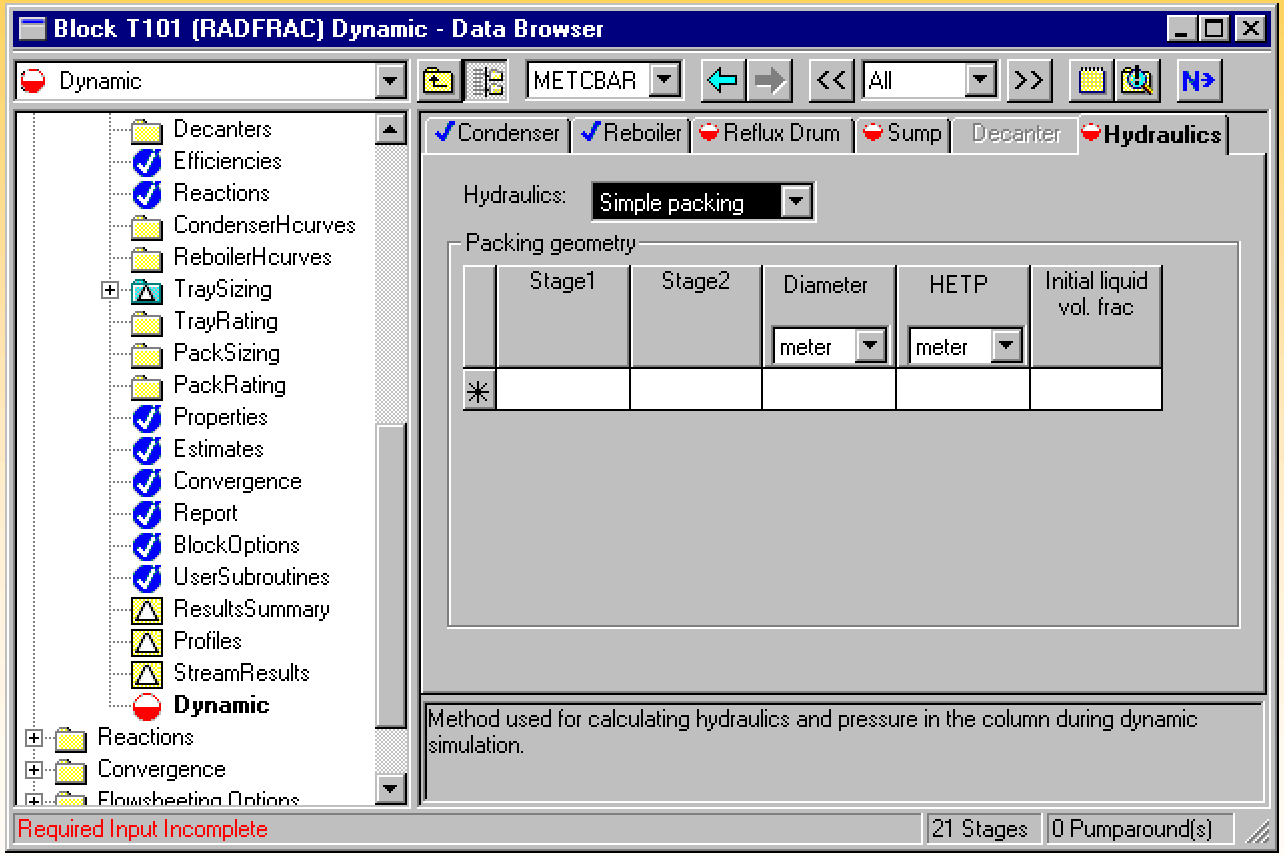
Initial Condition



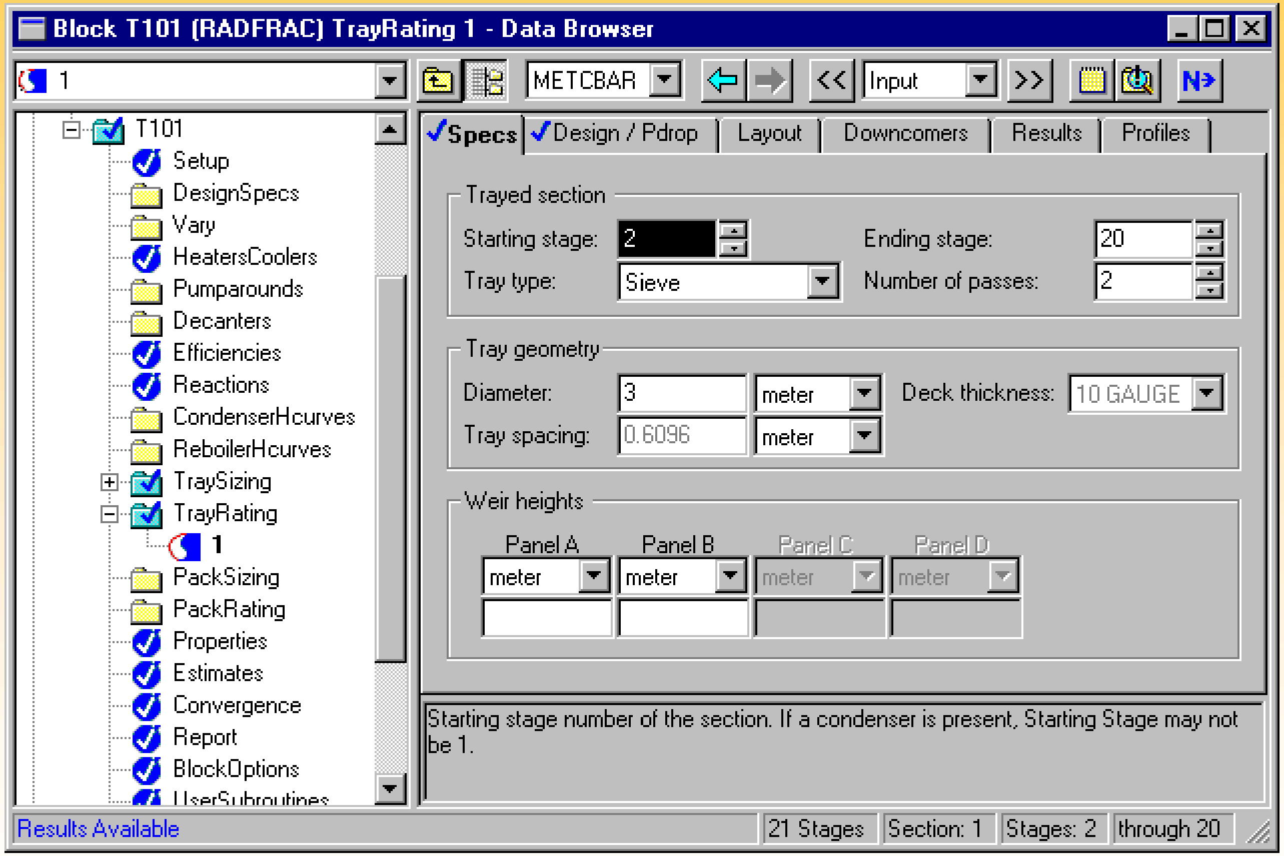
RadFrac Hydraulics

- Simple
  - Tray
  - Packing
- Rigorous (vendor correlations) with pressure update
  - Trays
  - Packing

Hydraulics for Radfrac

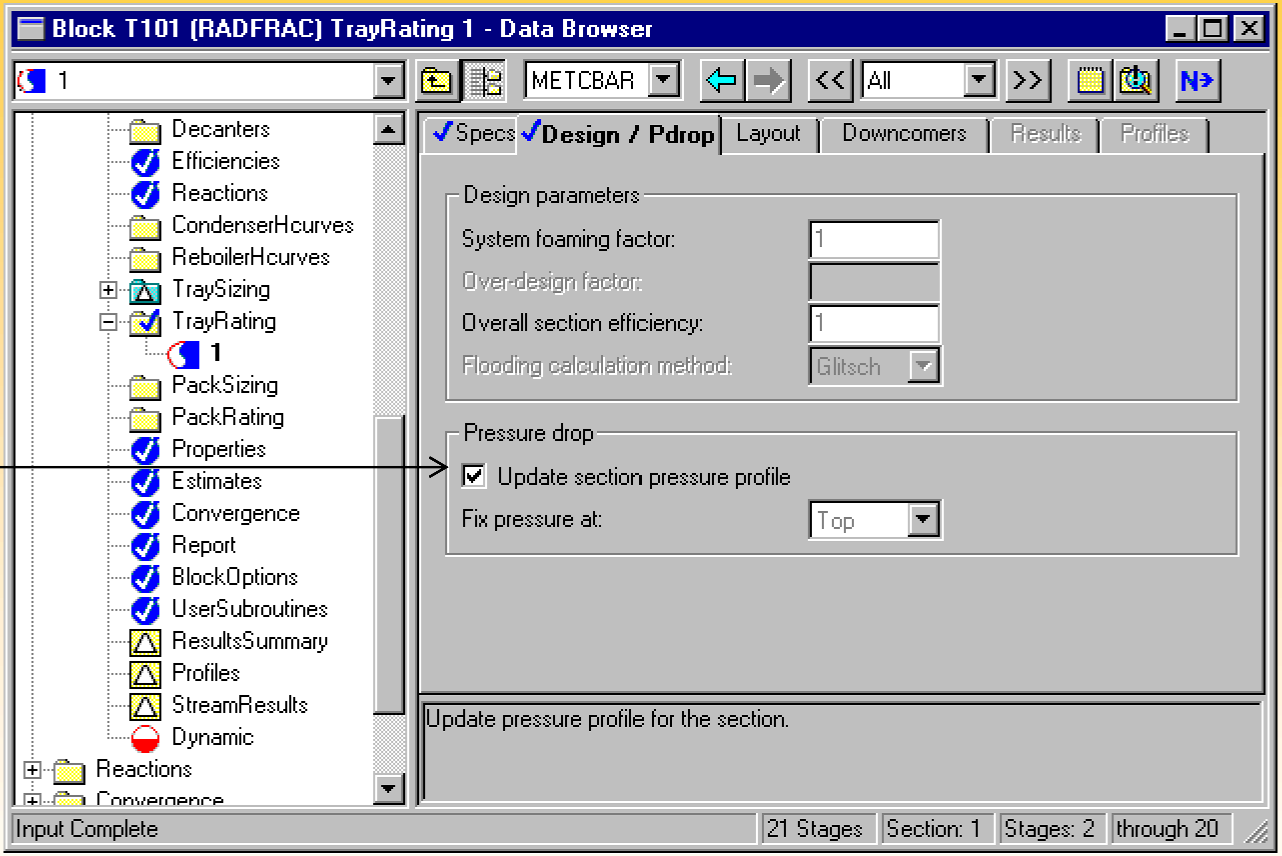


Radfrac Rating - Rigorous Hydraulics



Radfrac Rating Pressure Update

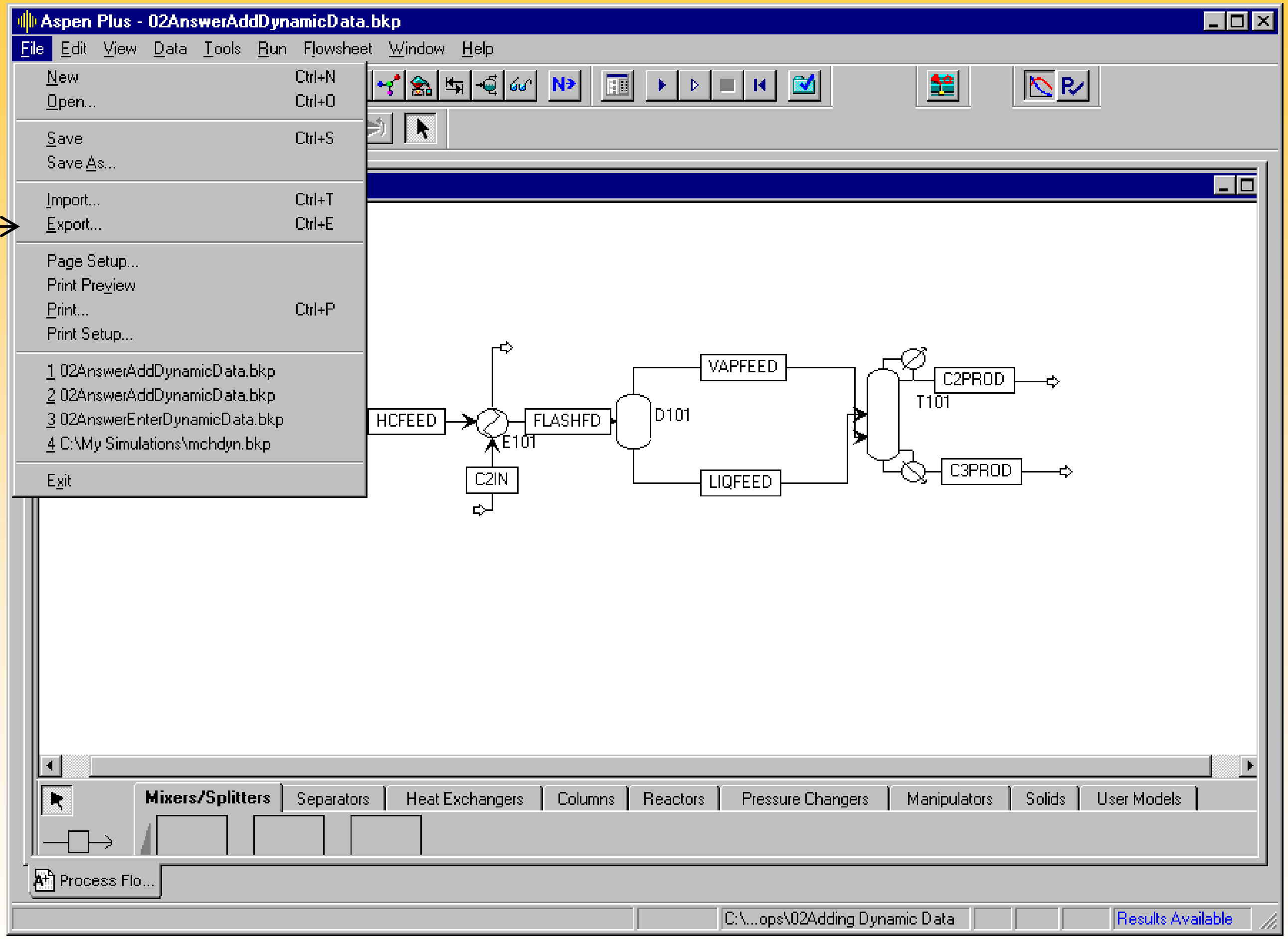
Pressure update box checked



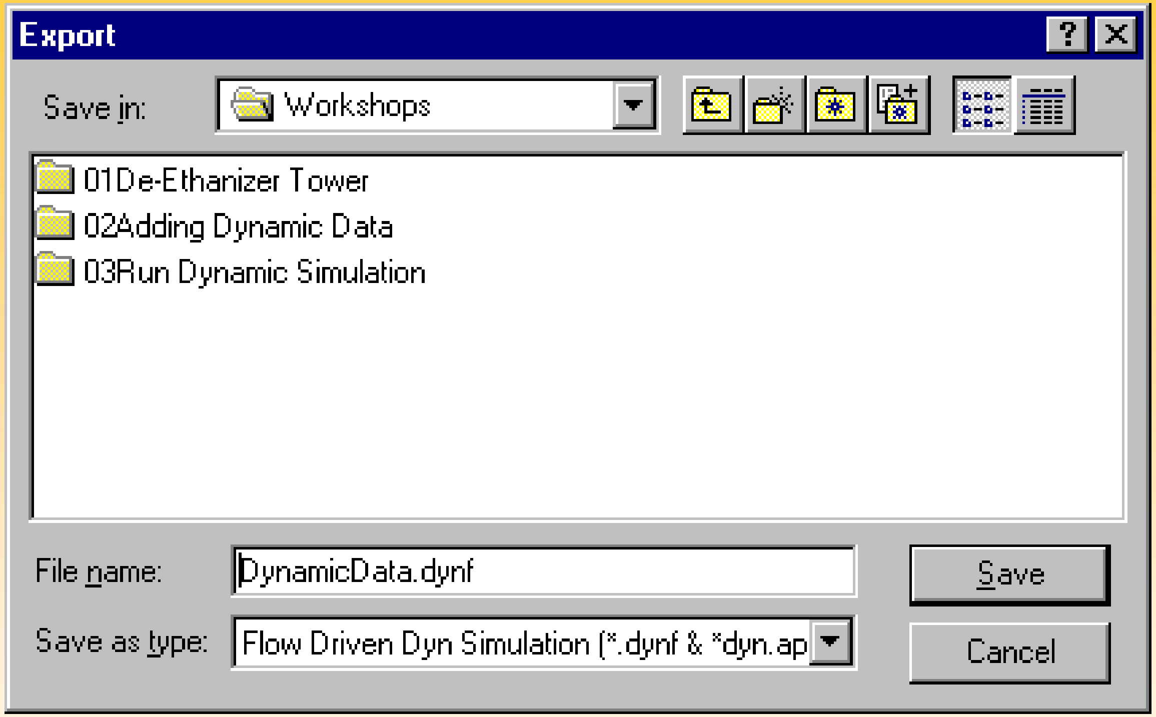
Exporting the Dynamic Simulation

Menu bar

Export file(from file menu)



Exporting the Dynamic Simulation



Note:
You can export only simulations with status of:
Results Available
Results with Warnings

Workshop (15 min): Adding Dynamic Data

Objective:

- Use Aspen Plus to add dynamic data to the steady state simulation.
- Perform a Radfrac block tray rating calculation to generate the column hydraulics.

Workshop: Adding Dynamic Data *(1)*

1. Load the file Start-AddDynData.bkp

2. Add dynamic data (see following data slides) to the steady state problem from the previous workshop.

3. Include a tray rating (TrayRating data sheet) section to calculate the column
4. Run the steady state simulation

5. Export the Aspen Dynamics problem definition files as a flow driven simulation file.

6. Save your simulation as a backup file.

Should there be a difference in results with and without dynamic data as seen in the Aspen Plus steady state simulations?

Workshop: Adding Dynamic Data *(2)*

T101 De-ethanizer Column:

Reflux Drum: Horizontal vessel
Length: 5 m, Diameter: 2 m

Reboiler Sump: Height = 3 m , Diameter = 2.8 m (from tray sizing result)

Condenser: Constant temperature (-45 C) cooling medium

Reboiler: LMTD heat transfer option,
Quench water medium temperature: 80 C
Temperature approach: 5 C

Tray Hydraulics: Rigorous (TPSAR) calculations, with pressure profile update option - TrayRating data sheet, Design / Pdrop tab

Workshop: Adding Dynamic Data *(3)*

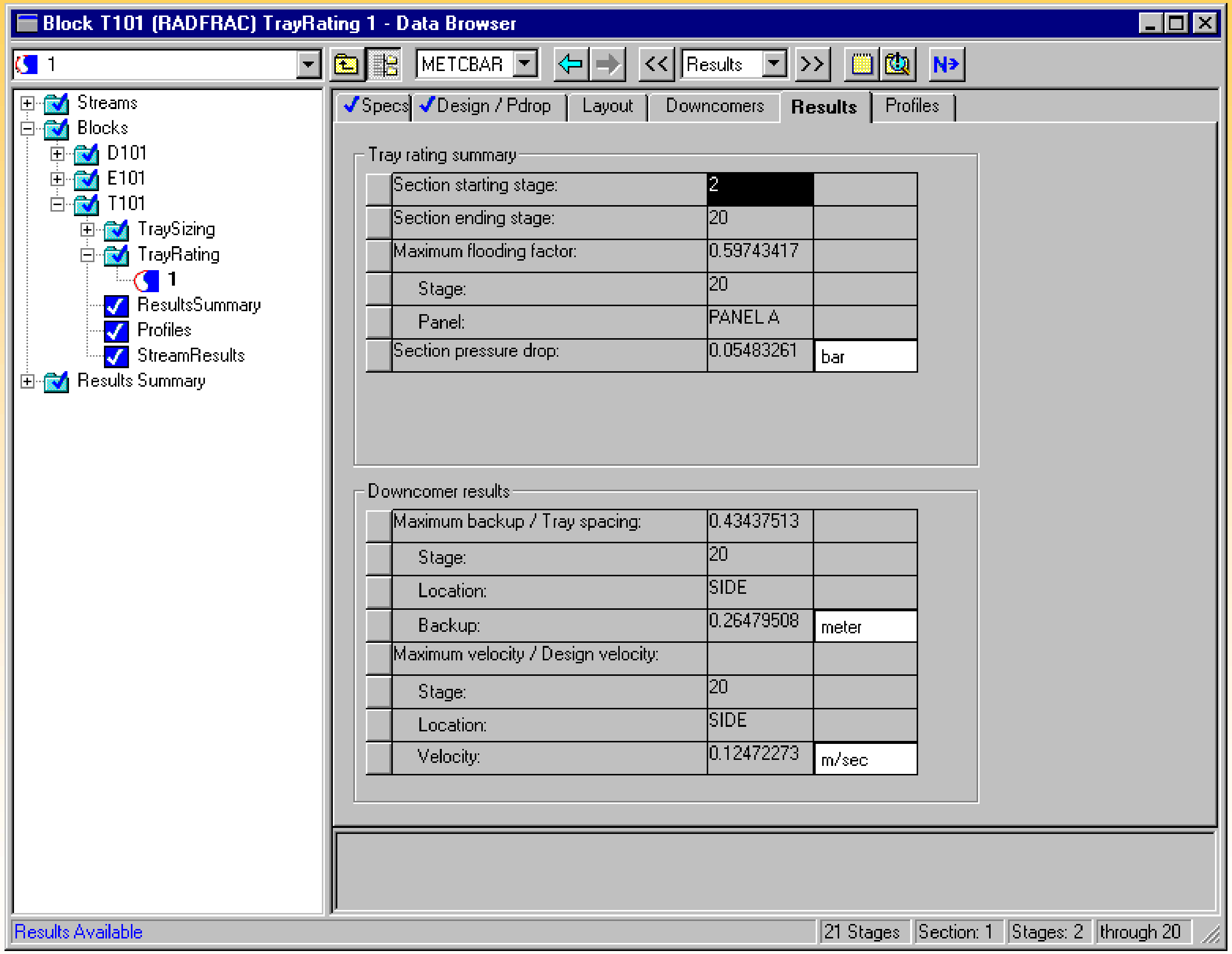
Tray Rating for T101 Column
Trayed section: Stages 2 to 20
Sieve Tray, 2-pass
Diameter = 2.8 m (from tray sizing results)
Update section pressure profile

E101 Pre-heater
Assume instantaneous (steady state) operation

D101 Flash drum:
Vertical vessel, with constant heat duty heating option
Length = 3m, Diameter = 2m
Initial liquid volume fraction = 0.5

Workshop: Adding Dynamic Data *(4/4)*

Tray Rating Results Summary



Adding Dynamic Data

- Review

Reach Your
True
Potential

Running the Dynamic Simulation

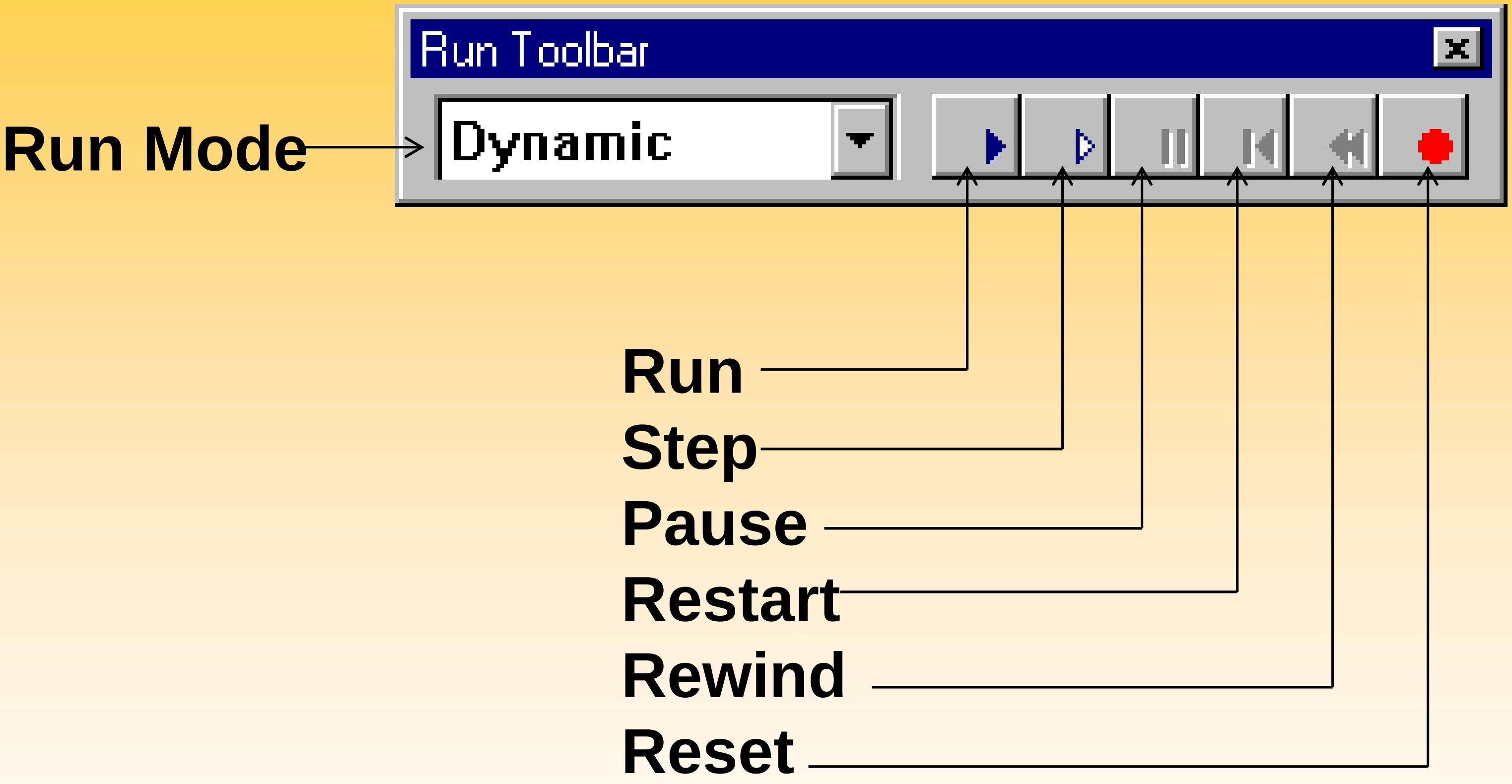
Objective:

Describe and become familiar with the user interface features required for running dynamic simulations

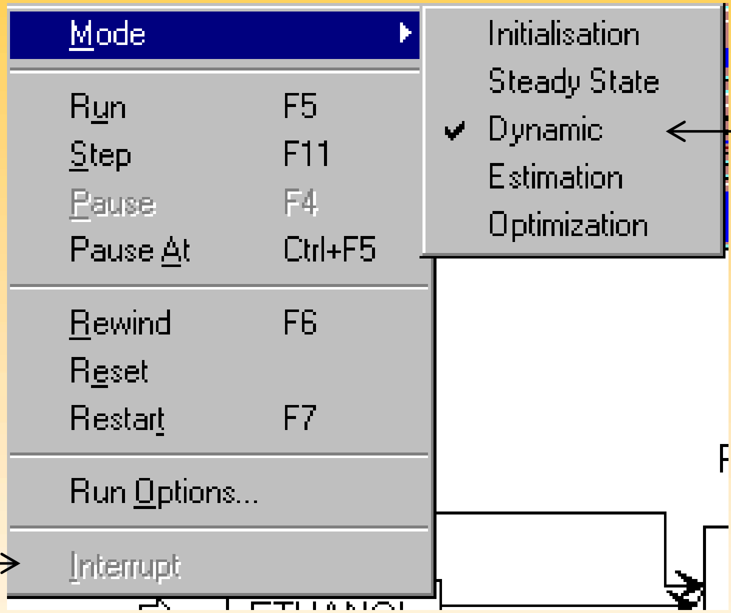
Running the Dynamic Simulation

- Run Control
- Tools
  - Run Options
  - Snapshots
  - Results Displays
  - Units of Measure
  - Variable Find
- Specification Status and Status Bar

Run Control Buttons



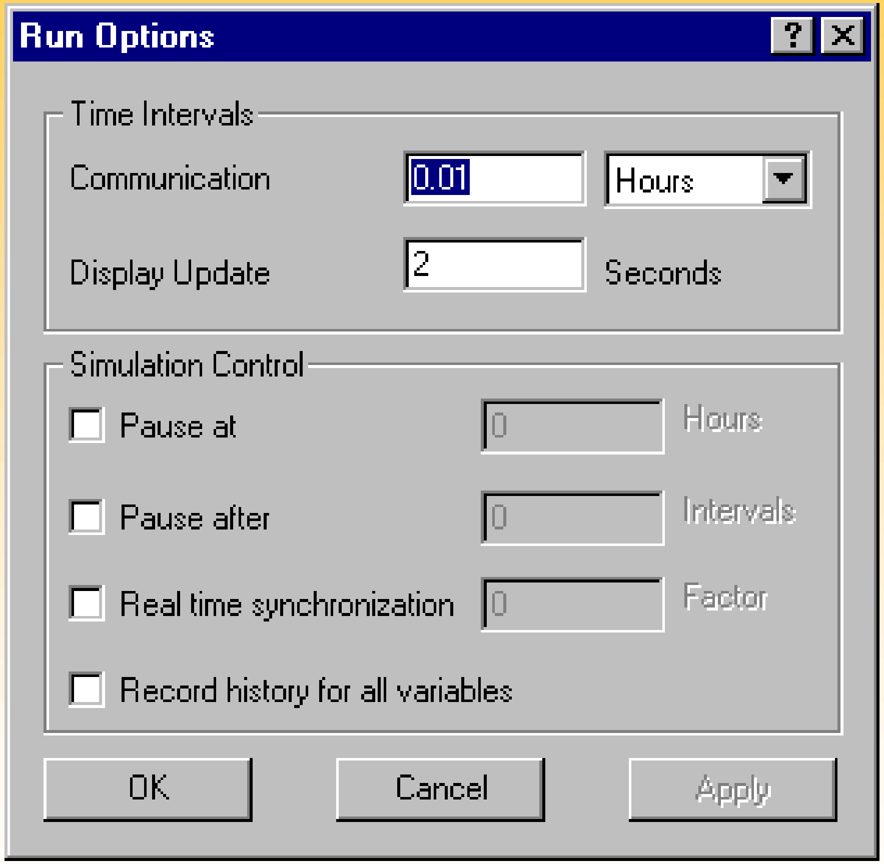
Run Menu



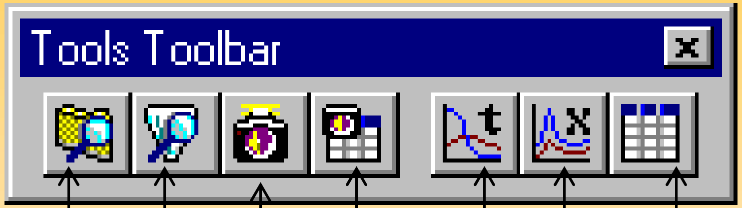
Run Modes

Interrupt Run

Run Options


Run Options
Time Intervals
Communication
0.01
Hours
Display Update
2
Seconds
Simulation Control
Pause at
0
Hours
Pause after
0
Intervals
Real time synchronization
0
Factor
Record history for all variables
OK
Cancel
Apply

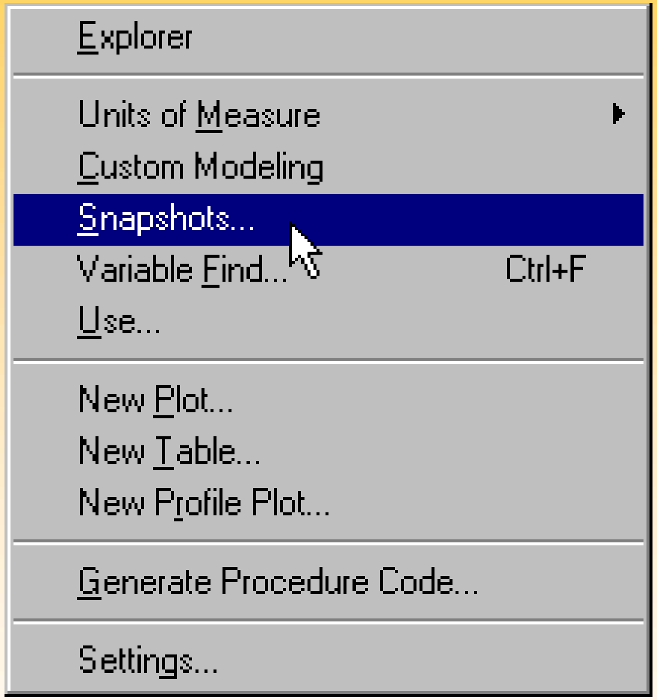
Tools Buttons



Open Explorer
Variable Find
Snapshots
Initialize Simulation

New Table
New Profile Plot
New Plot

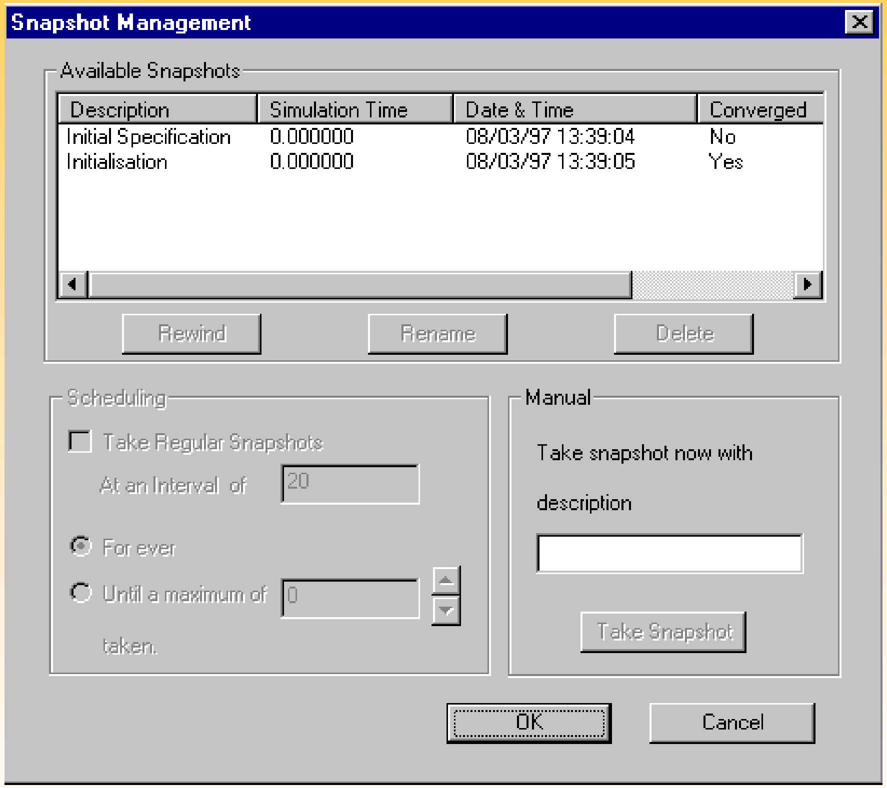
Tools Menu - Snapshots



Snapshots

- Snapshot Management
- Use of snapshots
  - Initialization
  - Restart
  - Rewind

Snapshot Management



Snapshot Management

- Automatically Saved Snapshots
  - Initial specification
  - Dynamic initialization (converged) at time zero

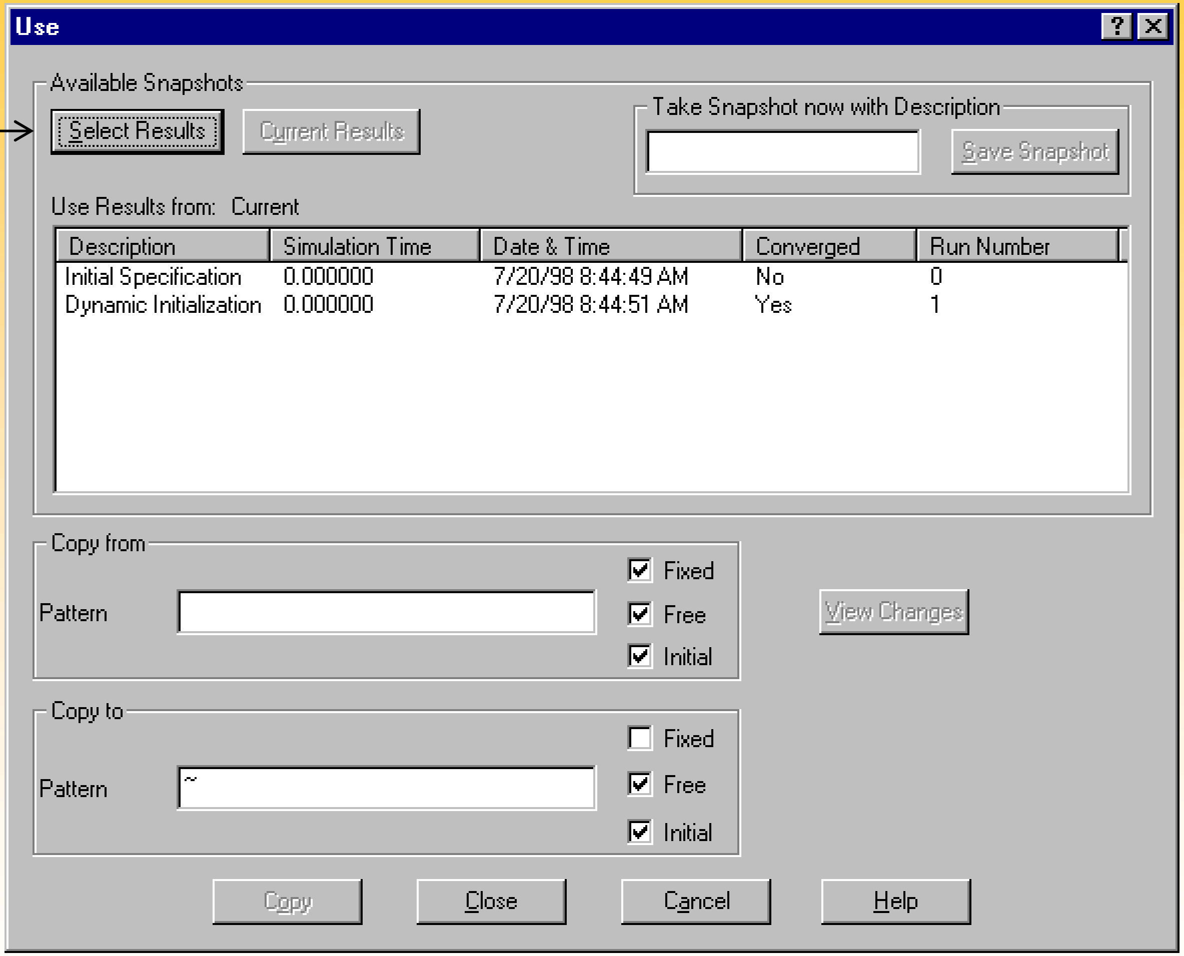
- New snapshots can be created
  - Take regular snapshots
    - Specify interval
  - Take manual snapshots

Use of Snapshots

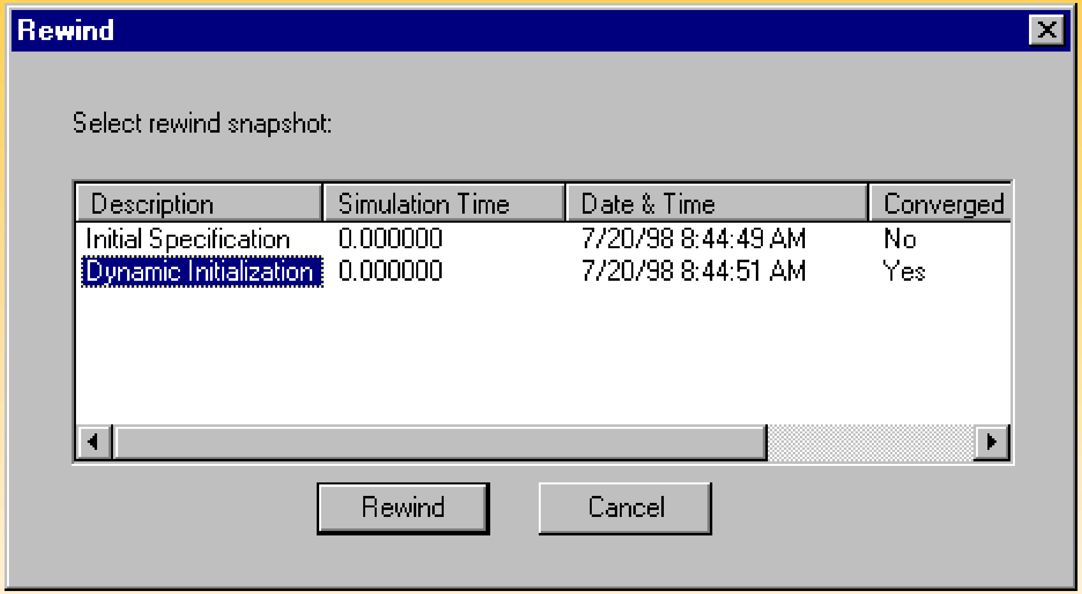
- Restart simulation
  - Time zero - snapshot selected automatically
- Rewind Dynamic Simulation
  - Specify snapshot (and time) to rewind to
- Initialize simulation

Use Form

Archived Snapshots



Rewind Form

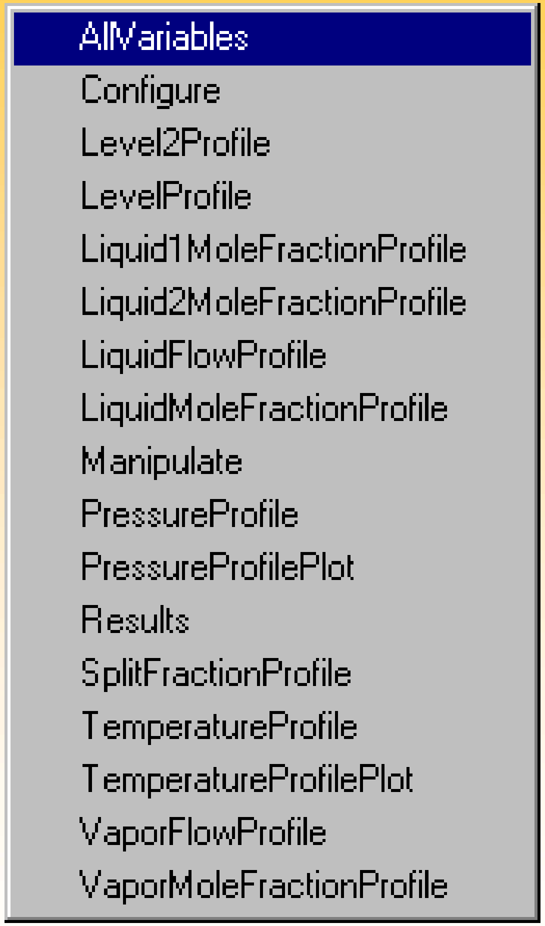


- Select Snapshot
  - Automatically selects simulation time

Results Displays

- Predefined
  - Tables
  - Plots
    - Time series
    - Profiles (stage-wise processes)
- Custom
- Access Results using OLE Automation

Results Display Forms



Results Tables

- Predefined Tables
  - AllVariables
  - Configure
  - Manipulate
  - Results
  - Profiles (stage-wise processes)

Predefined Tables

This table	Lists
AllVariables	All variables for the block.
Configure	The variables and parameters that control the configuration of the block. These are determined from your Aspen Plus® specification and will not normally be changed. However for control blocks that you add to the simulation you can use this table to configure the block.
Manipulate	Variables that you can manipulate during the dynamic simulation, either manually from the table or by connecting them to the output of a controller.
Results	The key results for the block.

AllVariables Table

Table STREAMS("ACETATE").AllVariables

	Value	Units	Description	Spec
CompBasis	Mole-Flow		Composition basis	
ComponentList	Type1			
F	78.5811	kmol/h	Total mole flow	Free
Fcn("ACETATE")	23.4427	kmol/h	Component mole flow	Free
Fcn("ACETIC")	14.8571	kmol/h	Component mole flow	Free
Fcn("ETHANOL")	11.2878	kmol/h	Component mole flow	Free
Fcn("WATER")	28.9936	kmol/h	Component mole flow	Free
FeedIndex	[]			
FlowBasis	Mole		Flow basis	
Fm	4000	kg/h	Total mass flow	Free
Fmcn("ACETATE")	2065.45	kg/h	Component mass flow	Free
Fmcn("ACETIC")	892.205	kg/h	Component mass flow	Free
Fmcn("ETHANOL")	520.017	kg/h	Component mass flow	Free

Results Table

Table STREAMS("4").Results

	Description	Value	Units
F	Total mole flow	1715.07	lbmol/h
Fm	Total mass flow	161040	lb/h
T	Temperature	333.226	F
P	Pressure	20.1999	psi
h	Molar enthalpy	-0.046109	MMBtu/lbmol
MW	Molar weight	93.8968	lb/lbmol
zn(*)			
Zn("MCH")	Mole fraction	0.0023337	lbmol/lbmol
Zn("PHENOL")	Mole fraction	0.88323	lbmol/lbmol
Zn("TOLUENE")	Mole fraction	0.11444	lbmol/lbmol
zmn(*)			
Zmn("MCH")	Mass fraction	0.0024403	lb/lb
Zmn("PHENOL")	Mass fraction	0.88526	lb/lb
Zmn("TOLUENE")	Mass fraction	0.1123	lb/lb

Manipulate Table

Table STREAMS("2").Manipulate

	Description	Value	Spec	Units
FR	Specified total molar flow	1515.08	Free	lbmol/h
T	Temperature	220	Fixed	F
P	Pressure	20	Fixed	psi
FcR(*)				
FcR("MCH")	Specified component mole flow	0	Fixed	lbmol/h
FcR("PHENOL")	Specified component mole flow	1515.08	Fixed	lbmol/h
FcR("TOLUENE"	Specified component mole flow	0	Fixed	lbmol/h

Configure Table

Table STREAMS("2").Configure

	Description	Value	Units	Spec
ComponentList		Type1		
ValidPhases	Valid phases	Vapor-Liquid		
FlowBasis	Flow basis	Mole		
CompBasis	Composition basis	Mole-Flow		
TotFlowSpec	Total flow is specified	False		
PDriven	Model is pressure driven	False		
Solvent	Component ID of solvent			
FR	Specified total molar flow	1515.08	lbmol/h	Free
T	Temperature	220	F	Fixed
P	Pressure	20	psi	Fixed
FcR(*)				
FcR("MCH")	Specified component mole flow	0	lbmol/h	Fixed
FcR("PHENOL")	Specified component mole flow	1515.08	lbmol/h	Fixed
FcR("TOLUENE"	Specified component mole flow	0	lbmol/h	Fixed

Profile Table

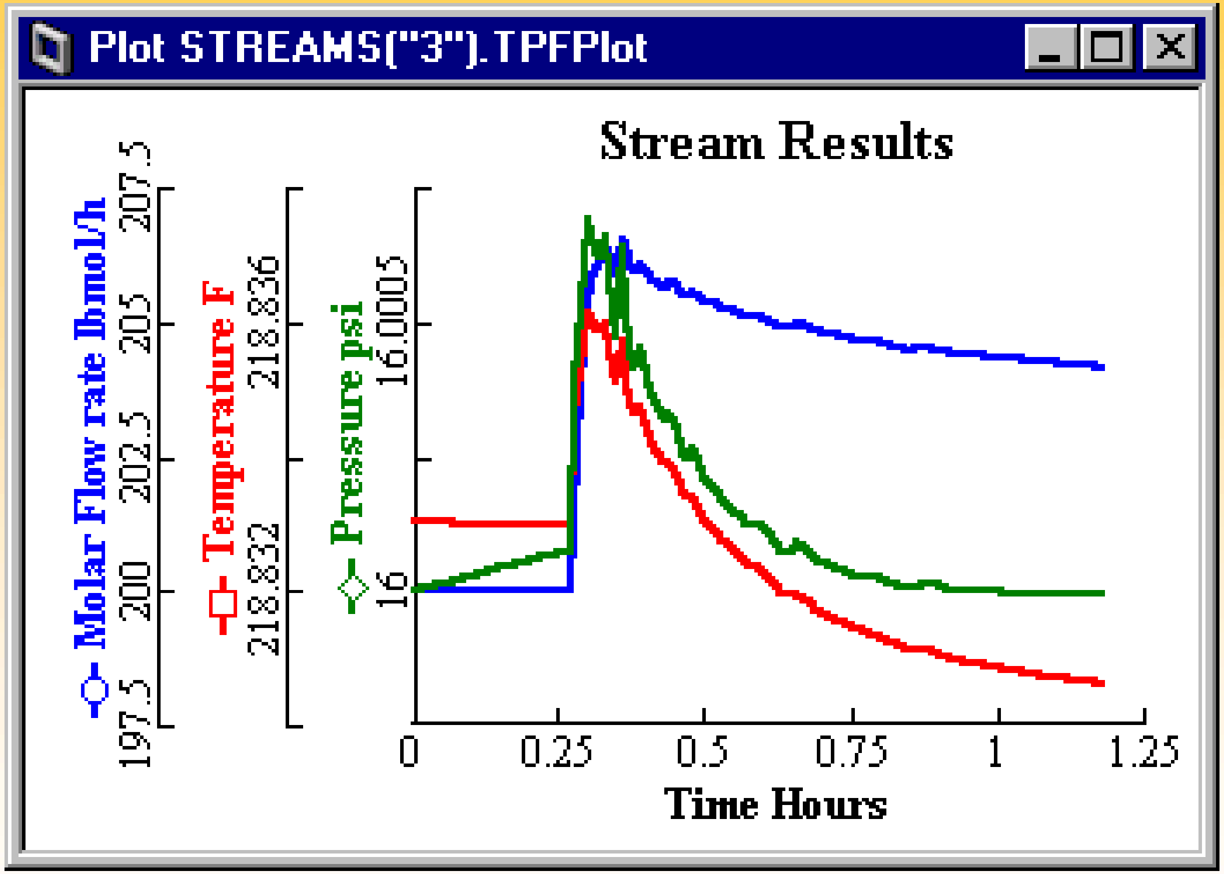
Table BLOCKS("B1").TemperatureProfile

	Description	Value	Units
stage(*).T			
Stage(1).T	Temperature	218.833	F
Stage(2).T	Temperature	219.697	F
Stage(3).T	Temperature	220.601	F
Stage(4).T	Temperature	221.605	F
Stage(5).T	Temperature	222.876	F
Stage(6).T	Temperature	225.172	F
Stage(7).T	Temperature	237.407	F
Stage(8).T	Temperature	238.361	F
Stage(9).T	Temperature	239.389	F

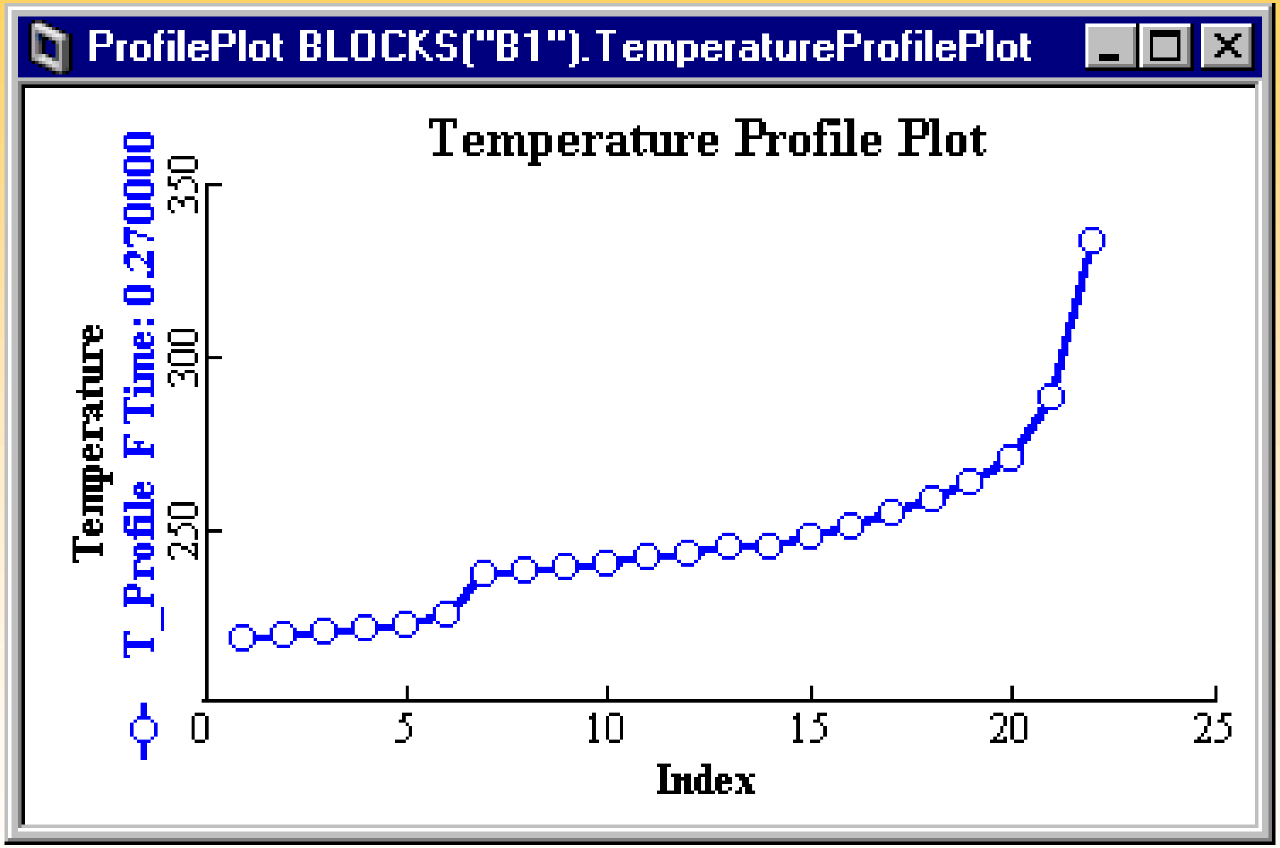
Displaying Results - Plots

- Plots
  - Default
    - Time series
    - Profiles - stage-wise processes
    - FacePlate - PID controller

Time-Series Plot



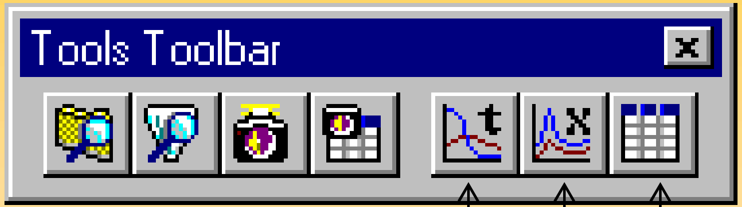
Profile Plot



Custom Results

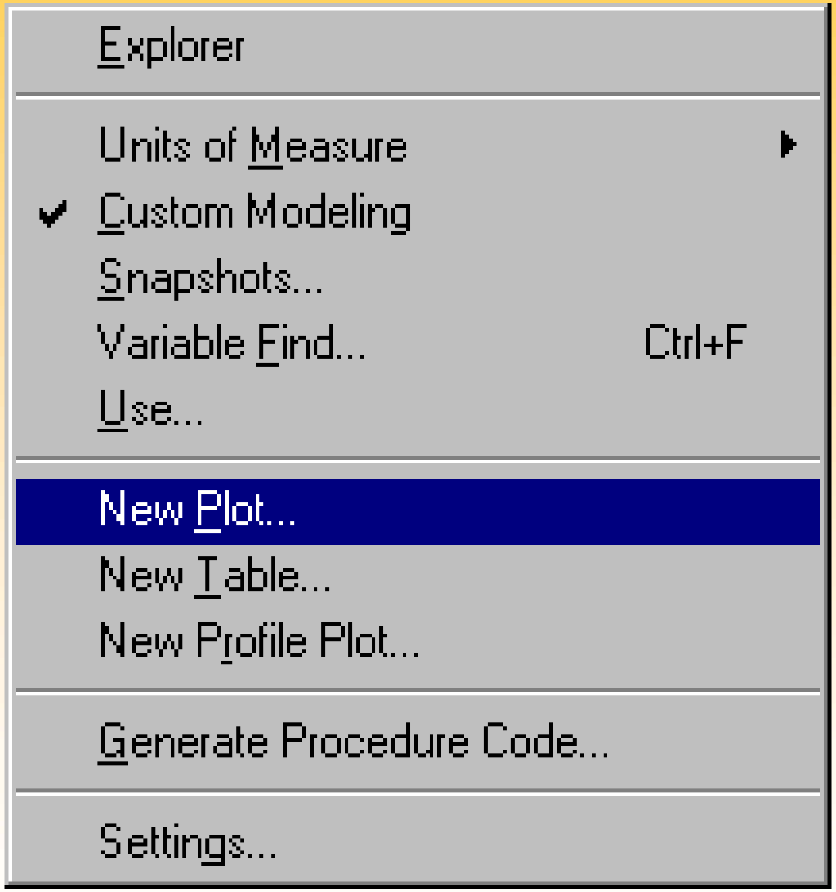
- Tables
  - Drag and drop variables from tables
  - Auto-generate custom table from Variable Find tool
- Time series Plot
  - Drag and drop variables from tables
- Profile Plot
  - specify array variable to profile

Custom Results Buttons



New Plot
New Profile Plot
New Table

Tools Menu - Custom Results



Custom Table from Variable Find

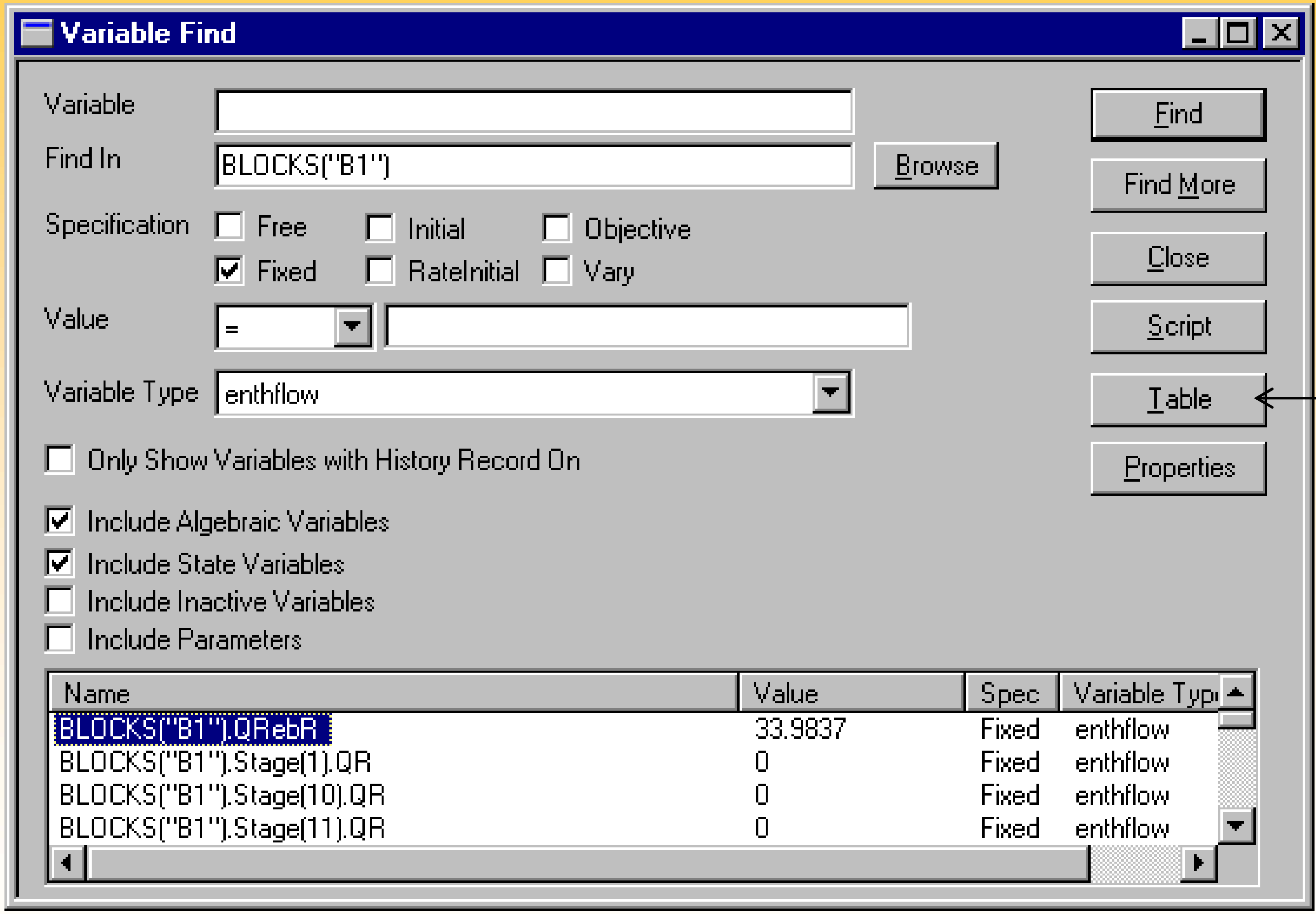
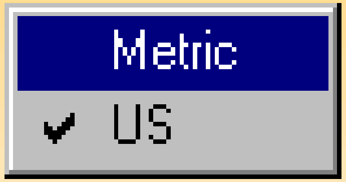


Table button

Units of Measure

- ENG or SI/Metric derived
  - US
  - Metric
- Access from Toolbar



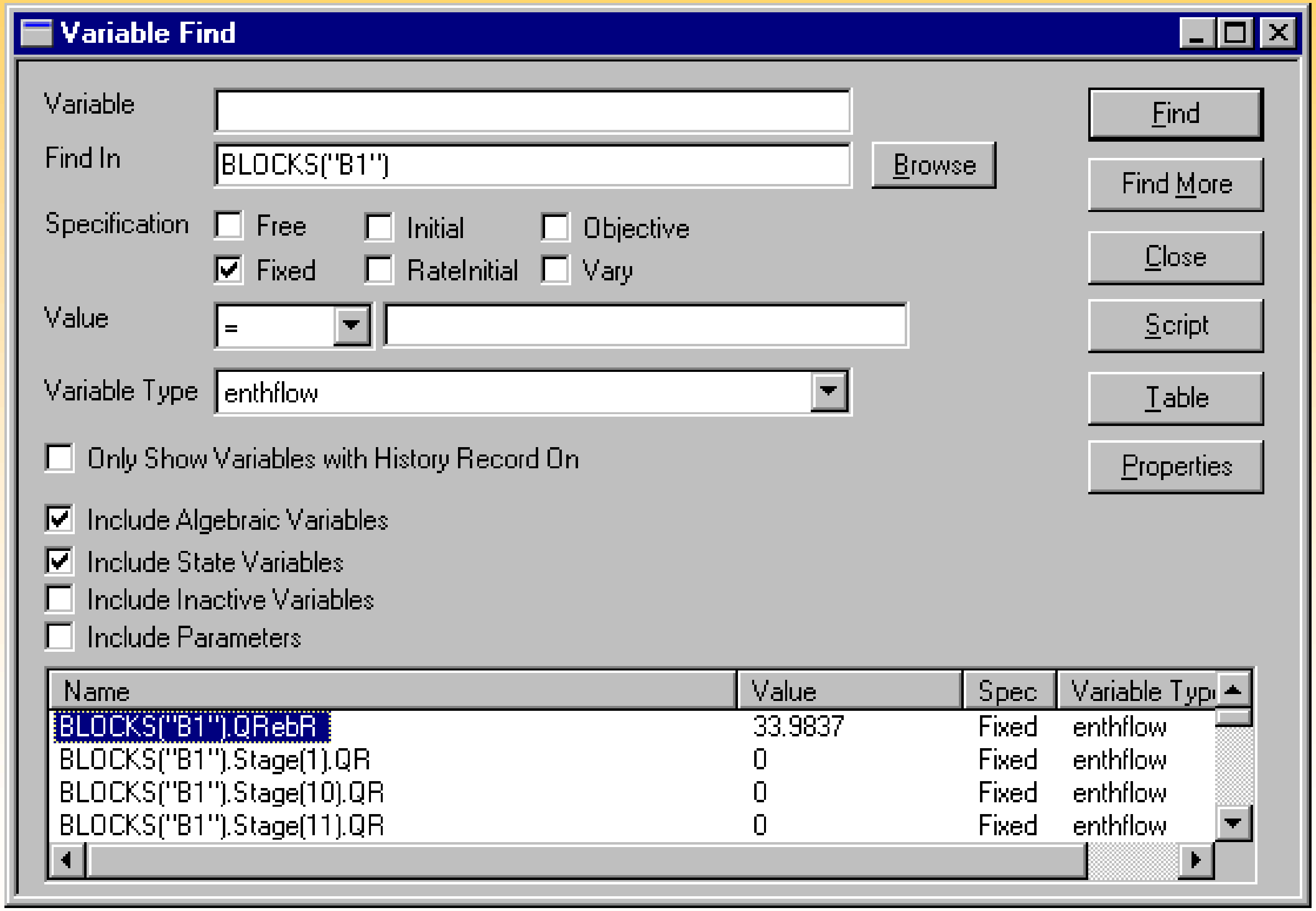
If Aspen Plus input data units of measurement are:	Aspen Dynamics defaults to:
ENG, or is derived from ENG	Aspen Dynamics US units
SI or MET, or is derived from SI or MET	Aspen Dynamics metric units

Variable Find

- Find and List Simulation Variables
- Generate Scripts
- Generate Customized Results Tables
- Modify Properties of Variables

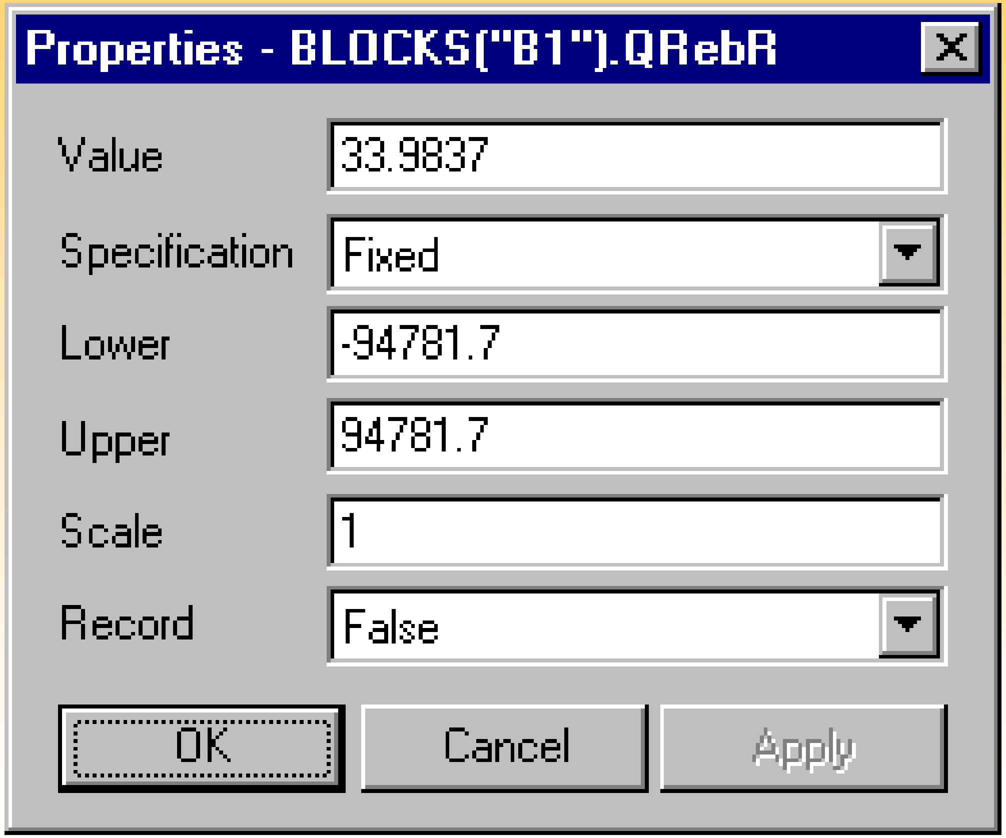
Variable Find

Variable Find Form



Variable Find

Variable Properties



Variable Find

- Variable Name Patterns
  - Access variable names with patterns containing Wildcards
    - Variable find operation
    - Use (snapshot) operation
  - Paths to variable names are segmented in fields
    - Fields delimiters are:
      - .   (period)
      - ( )   (parenthesis)

Variable Name Patterns - Wildcards

Symbol	Meaning
*	Finds zero or more characters for the current name field
~	Finds zero or more name fields
?	Finds any single character present in the specified name field

Variable Find

- Variable Name Patterns - Examples
  - * matches zero or more characters in path statement
    - x* matches x124
    - x* will not match x(1) or x.y
  - ~ matches zero or more path segments
    - x~ will match x(1) or x.y
    - x~ will match x124
  - All 4 examples below produce the same result
    - Blocks(“T101”).Stage(*).X(*)
    - Blocks(“T101”).S*(*).X(*)
    - Blocks(“T101”).S*~(*).X(*)
    - Blocks(“T101”).S*~(*).X~

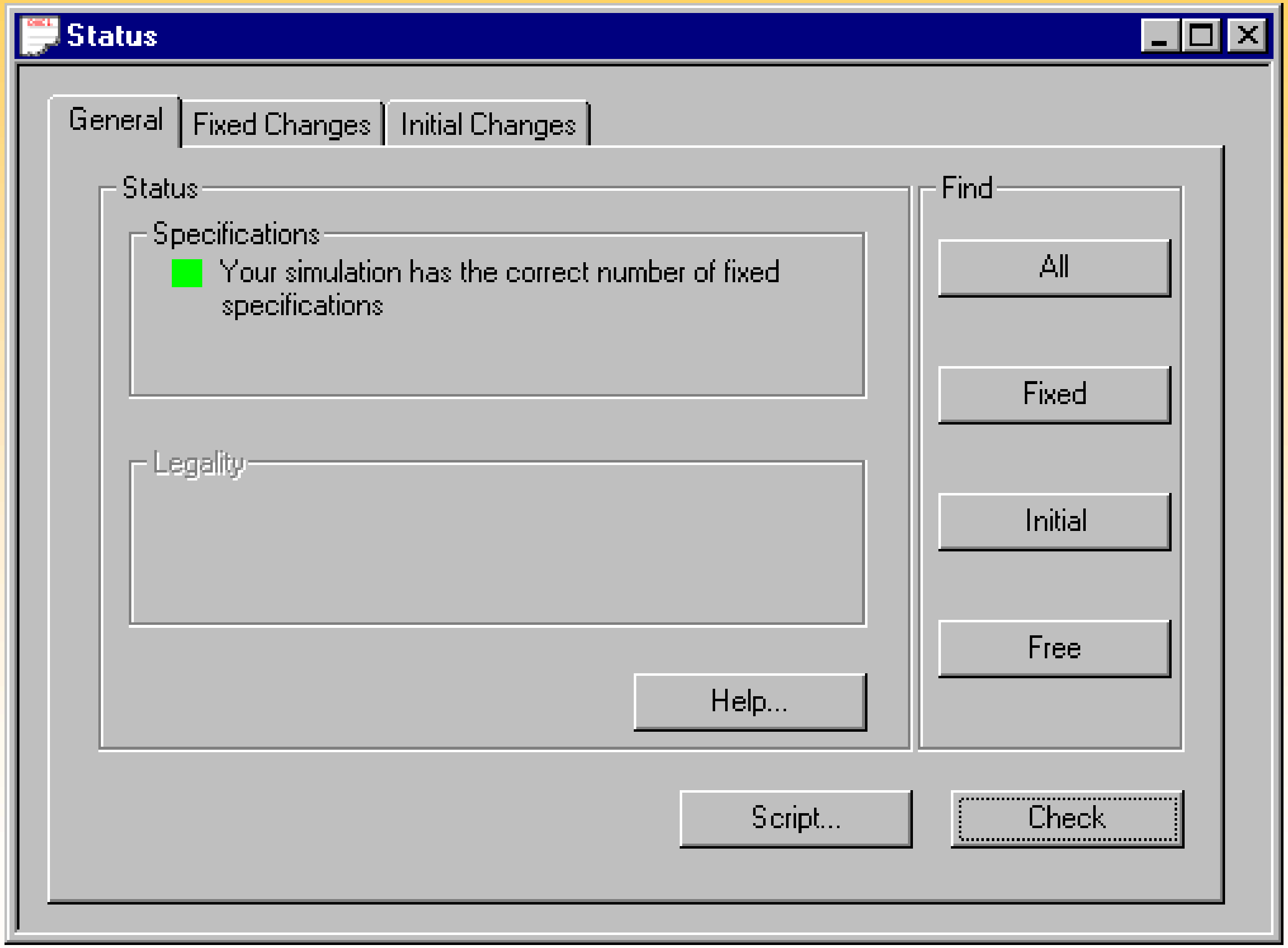
Note: For more examples, visit the online help

Specification Status

- Specification Status on Status Bar
  - Green box - degrees of freedom is satisfied
  - Red box - Number of fixed variables is either over-specified or under-specified
  - Green box with red triangle - Number of initial variables is either over-specified or under-specified
- Automatic Specification Update as Flowsheet is Modified
  - Details available in Specification Status form

Specification Status

Specification Status Form

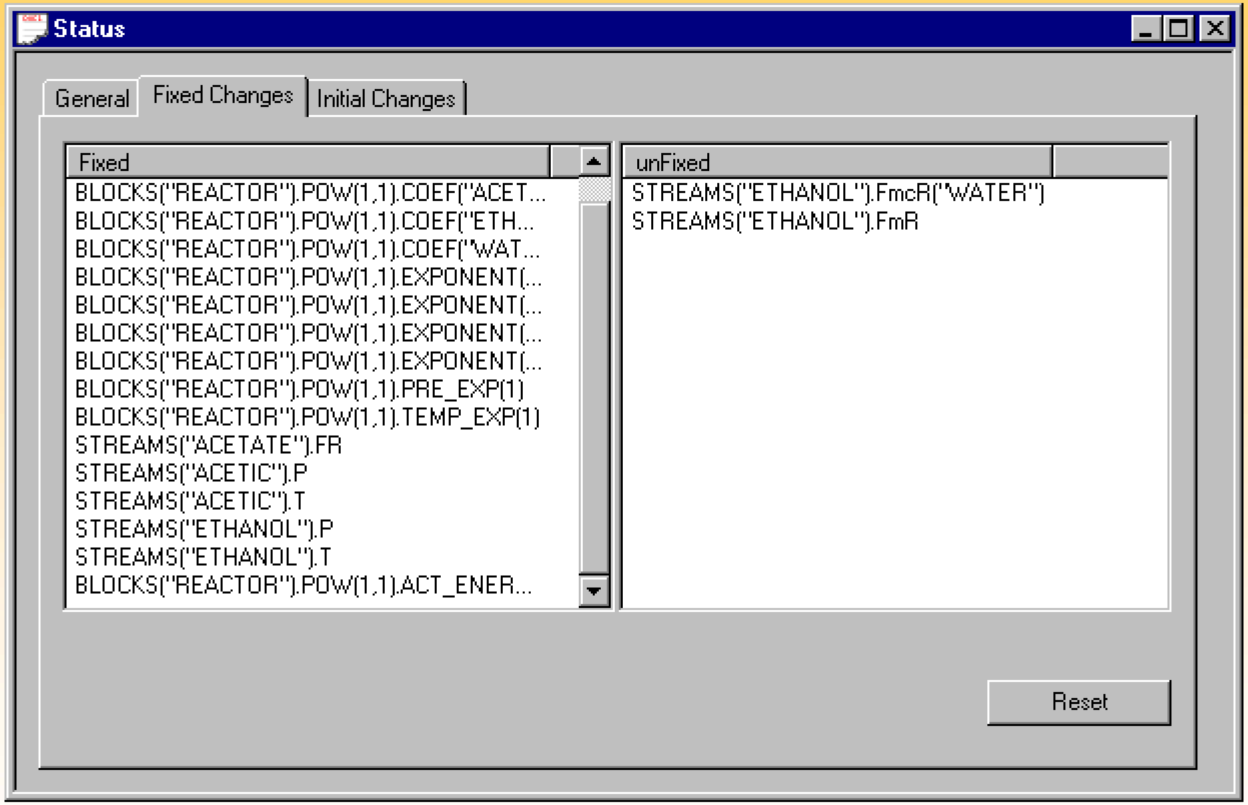


Specification Status

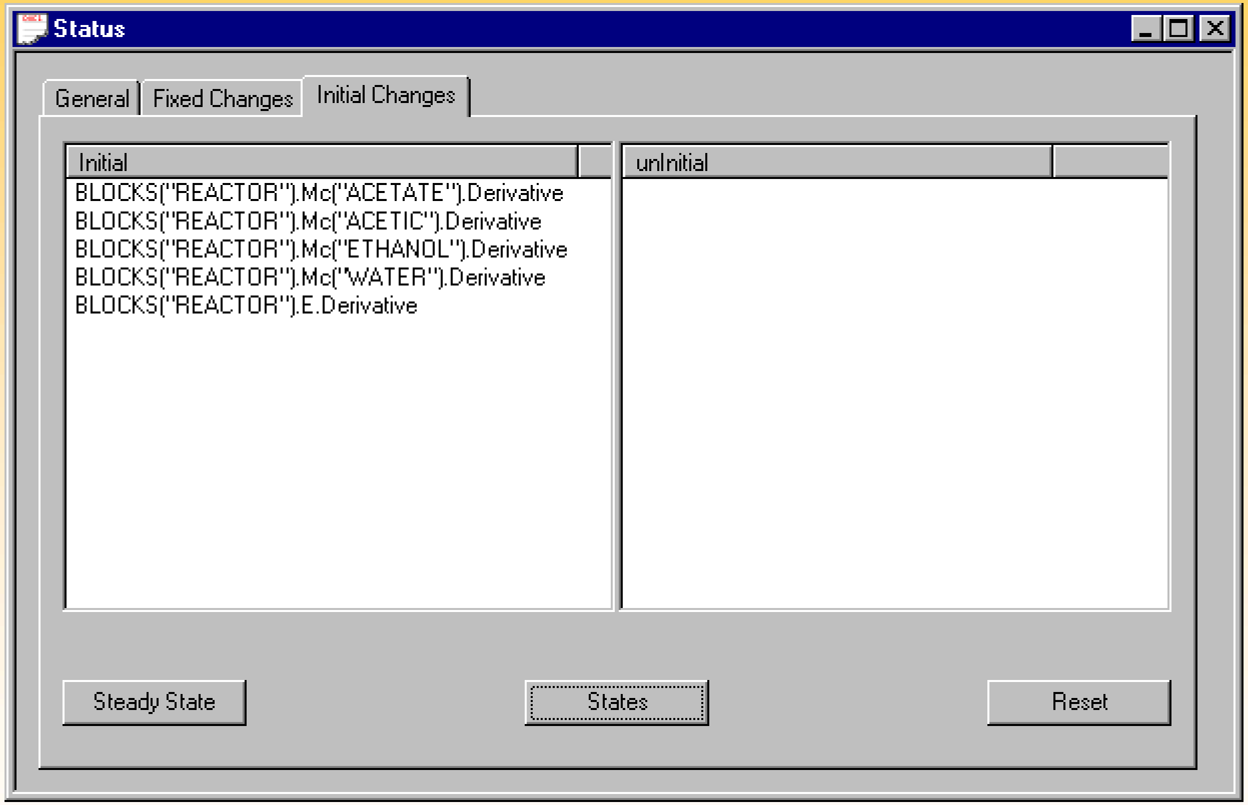
- Specification Status Form
  - Records Specification Changes
    - Fixed and unfixed (Freed) variables
    - Initial and uninitialed variables
  - Initialize Simulation State Variables & Derivatives
    - Steady state conditions
  - Launch Variable Find Form
  - Create Flowsheet Script

Specification Status

Fixed and unFixed Changes Form



Initialize Simulation



Workshop (60 min): Dynamic Simulation

Objective:

- Experience and become familiar with key features of Aspen Dynamics
  - Run a dynamic simulation and implement a step change in Aspen Dynamics
  - Create custom results tables, time series plots and profile plots
  - Modify plot properties

Getting Help on Using Aspen Dynamics

If you want help about	Do this
A particular topic	From the Help Topics dialog box, click the Index tab.
A form or field	On the ASPEN PLUS toolbar, click the What's This button then click the field or form.
A dialog box	Click the Help button on the dialog box.
The item the cursor or mouse pointer is on	Press F1

Workshop: Dynamic Simulation *(1)*

1. Open the dynamic problem definition file Start-RunDynSim.dynf

2. Create a New Plot to observe

a) The change in the specified hydrocarbon feed (stream HCFEED) total mass flow rate (variable FmR from the Manipulate table)

Which variable in stream HCFEED Results table is equivalent to variable FmR in the Manipulate table?

b) The response of the flash block D101 products (streams VAPFEED and LIQFEED) flows (variables Fm and Fm from their respective Results tables)

c) The change in the flash block D101 liquid level (variable Level from the Results table)

Note: The full path for a stream or block variable name is:

STREAMS(”STREAMID").VariableName,

BLOCKS(”BLOCKID").VariableName

Workshop: Dynamic Simulation *(2)*

3. Open the controller block LC1 (flash block D101 level controller) FacePlate and use its plot button to open the associated ResultsPlot form.

4. Use the following steps to create a new profile plot to display the column ethane and propane liquid phase compositions.

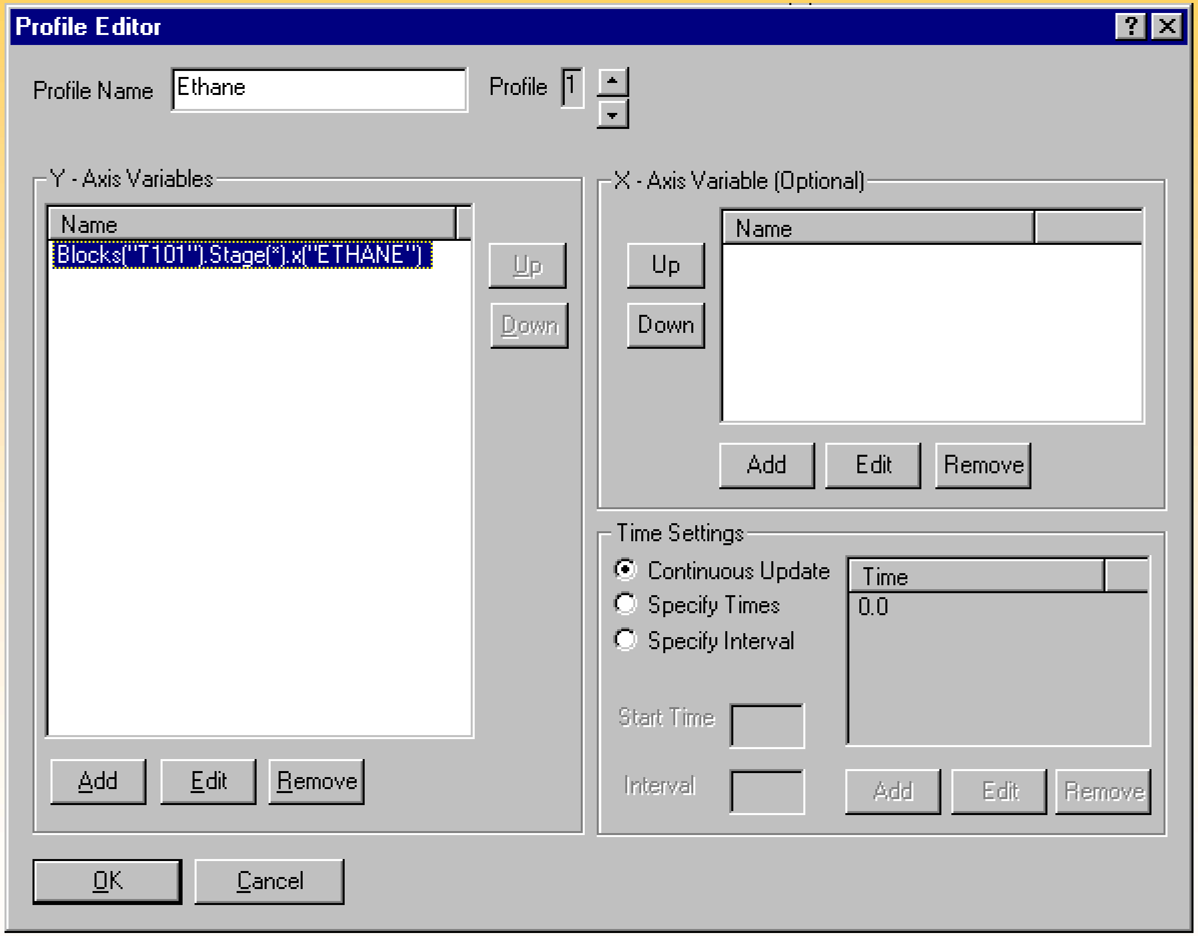
a) Tools menu/New Profile Plot
b) Enter the flowsheet plot name C2_C3_Split to create an empty profile plot
c) On any space in the empty plot, RMB to bring up the plot pop-up menu
d) Select Profile Variables to bring up the Profile Editor
e) For Profile 1, enter Ethane in the Profile Name field
f) Click on the Add button under the Y-Axis Variables section
g) Enter the variable name for the first profile:

Blocks(“T101”).stages(*)x.(“Ethane”)

The profile editor should look like the picture below

Workshop: Dynamic Simulation *(3)*

Profile Editor



Workshop: Dynamic Simulation *(4)*

h) Step the Profile value to 2
I) For Profile 1, enter Propane in the Profile Name field
j) Click on the Add button under the Y-Axis Variables section
k) Enter the variable name for the second profile:

Blocks(“T101”).stages(*)x.(“Propane”)

l) Ok to accept the changes in the Profile Editor.

5. From the Run menu, set the simulation to pause at time 0.1 hours

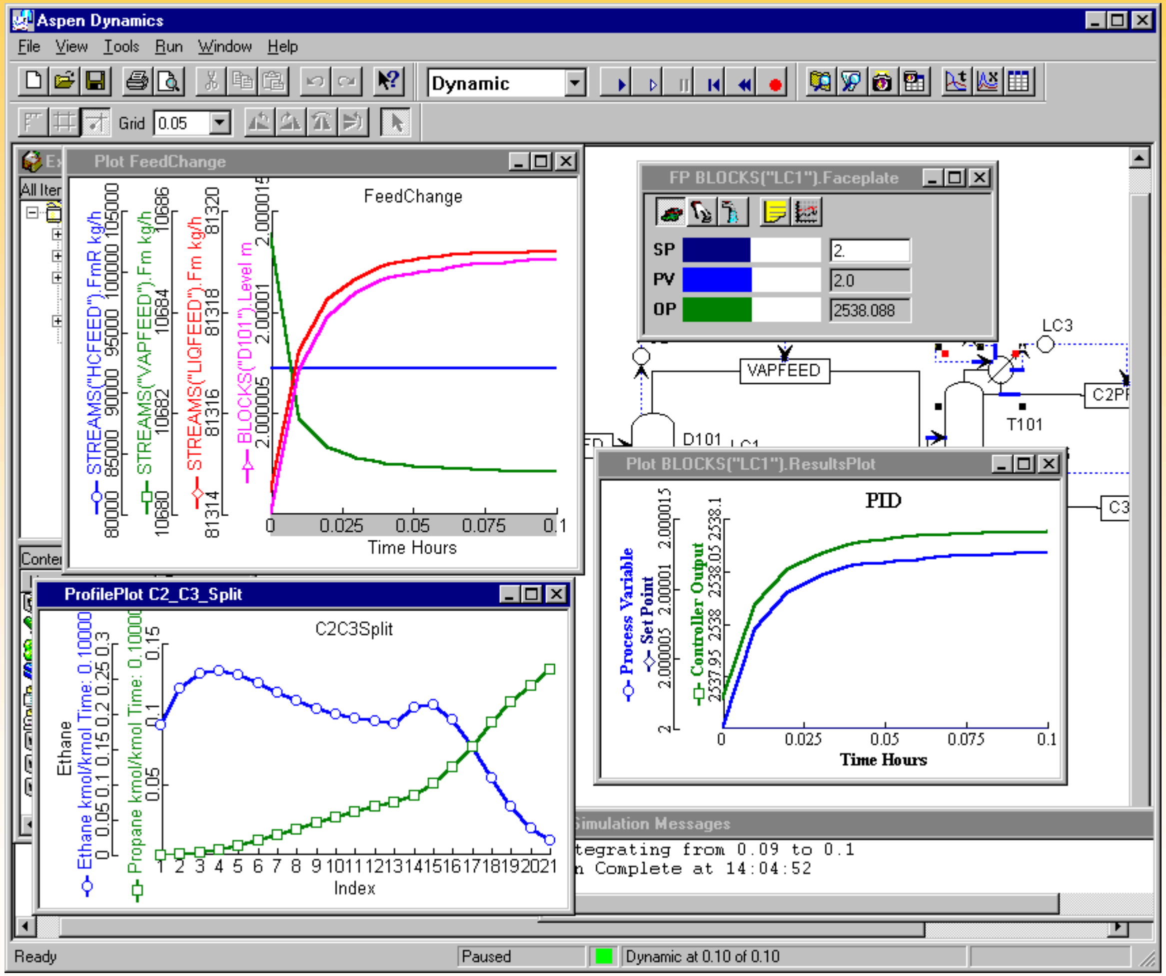
6. Run the simulation in dynamic mode to time 0.1 hours

7. When the simulation completes at time 0.1, zoom full on the two time series (not the profile plot)

Can you reproduce the following picture?

Workshop: Dynamic Simulation *(5)*

Results at simulation Time 0.1 Hours



Workshop: Dynamic Simulation *(6)*

6. Use the RMB pop-up menu to bring up the Profile Editor again. Under the Time Settings section, click on the Specify Times radio button and add a time of 0.25

11. Open the hydrocarbon feed Manipulate table and increase the hydrocarbon feed total mass flow rate by 20% from 94,000 to 110,400 kg/hr.

12. Set the simulation to pause at time 0.25 hours

13. Run the simulation to completion

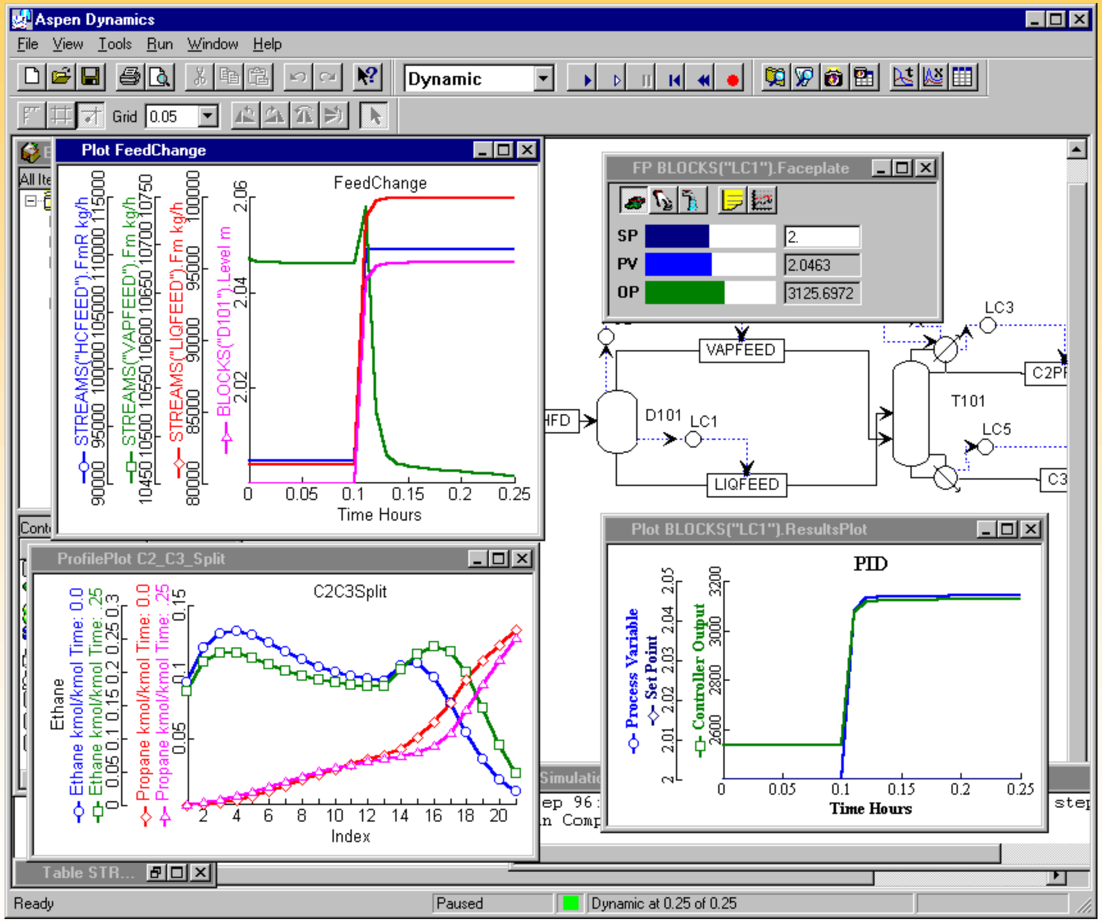
14. When the simulation completes at time 0.25, zoom full on the two time series (not the profile plot)

Can you reproduce the pictures following? You will need to modify the plot properties (axis range, axis map, grid interval, etc.)

Tip: For better performance, close any applications (e.g. Aspen Plus, Internet Browsers, etc.) and windows (tables, plots, etc….) you do not need.

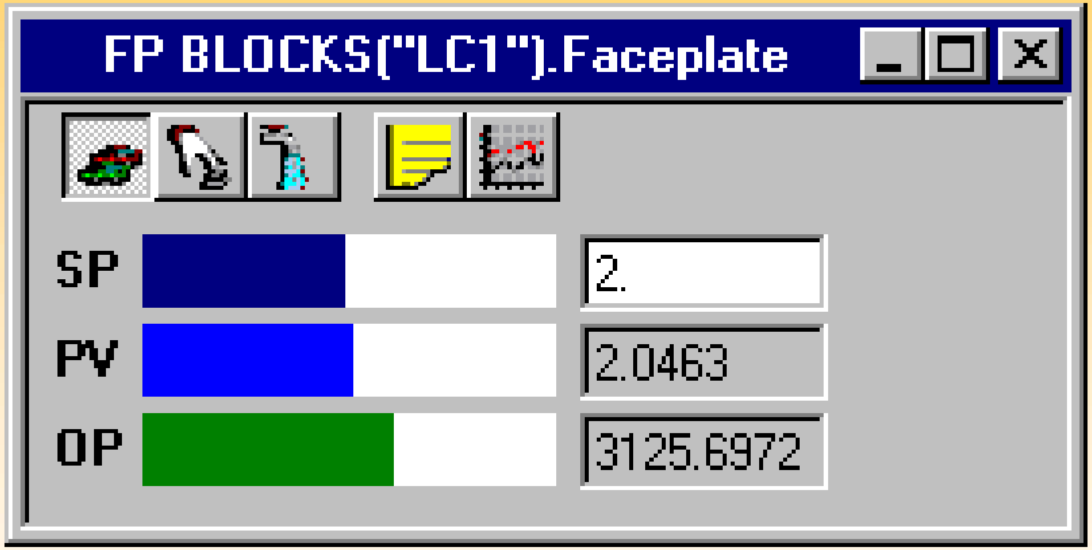
Workshop: Dynamic Simulation *(7)*

Results at simulation Time 0.25 Hours



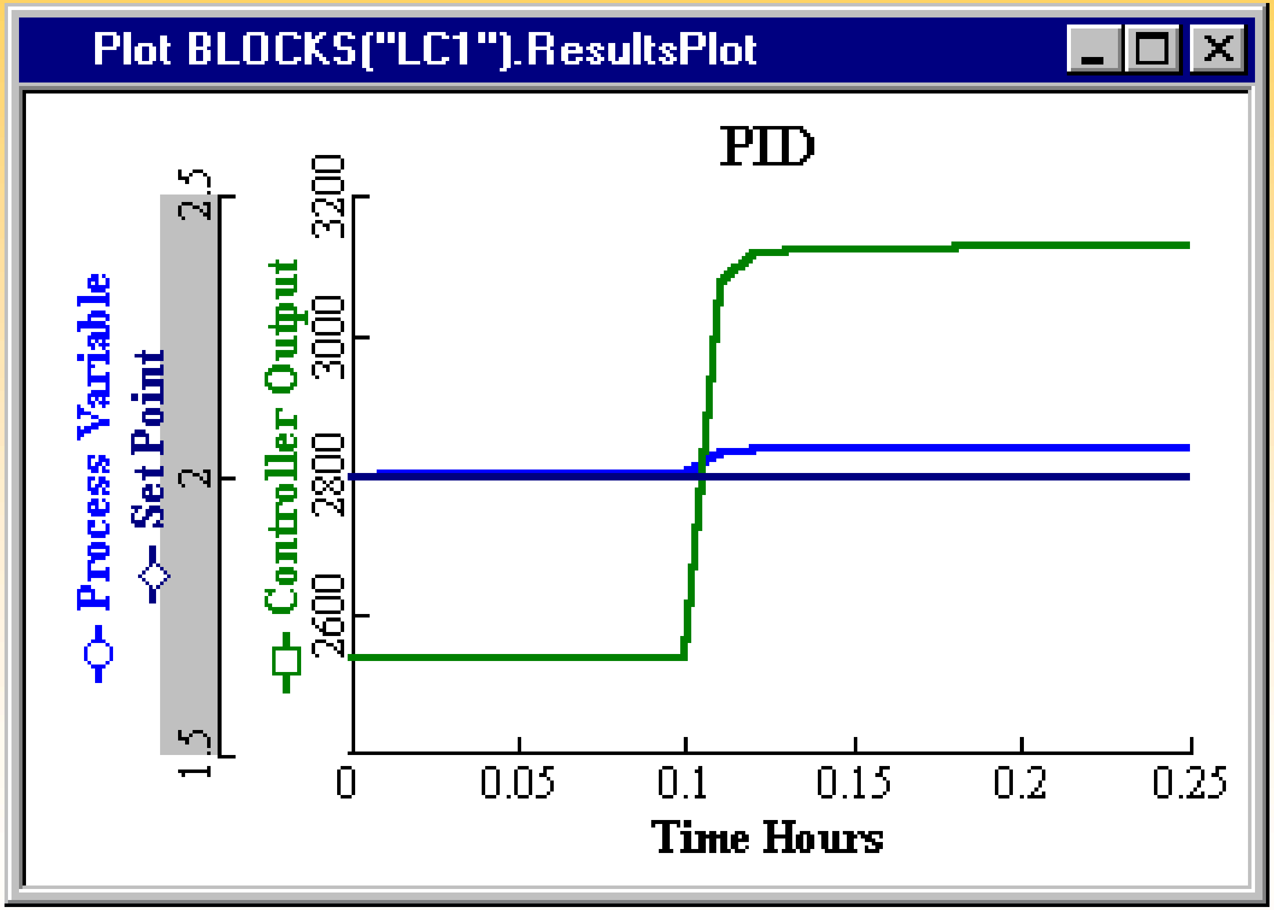
Workshop: Dynamic Simulation *(8)*

Controller LC1 FacePlate at simulation Time 0.25 Hours



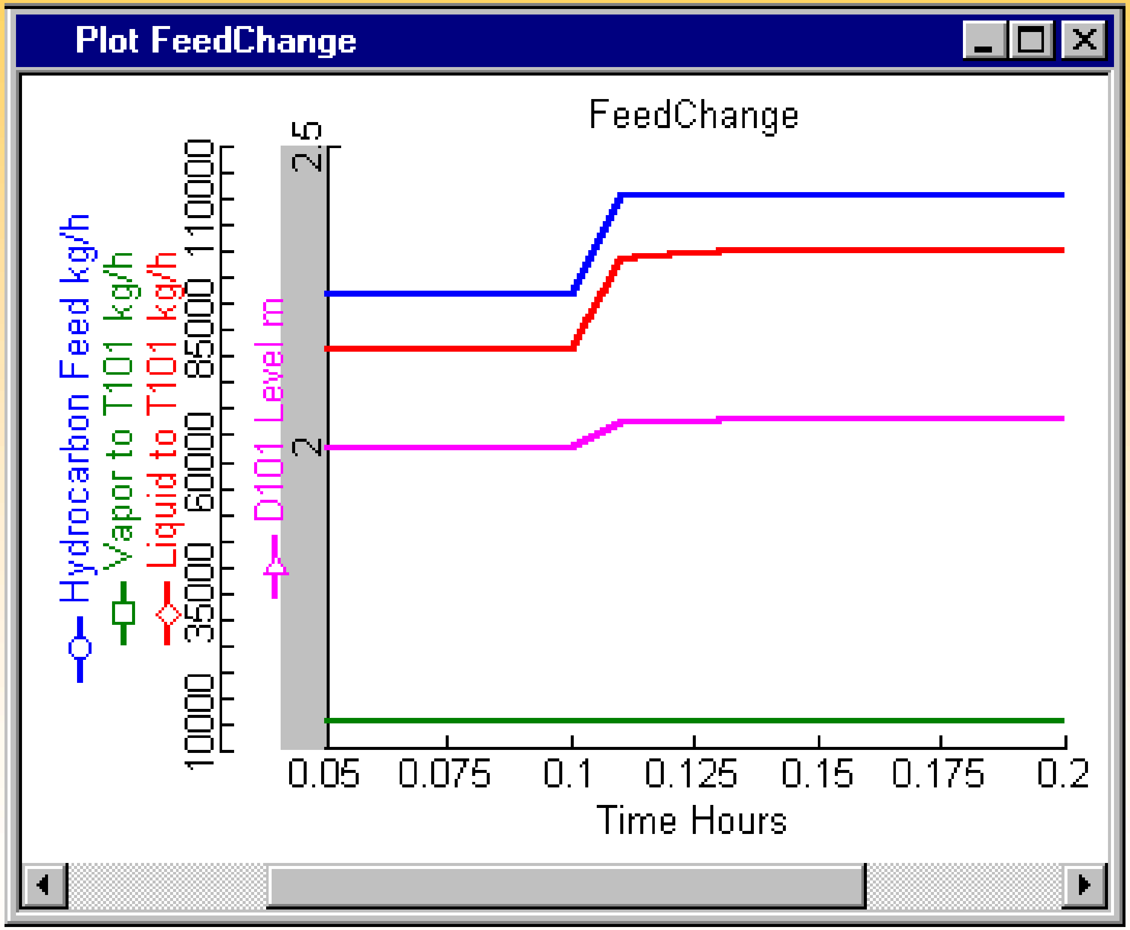
Workshop: Dynamic Simulation *(9)*

Controller LC1 Results Plot at simulation Time 0.25 Hours



Workshop: Dynamic Simulation *(10)*

Hydrocarbon Feed Flow and Flash Drum Level History



Workshop: Dynamic Simulation *(11/11)*

What effect is this disturbance likely to cause to the plant?

Which variables are most likely to be affected?.

Does the flash drum level controller response indicate a well-tuned controller? Why does the level controller not return to its set-point?

15. Save your problem as an Aspen Dynamics Language (*.dynf) file type

Dynamic Simulation

- Review

System Working Files

- RUNID.BKP — Aspen Plus backup
- RUNID.APW — Aspen Plus (binary) document
- RUNIDDYN.APPDF — Aspen Dynamics problem physical properties definition file
- RUNIDDYN.OBJ — Aspen Dynamics user FORTRAN object library
- RUNIDDYN.HIS — Aspen Dynamics run history
- RUNID.DPL — Aspen Dynamics log file (file export/translation)

System Working Files

- PCHECK.LOG — Pressure Checker log file
- RUNID.DYNF — Aspen Dynamics problem file for flow driven simulations
- RUNID.DYND — Aspen Dynamics problem (binary) document
- ..\RUNID — Aspen Dynamics working problem system files subdirectory, including snapshots (binary *.snp files)

Reach Your
True
Potential

Capabilities & Key Modeling Features

Objective:

Learn about the capabilities and limitations of Aspen Dynamics. Understand the basic modeling philosophy and underlying general assumptions

Capabilities & Key Modeling Features

- Supported Features
- Key Dynamic Modeling Features

Supported Features

- Physical properties
  - Full three-phase capabilities
  - Electrolyte simulations with apparent approach

Note: True approach is not supported for electrolytes

Supported Features

- Component Types

Component	Type
Conventional	Conventional component
Solid	Conventional solid component (when used as a salt)
Pseudocomponent	Pseudocomponent
Hypothetical-Liquid	Hypothetical liquid component for pyrometallurgical applications

Note: Use of solids that are salts and appear in electrolyte salt chemistry is supported. Other types are not supported

Supported Features

- Streams and Stream types
  - Stream class CONVEN must be used in Aspen Plus
  - Stream models have no dynamic features

Type of Stream	Model Name
Material	MaterialStream
Heat	HeatStream
Work	WorkStream

Note: Other stream types are not supported

Supported Features

- Streams and Stream Types
  - Feed Streams
    - Variables that have a “Fixed” spec in the dynamic simulation can be changed (manually or with a controller)
    - Material Streams
      - Aspen Plus specified variables map directly with the dynamic simulation fixed variables
    - Heat stream duty is a fixed variable
    - Work stream power is a fixed variable

- Note: Total flow rate must be specified in Aspen Plus to be manipulable in the dynamic simulation

Supported Features

- Unit Operations

Mixers/ Splitters	Separators	Heat Exchangers	Columns	Reactors	Pressure Changers	Manipulators
Mixer	Flash2	Heater	Distl	RStoic	Compr	Dupl
FSplit	Flash3	HeatX	RadFrac	RYield	MCompr	Mult
	Decanter		Extract	RGibbs	Pump	
	Sep			RCSTR	Valve	
	Sep2			RPlug	Pipe	

Supported Features

- Modes of Operation

Instantaneous Only	Dynamic Only	Dynamic & Instantaneous
FSplit	Decanter	Mixer
Sep	Distl	Flash2
Sep2	Radfrac	Flash3
Heater	Extract	HeatX
Pump	RCSTR	RStoic
Dupl	Rplug	RYield
Mult	Pipe	RGibbs
Valve		Compr
		MCompr

General Assumptions & Rules

- Perfectly Mixed Systems
- All phases in equilibrium at all times, except when:
  - Entrainment is allowed
  - Efficiency (Murphree or Vapor) is specified
- Kinetic (including user kinetics) reaction types only are supported

Pressure and Flow Determination

Dynamic Feature	Pressure Determination	Flow Rate Determination
Instantaneous	Fixed at steady-state value	From material balance. Total outlet flow rate is always equal to inlet flow rates.
Vapor holdup is modeled	Temperature and composition in vessel	Vapor flow manipulated to control pressure
Liquid holdup is modeled	Fixed at steady-state value	Liquid flow manipulated to control level

Separators

- Flash2
- Flash3
- Decanter
- Sep
- Sep2

Flash2, Flash3 & Decanter

- Duty is always specified as “Fixed”
  - Can manipulate manually or with a controller

Flash3 & Decanter Level Controllers

Controller added	When vessel type is	Measured variable	Manipulated variable
Liquid Level	Vertical or horizontal	Overall liquid level	Liquid 1 outlet flow rate
Interface Level	Vertical or horizontal	Liquid interface level	Liquid 2 outlet flow rate

Heat Exchangers

- Heater
- HeatX

Heater & HeatX

- The pressure drop is related to the outlet volumetric flow rate by:

$$\Delta P = K * Rho * Fv\_Out^{2}$$

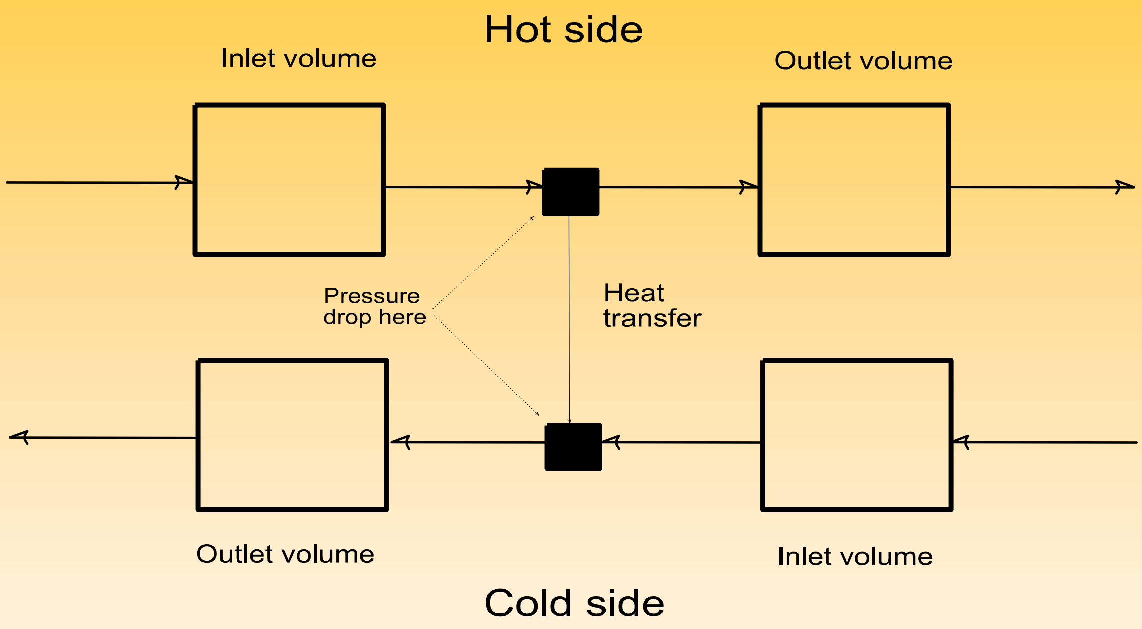
Where:

K	=	Constant determined by fitting to steady-state conditions
Δ P	=	Pressure drop
Rho	=	Mass density at outlet conditions
Fv_out	=	Outlet volumetric flow rate

HeatX

- Overall heat transfer coefficient is constant
- LMTD correction factor is constant
- Dynamic mode operation
  - Dynamic characteristics are modeled using volume holdups on each side of exchanger
    - Total volume is split between two volumes
  - Pressure drop is assumed to occur between inlet and outlet volumes

HeatX - Dynamic Mode Operation



Volume = (residence time) * (steady state volumetric flow rate)/2

Adjust volume to fit plant data

Reactors

- RStoic
- RYield
- RGibbs
- RCSTR
- RPlug

Note: User reaction kinetics subroutines are supported

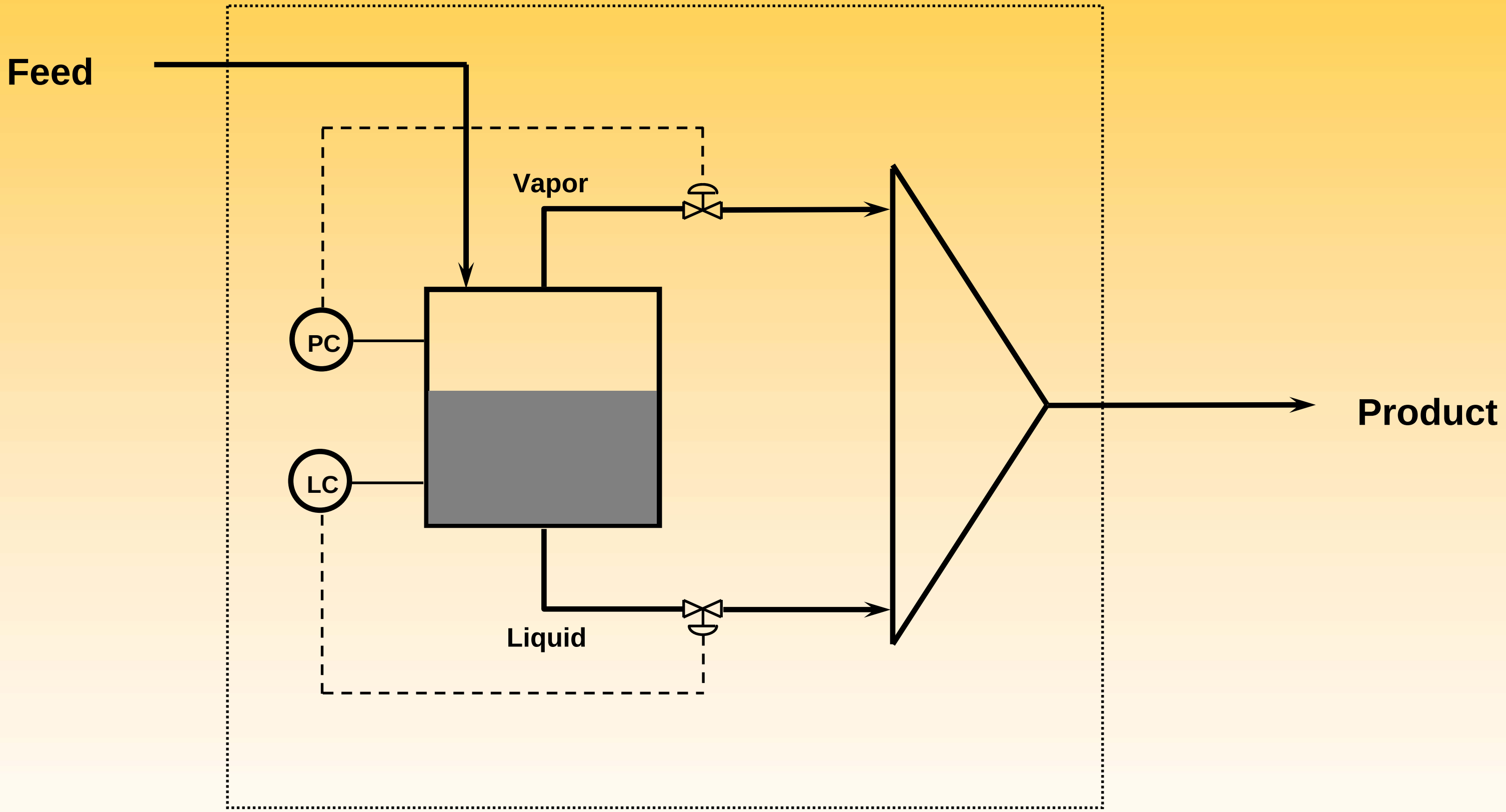
Rstoic, RYield and RGibbs

- Dynamic Modes of Operation are:
  - Stirred tank (CSTR) geometry
  - Tubular or Plug flow reactor (PFR) geometry
- Reactions equations are applied at outlet conditions
  - Allows reaction specification to be satisfied
  - Reactions are instantaneously applied at the outlet
- CSTR mode reactors can have inventory controllers
  - Level
  - Pressure

RCSTR

- Temperature controller is automatically added when constant duty heat transfer option is specified
  - Controller manipulates duty
- Internal Controls
  - Model enables the outlet flow of each phase to be manipulated independently
  - Vapor and liquid phase flows are mixed at the outlet of the reactor
- Can modify reactor configuration for vapor only (vent) flow and liquid only (product) streams

RCSTR - Internal Controls



RPlug

- Supports Liquid phase and Vapor phase reactions
- User must specify NPHASE = 1
- Model assumes:
  - No axial mixing
  - No axial heat conduction
- Heat transfer effect between catalyst and process fluid is modeled

RPlug

- The pressure drop is related to the outlet volumetric flow rate by:

$$\Delta P = K * Rho * Vel^{2}$$

Where:

K	=	Constant determined by fitting to steady-state conditions
Δ P	=	Pressure drop
Rho	=	Mass density at outlet conditions
Vel	=	Fluid Velocity

- Coolant pressure drop is fixed

Rplug - Cooling Options

Cooling Type	Description
TCOOL_SPEC	Reactor with constant cooling temperature
ADIABATIC	Adiabatic reactor
CO-COOL	Reactor with co-current external coolant
COUNTER-COOL	Reactor with counter-current external coolant

T_SPEC option is not supported

(Use high flow rate coolant for constant reactor temperature)

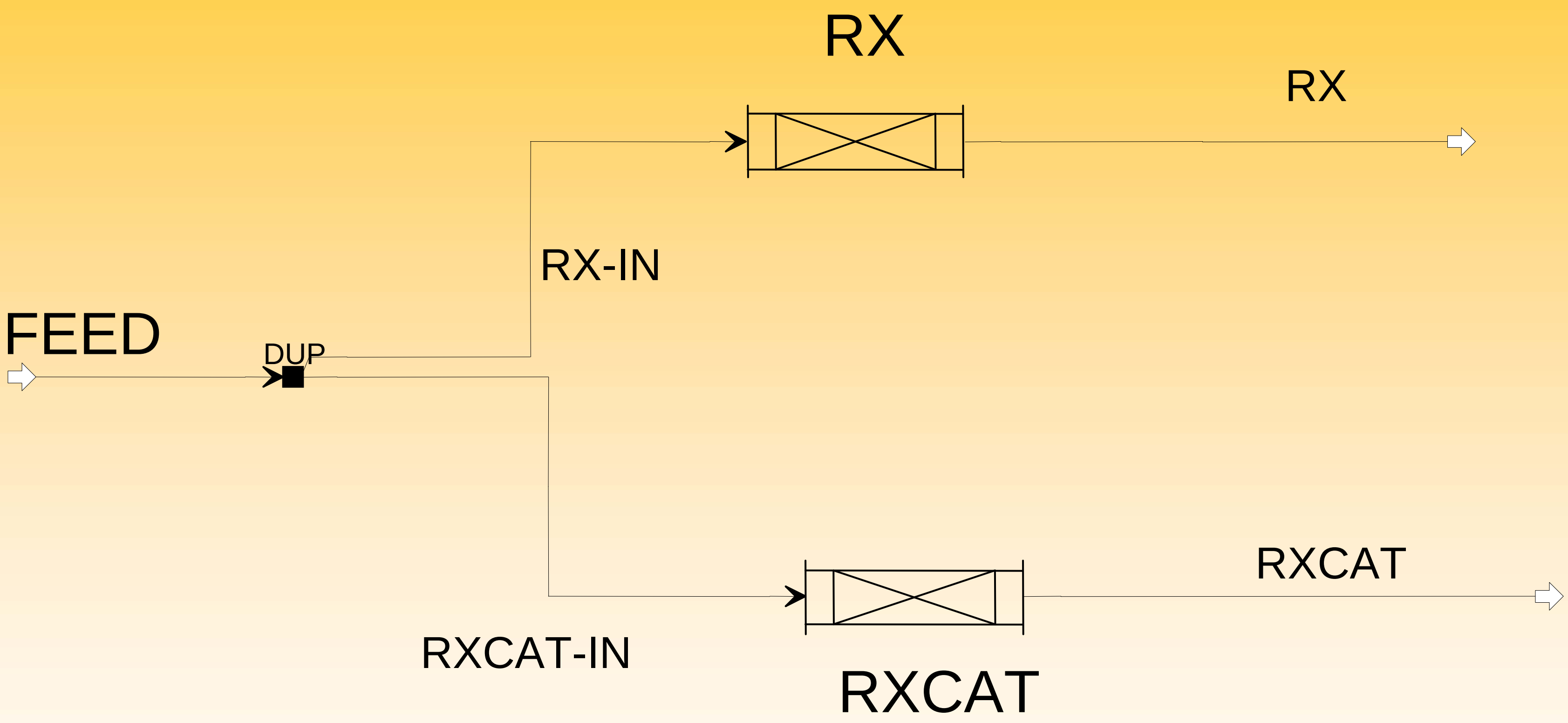
RPlug Catalyst Heat Transfer

If you choose	Specify	Description
No heat transfer (default)	No additional input	No catalyst present, or the effect of heat transfer between catalyst and process fluid on the reactor dynamics is neglected.
Heat transfer at equal temperatures	Voidage fraction of catalyst Heat capacity of catalyst Mass density of catalyst	There is very fast heat transfer between the catalyst and the process fluid, and they are assumed to be always at the same temperature
Heat transfer at different temperatures	Voidage fraction Heat capacity of catalyst Mass density of catalyst Specific surface area of catalyst Overall heat transfer coefficient	This is the most rigorous option. Heat transfer between the catalyst and process fluid is determined by their temperature differential, contact area, and overall heat transfer coefficient

Workshop (30 min): RPlug Thermal Inertia

- Compare RPlug reactor dynamics with and without catalyst thermal inertia effects
- Become acquainted with the dynamic operation of the RPlug model

Workshop: RPlug Thermal Inertia *(1)*



Workshop: RPlug Thermal Inertia *(2)*

Property: PR-BM

<u>Feed</u>

Temperature = 380 C

Pressure = 35 bar

Water = 35 kmol/h

Carbon Monoxide = 10 kmol/h

Carbon dioxide = 5 kmol/h

Hydrogen = 35 kmol/h

Nitrogen = 15 kmol/h

<u>Reactor</u>

Process Side Pressure drop = 0.5 bar

Adiabatic reactor

Valid-Phases: Vapor Only

Length = 2.0 m

Diameter = 0.5 m

Workshop: RPlug Thermal Inertia *(3)*

Reaction: specified as 2 kinetic reactions

Water + Carbon Monoxide <--> Hydrogen + Carbon dioxide

Catalyst Data

Voidage fraction = 0.40

Heat capacity = 1.5 KJ/kg-k

Mass density = 3500 kg/m3

Specific surface area = 1000 m2/m3

Overall heat transfer coefficient = 500 Kcal/hr-m2-K

Workshop: RPlug Thermal Inertia *(4)*

You are supplied with a backup file StartRPlugInertia.bkp

1. Load the backup file in Aspen Plus

2. Run the simulation and view the steady state results.

3. Follow the steps below to create a plot to view the profile of one reactors temperature, carbon monoxide mole fraction and hydrogen mole fraction along its length

a) Go to the RPlug block results Data Browser

b) Click on profiles in the block tree-list to bring up the Profiles Data Browser

c) Click on the “Reactor Length” column label to highlight the whole column

Workshop: RPlug Thermal Inertia *(5)*

d) Go to the Plot menu and select “X-Axis Variable” to make the reactor length the x-axis

e) Click on the “Temperature” column label to highlight the whole column

f) Go to the Plot menu and select “Y-Axis Variable” to select temperature as a profile variable

g) Go to the Plot menu and select “Display Plot” to bring up the temperature profile

h) Pull down the “View” field list and select “Molar composition”

i) Click on the Length column label to highlight the Length column

j) Go to the Plot menu and select “X-Axis Variable” to select length as

the X-axis

Workshop: RPlug Thermal Inertia *(6)*

k) Click on the CO (carbon monoxide) column label to highlight the column

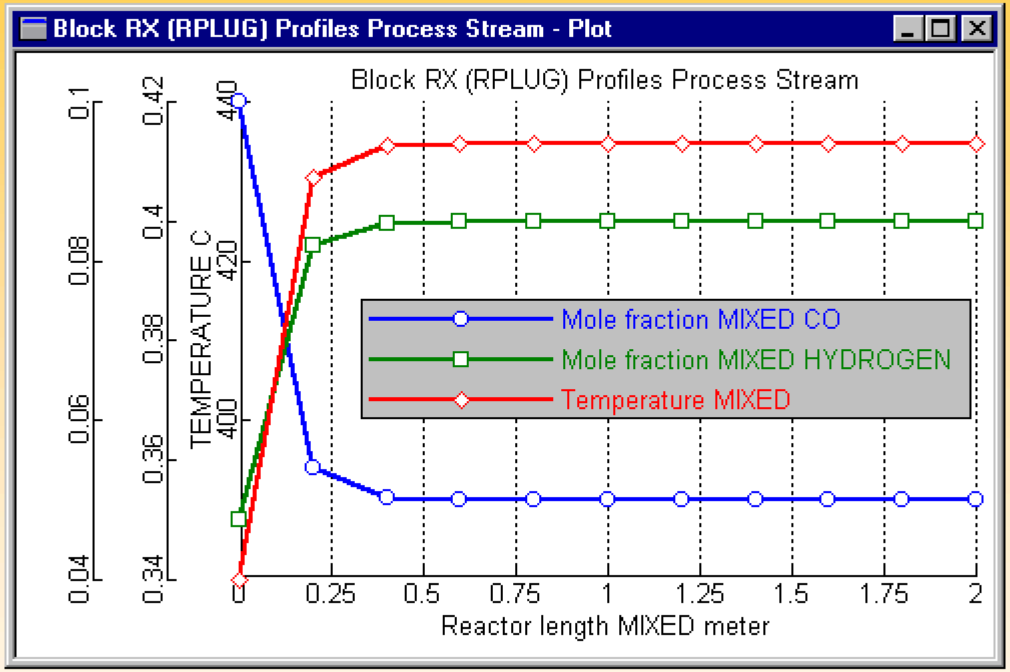
l) Go to the Plot menu and select “Y-Axis Variable” to select carbon monoxide as a profile variable

m) Go to the Plot menu and click on “Add New Curve” to add the carbon monoxide profile to the existing plot

n) Select “Block RX(RPLUG) Profiles Process Stream” from the Plot Window List dialogue box and OK to add to the existing plot

o) Repeat the selection process *(steps 2.9 - 2.14*) for hydrogen to add the hydrogen composition bed profile to the existing plot

Workshop: RPlug Thermal Inertia *(7)*



Reactor Steady State Profile

Workshop: RPlug Thermal Inertia *(8)*

4. Add the supplied catalyst data for the RXCAT block.

5. Re-Run the simulation

6. Export the dynamic simulation problem files.

7. Open the dynamic problem files with Aspen Dynamics

8. Create a single custom profile plot to compare the bed temperature along the length of both reactors.

9. Create a time series plots to compare the reactor product stream

   outlet temperatures and Carbon dioxide compositions.

10. Run the simulation to time 1 hour

Tip: use the “pause at” option

Workshop: RPlug Thermal Inertia *(9)*

11. At time 1 hour, use the manipulate table to step the feed stream

    temperature from the current value to 400 C.

12. Continue the simulation and observe and compare the dynamic responses whilst allowing the reactors to return to steady state.

13. Restart the simulation (time zero hours)

14. Run the simulation to time 1 hours.

15. At time 1 hours, step the carbon monoxide feed flow to 12 kmol/h

16. Continue the run and observe and compare the dynamic

    responses whilst allowing the reactors to return to steady state

17. Repeat the steps *(c to f)* above for a decrease in pressure to 30 bar

Workshop:RPlug Thermal Inertia *(10/10)*

Which catalyst characteristic (voidage fraction, specific heat capacity, mass density, specific surface area, overall heat transfer coefficient) would have most influence on the thermal inertia?

Which reactor model (with/without catalyst thermal inertia) would you expect to return to steady-state the quickest? Can you explain why?

What happens to the simulation when the feed temperature is increased? Why is this?

What other variables are worth observing for the response to a change in the feed conditions ? What other variables are worth manipulating?

Workshop: RPlug Thermal Inertia

- Review

Columns

- Distl
- RadFrac
- Extract

RadFrac

- Reactive distillation is supported
  - Reaction holdup is a fixed ratio of actual stage holdup and the specified reaction holdup
- Weeping is modeled in trays
- User-KLL, polynomial KLL, VL1/LL prop-sections are not supported
- Different VL1 and VL2 efficiencies are not supported
- Pseudo streams are not supported

RadFrac

- Five Key Model Elements
  - Overhead system
  - Bottoms system
  - Stages
  - Decanter
  - Pumparound

RadFrac Overhead System

- Condenser
  - Dynamic effects are not modeled
    - Assumes instantaneous operation
- Reflux drum
  - Liquid reflux flow rate is fixed
  - Vapor and liquid holdups are modeled
  - Reflux flow hydraulics are not modeled

RadFrac Bottoms System

- Thermosyphon reboiler
  - Dynamic effects are not modeled
    - Assumes instantaneous operation
  - Recirculation rate is a function of duty

$$\text{Recirculation\_Rate} = R * \text{Duty}^{1/3}$$

where :

Constant R is determined from steady state results

RadFrac Decanter

- Decanter
  - Vapor holdup is not modeled
  - Flow rate of the first liquid phase is manipulated to control the total liquid level
  - Flow rate of second liquid phase is manipulated to control the interface level

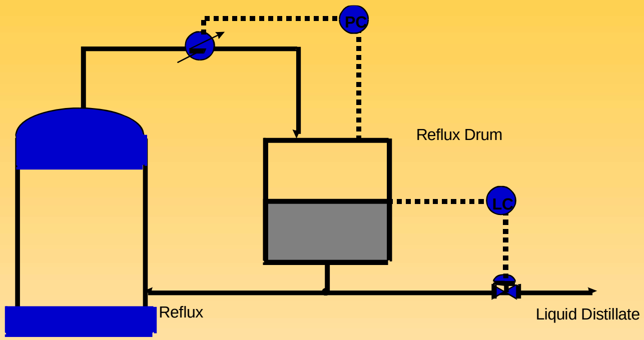
RadFrac Pumparound

- Pumparound
  - Assumes instantaneous operation

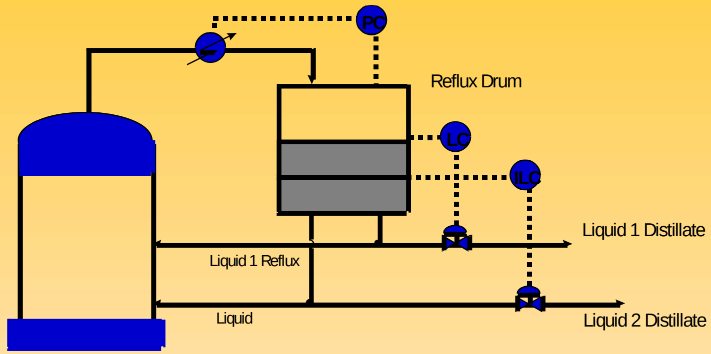
RadFrac Stages

- Top Stage Pressure
  - Determined from stage temperature and composition
- Other Stages
  - Pressure difference calculated from pressure drop flow equation
  - Flow rates are related to liquid holdup with hydraulics equation
- Stage Product Streams
  - Flow rate is fixed at steady-state value

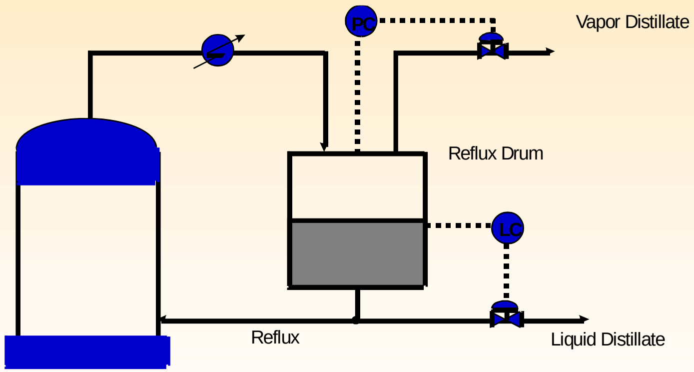
RadFrac Inventory Control



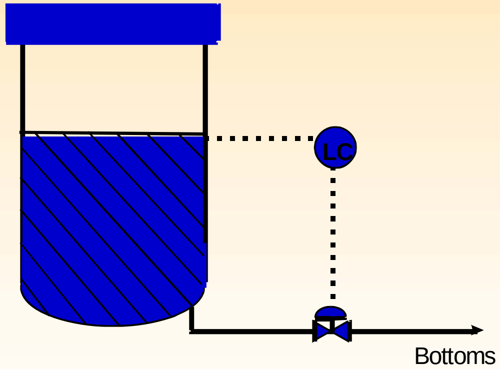
Typical overhead inventory control configuration for a column with no vapor distillate.



Typical overhead inventory control configuration for a column with liquid 1 and liquid 2 distillates.



Typical overhead inventory control configuration for a column with vapor distillate.

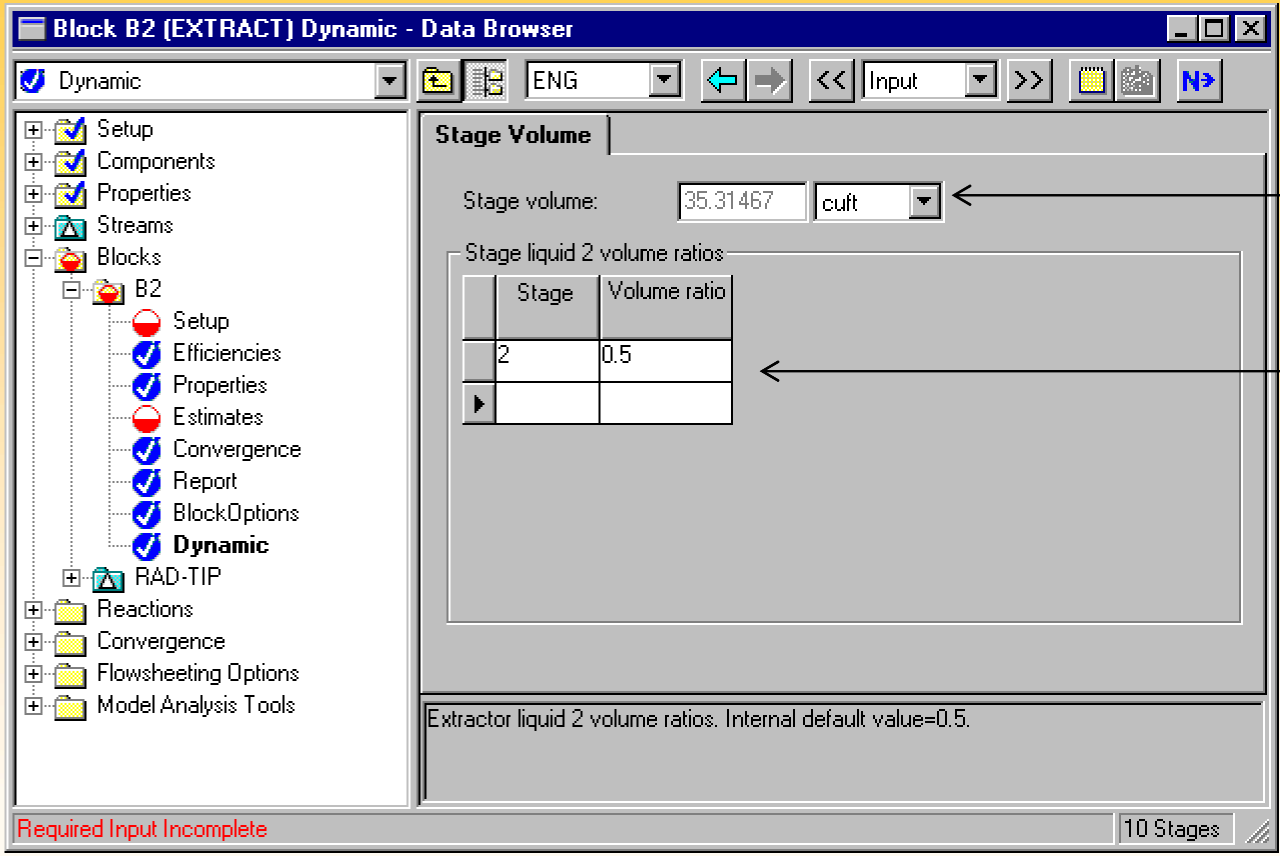


Default sump inventory control configuration.

Extract

- Assumes instantaneous equilibrium
- Assumes equi-volume stages
- Assumes a constant 2nd liquid phase volume fraction
- Stage or component efficiencies are allowed
  - Constant throughout simulation
- Pressure/Flow effects
  - Pressure at each stage is fixed at the steady state value
- User KLL subroutines is not supported
- Pseudo streams are not supported

Extract Dynamic Form



Equi-volume Stages

Liquid 2 volume ratio default = 0.5

Pressure Changers

- Pump
- Valve
- Pipe
- Compr
- MCompr

Valve

- Instantaneous mode only
- Flow through valve is a function of the upstream and downstream pressures

Pipe

- Supported Solution Methods
  - Integrate
  - Constant dP/dL
    - Outlet flow rate always equal to inlet flow rate
- Assumptions
  - One-dimensional fully developed flow
  - Perfect plug flow (no axial mixing)
- Entrance Effects not Modeled

Compr and MCompr

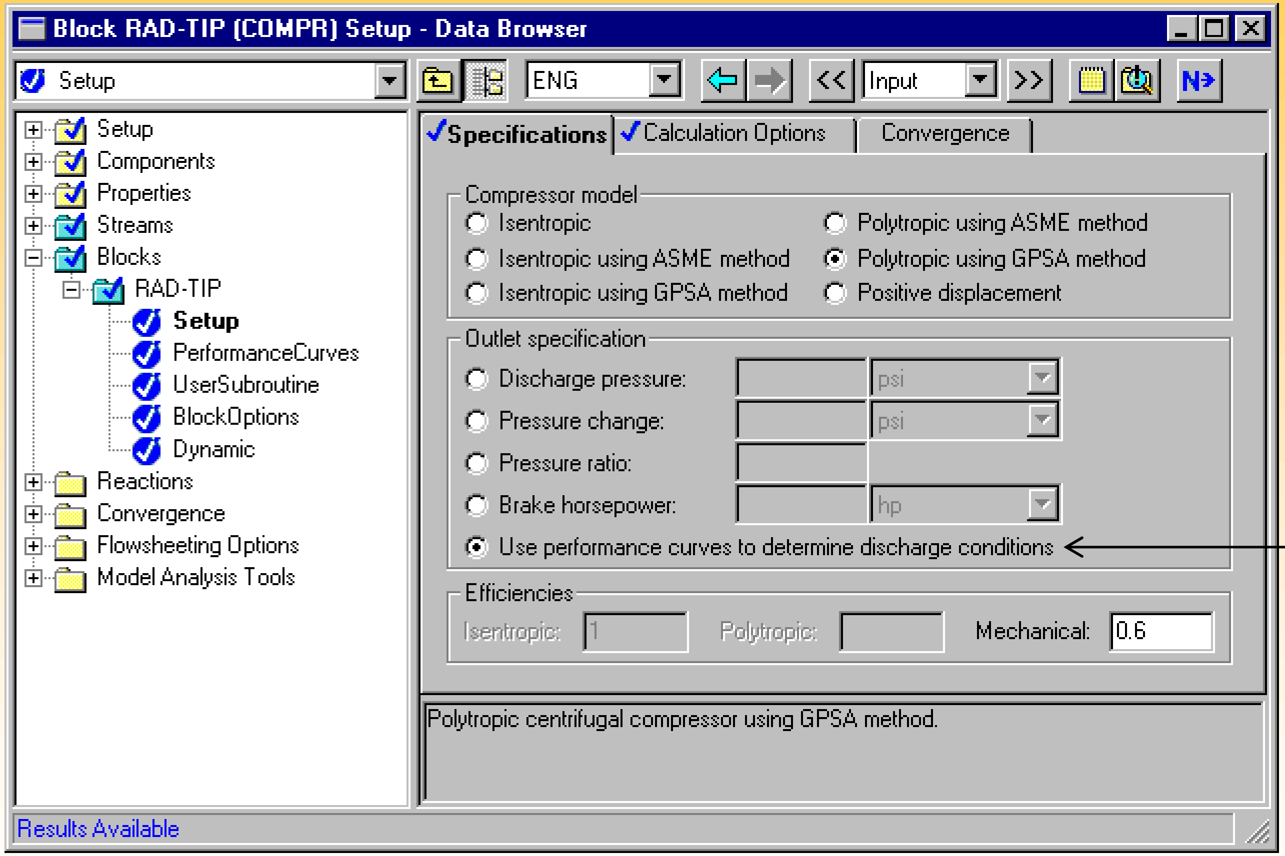
To	Do this
Ignore inertia effects	Select the Instantaneous option
Model the effect of inertia on compressor speed	·Select the Dynamic option ·Enter the moment of inertia ·Enter driver gear ratio (compressor speed/driver speed)

Compr and MCompr

- For dynamic Compressors:
  - Include performance curves
    - Single curve at reference speed

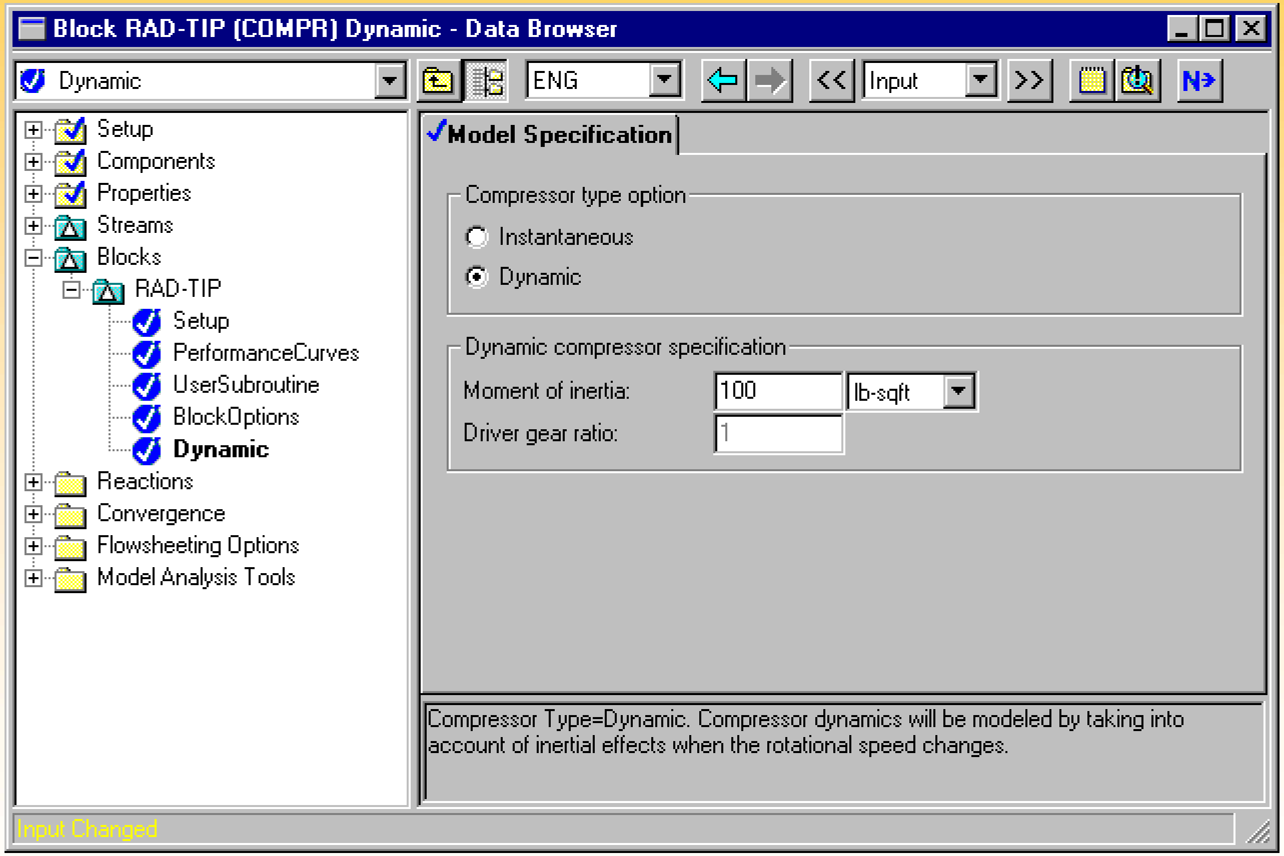
      OR
    - Multiple curves at different speeds

Performance Curves Specification



Specify Performance Curves

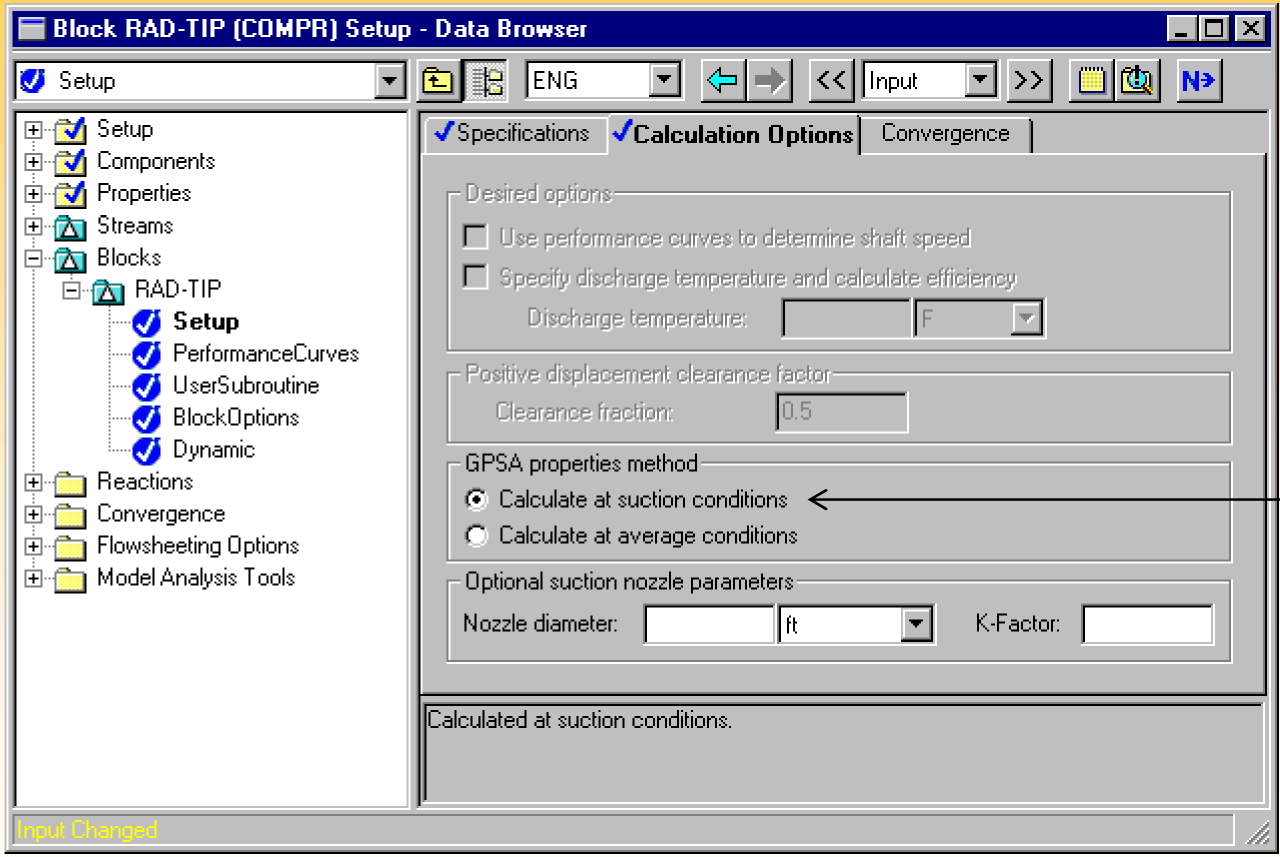
Compressor Dynamic Form



Compr and MCompr

- Supported Compressor types
  - Isentropic
  - Isentropic ASME method
  - Isentropic GPSA method
    - Basis - suction conditions
  - Polytropic ASME method
  - Polytropic GPSA method
    - Basis - suction conditions
  - Positive displacement

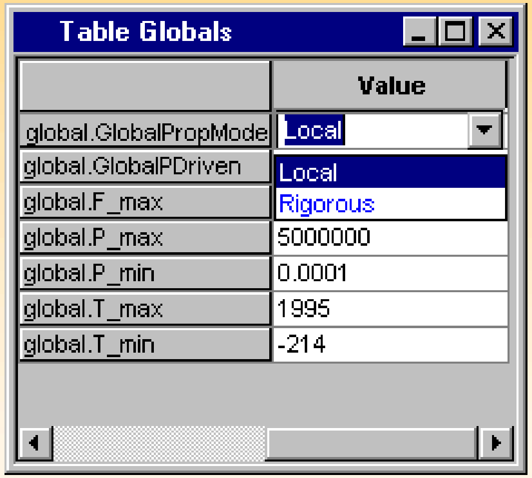
GPSA Properties Method



Supported GPSA calculation method

Key Dynamic Modeling Features

- Physical Properties Calculations
  - “Local” Property Models (default)
  - Rigorous physical properties calculations



Key Dynamic Modeling Features

- Physical Properties Calculations
  - Local property models
    - Used to calculate physical properties such as enthalpy, entropy, density, K-values
      - Properties are modeled on simple functions of temperature and pressure
      - Faster to evaluate than full physical properties calculations
      - Accuracy is comparable to using full physical properties
        - Local property parameters are updated at every integration step for accuracy

Key Dynamic Modeling Features

- Physical Property Calculations
  - Local property model example for equation to calculate liquid molar enthalpy.

$$h_L = \sum_{i=1}^{nc} xi \,.\, (A_i + B_i \,.\, T)$$

Where:

h_L = Liquid molar enthalpy

x_i = Mole fraction of component ***i***

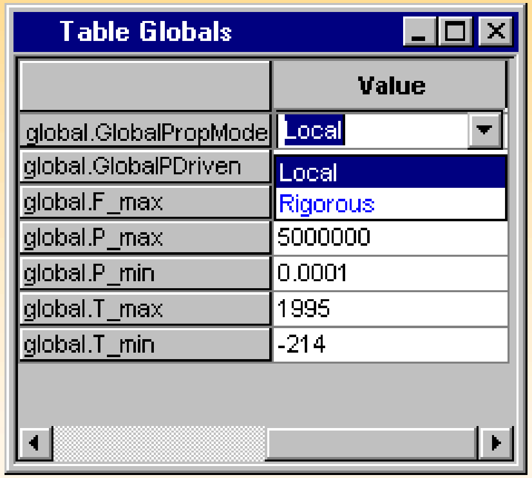
A_iB_i = Local property parameters for component ***i***

T = Temperature

nc = Number of components

Key Dynamic Modeling Features

- Physical Properties
  - Local Property Models
  - Rigorous properties



- Handling Full and Empty Vessels

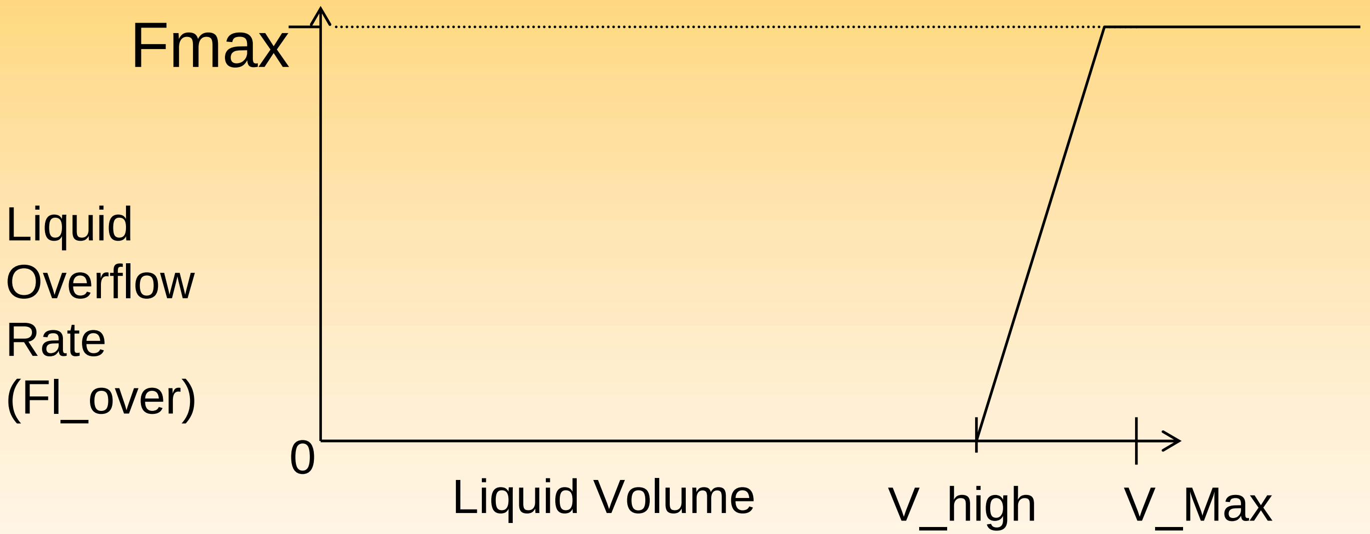
Key Dynamic Modeling Features

- Handling Full and Empty Vessels
  - Flow driven simulations allow change of flowrate directly by user or with controller
    - Can “remove” liquid from empty vessel flow
    - Can “add” liquid to full vessel where inlet flowrate is greater than outlet flowrate
  - Concept of “required” liquid outlet flow rate is introduced in the material balance for the vessel empty case
  - “Overflow” liquid flow is introduced in the material balance for vessel full case.

Note: Physical liquid overflow stream is not modeled

Key Dynamic Modeling Features

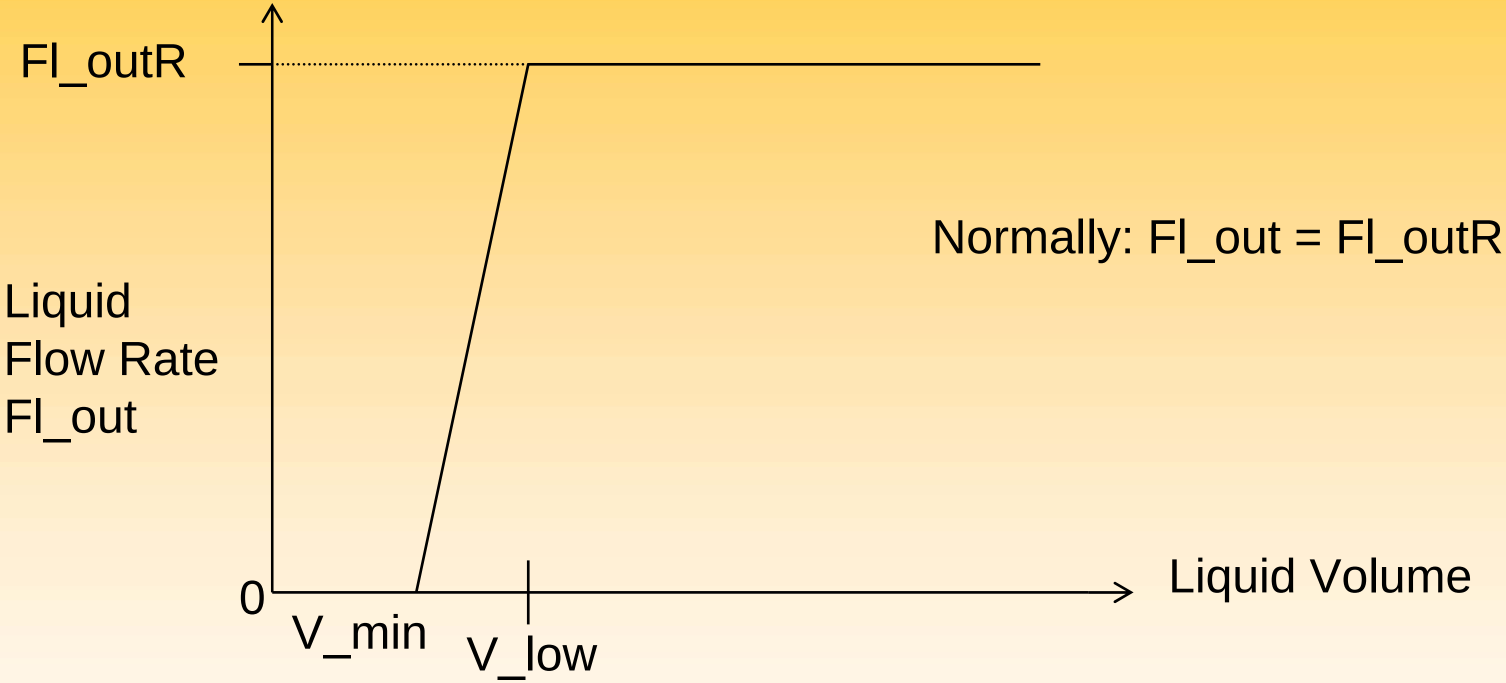
- Handling Full and empty Vessels - Overfilled Vessel



Fl_over - Liquid overflow rate
Fmax - Maximum allowable liquid flow
V_high - 99.5% of the vessel volume
V_Max - Vessel volume

Key Dynamic Modeling Features

- Handling Full and empty Vessels - Empty Vessels



Fl_outR - Required liquid outlet flowrate
Fl_out - Actual liquid flowrate
V_low - 0.5% of the vessel volume
V_Min - Zero volume

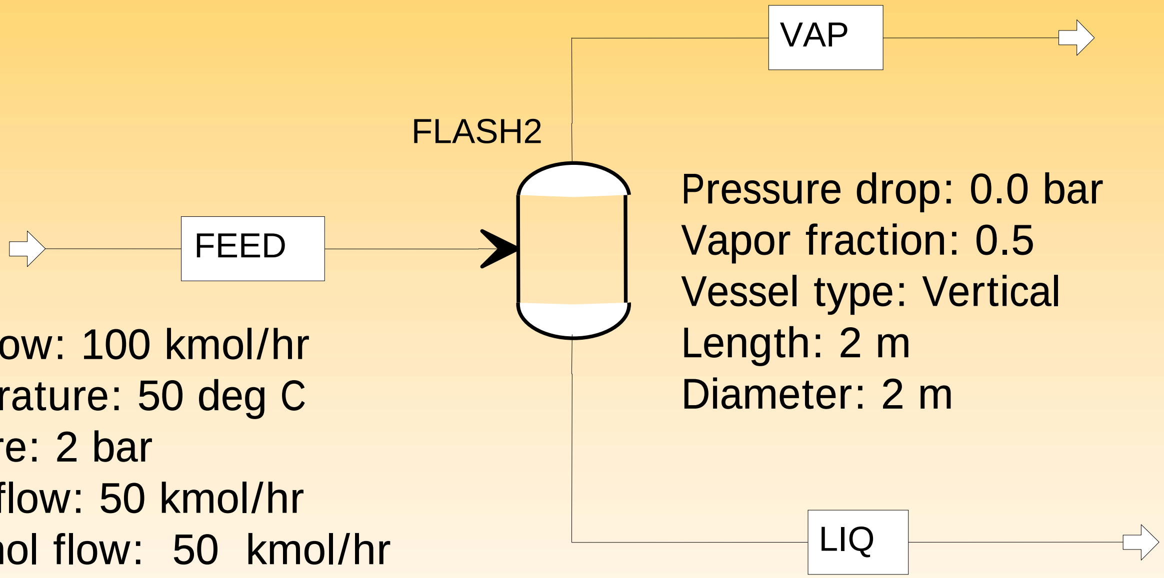
Workshop (45 min): Overfilled Vessel

Objective:

- Learn how overfilled vessels are handled
- Use the PID Control Block FacePlate

Workshop: Overfilled Vessel *(1)*

Property Method: NRTL



Total flow: 100 kmol/hr
Temperature: 50 deg C
Pressure: 2 bar
Water flow: 50 kmol/hr
Methanol flow: 50 kmol/hr

Pressure drop: 0.0 bar
Vapor fraction: 0.5
Vessel type: Vertical
Length: 2 m
Diameter: 2 m

Workshop: Overfilled Vessel *(2)*

The objective of this workshop is to demonstrate how liquid overflow is handled when the flash tank “overfills”. In actuality an overflow stream is not modeled in the flowsheet. Principally the “overflow” apart from satisfying the material balance, is there to allow the simulation to continue without failing, although it has some basis in reality.

1. Start Aspen Plus and load the file Start-OverfilledVessel.bkp from your workshop directory

2. Add the supplied dynamic data -see previous slide.

Tip: You must have the dynamic tool button down to access the dynamic data object under Blocks/Flash2. Expand the Blocks/Flash2 tree view to access dynamic data forms

3. Run the Aspen Plus steady state simulation

4. Export the dynamic problem files as a flow driven simulation

Workshop: Overfilled Vessel *(3)*

5. Save the backup file and exit Aspen Plus

6. Start Aspen Dynamics and load the generated dynamic problem file

7. Set your “flowsheet as wallpaper” from under the Window menu

8. Open the FacePlates for the level and pressure controllers on the flash drum.

9. Create a new plot to observe the vessel volume, liquid volume and vapor volume - modify the plot to have a time axis range of 0 to 1 hour and a single Y-axis

10. Create a second plot to observe the feed molar flow, vapor stream molar flow, liquid stream molar flow and the vessel liquid overflow rate - modify the plot to have a single Y-axis and a time axis range of 0 to 1 hour

11. Schedule regular snapshots to be taken every 0.2 hours

Workshop: Overfilled Vessel *(4)*

12. Set the simulation to pause at time 0.2 hours.

11. Run the simulation to 0.2 hours

12. Use the FacePlate button to switch the pressure controller to manual mode and set the output of the pressure controller to 0.0

What effect will this have on the flash vapor and liquid flows?

14. Set the simulation to pause again at time 0.4 hours

15. Run the simulation to time 0.4 hours

16. Use the FacePlate to switch off the liquid exit line flow in the same manner as the vapor exit line - change the controller mode to manual and set the output to 0.0

17. Set the simulation to pause again at 1.25 hours

18. Run the simulation to 1.25 hours

Workshop: Overfilled Vessel *(5)*

19. At time 1.25 hours, use the step tool button to step through the simulation till the liquid overflow kicks in.

At what time does the liquid overflow kick-in ?

What is the volume of the liquid in the vessel at the time when the liquid

overflow kicks in ?

What is the value of the liquid level when the vessel “overflows”?

The specified vessel length is 2 meters - why is the liquid level not equal to

this value?

Tip: The specified vessel length does not include the elliptical dished ends

What is the final (steady state) value of the variable Fl_Over?

Workshop: Overfilled Vessel *(6/6)*

Vessel Conditions at Time 1.29 Hours

Table MyVariables

	Description	Value	Units
BLOCKS("FLASH2").Vv	Vapor volume	0.041841	m3
BLOCKS("FLASH2").Vl	Liquid volume	8.33574	m3
BLOCKS("FLASH2").V	Vessel volume	8.37758	m3
STREAMS("LIQ").F	Total mole flow	0	kmol/h
STREAMS("VAP").F	Total mole flow	0	kmol/h
STREAMS("FEED").F	Total mole flow	100	kmol/h
BLOCKS("FLASH2").Level	Liquid level	2.91601	m
BLOCKS("FLASH2").Fl_over	Liquid overflow rate	125.889	kmol/h

Workshop: Overfilled Vessel

- Review

Reach Your
True
Potential

Scripts

Scripts

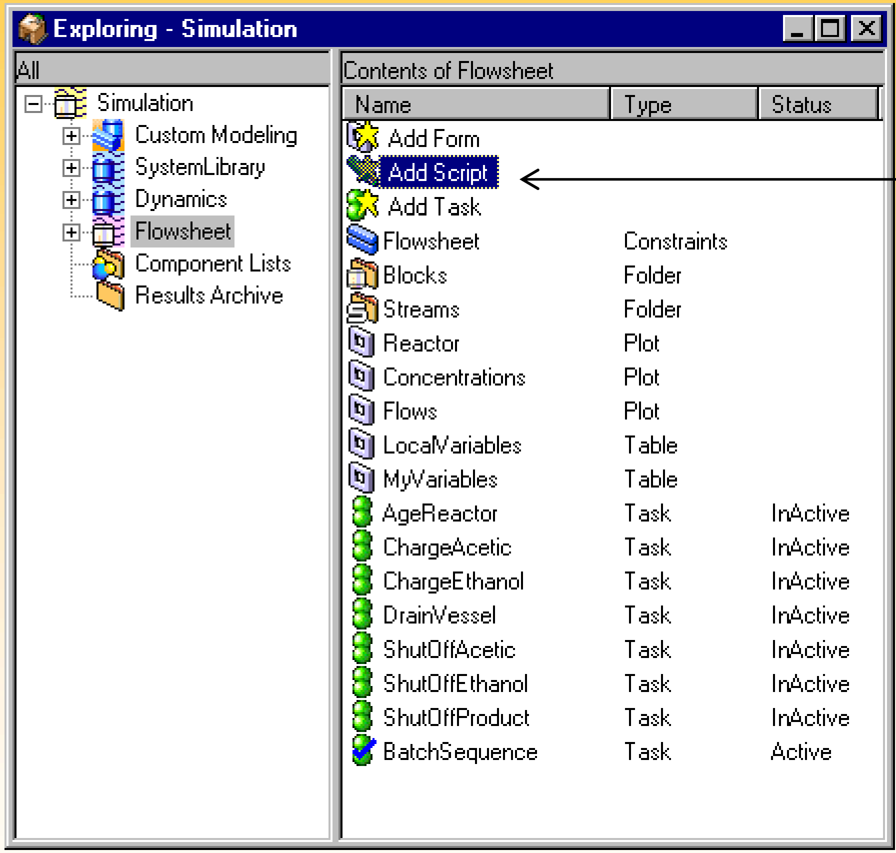
- Microsoft® Visual Basic® Scripting Edition (VBScript) Instructions
  - Automates simulation setup and control
- Add Scripts Manually
  - Simulation Explorer
- Auto-generate Scripts
  - Status window
  - Variable Find tool

Note: Microsoft® Visual Basic® Scripting Edition (VBScript) is automatically available with your installation.

Scripts

- Automate and Record Flowsheet Actions
  - Automate flowsheet problem specification
  - Automate simulation initialization
- Control Simulation Run Sequences with Automation Methods and Properties.
  - Define variable properties
- Define Units of Measure Sets
  - Store and apply different sets of specifications
- Call External Applications

Creating a Manual Script



Add Script Icon in Flowsheet folder

Auto-Generated Scripts

- Records changes made from Model Default Specification
  - FIXED and unFIXED (FREE)
  - INITIAL and unINITIAL

Advanced Scripts

- Invoke Scripts within Scripts
- Invoke scripts with External Visual Basic
- Execute Automation Methods
- Launch External Windows Applications
- Send messages to Simulation Window
- Use “FOR LOOPS” specifications

Syntax for Variable Assignments

- Flowsheet
  - Block.VariableName.Property = ######

- Example of Script at Flowsheet Level

  B1.Temp.Value= 550.0

  B1.Temp.spec = “Fixed”

  B1.X(“CO2”).Value = 0.03

  B1.X(“CO2”).Upper = 0.1

Scripts

- For more information and examples on Scripts, visit the Online Help.

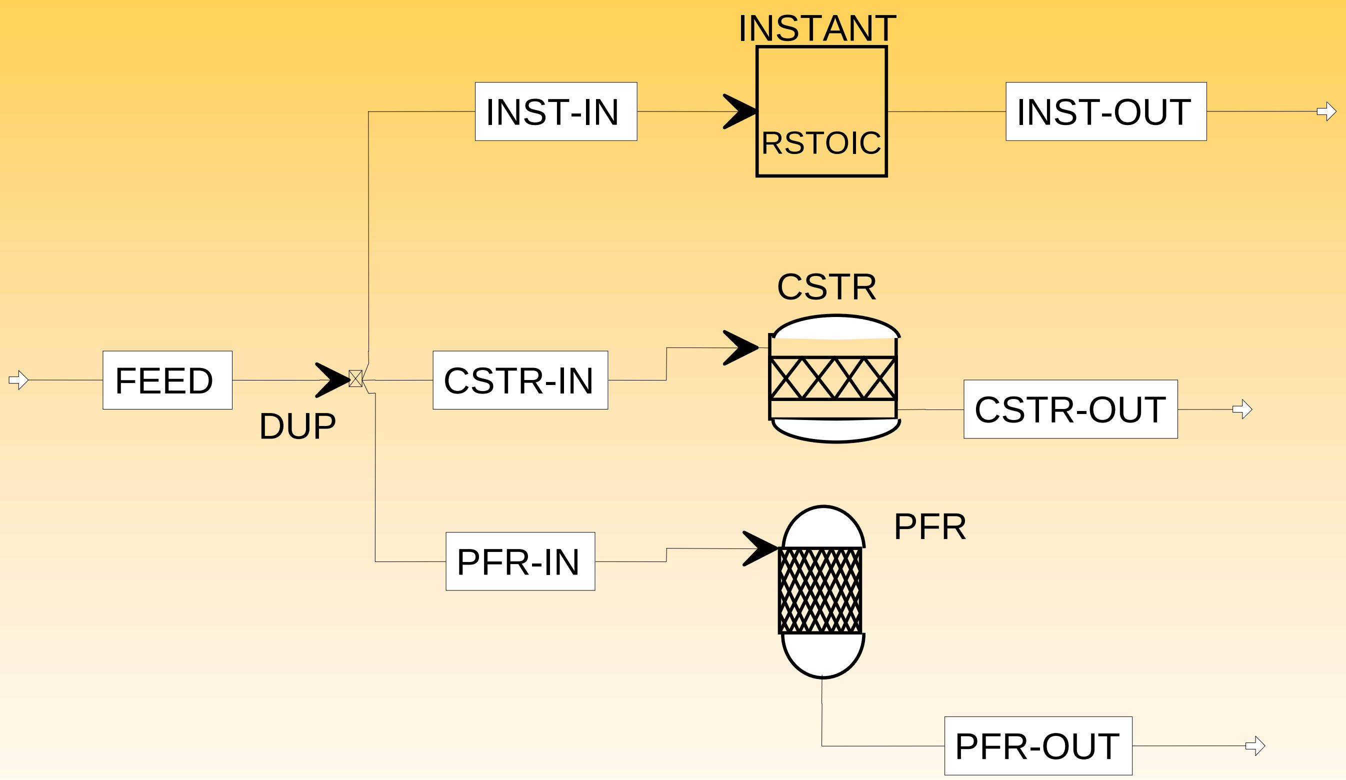
- VBScript help is available from the Microsoft web site as a free download:

  HTTP://WWW.Microsoft.com/VBScript

Workshop (30 min): Scripts

- Use Scripts to create specifications
- Use of Variable Find tool
- Become familiar with the RStoic reactor block dynamic simulation operating modes
- Customize Units of Measure (UOM)

Workshop: Scripts *(1)*



Workshop: Scripts *(2)*

Property: NRTL-RK

<u>Feed</u>

Temperature = 70 C

Pressure = 1atm

Water = 8.892 kmol/h

Ethanol = 186.59 kmol/h

acetic acid = 192.6 kmol/h

<u>Reactor</u>

Pressure drop = 0.2 bar

Temperature = 70C

Valid-Phases: Liquid-Only

Length = 3.5 m

Diameter = 1.5 m

Reactions: Ethanol + Acetic acid <---> Ethyl acetate + Water

Conversion = 70% of ethanol

Workshop: Scripts *(3)*

You are supplied with a backup file StartScripts.bkp

1. Load the backup file, and add the dynamic data supplied for the RStoic reactors operating in CSTR and PFR modes
2. Run the simulation in Aspen Plus and compare the steady-state results for the “different “ reactors.
3. Export the dynamic simulation problem files.
4. Open the dynamic problem file with Aspen Dynamics
5. Create a single time series plot to compare each reactor ethyl acetate product mole fraction. Add the feed component mole flow for ethanol on the same plot but use a separate axis.

Workshop: Scripts *(4)*

7. Auto-generate a Flowsheet Script to include the “spec” type and “value” of each feed stream component mole flow by following the steps below:

a) With the RMB, click on the FEED block and select “Find” to access the Variable Find tool window

b) Tick the “Fixed” specifications box to limit the variable search to variables specified as Fixed.

c) Click on Find to generate the variables requested

d) From the generated table, select all the listed as having Variable type “flow_mol”.

e) Click on Script to generate a Script in the Flowsheet folder

Workshop: Scripts *(5)*

8. Edit the Script to change the ethanol component mole flow in the feed

   from the current value to 200 kmol/h.

9. Save the Script - do not invoke the Script at this point.

10. Run the simulation to time 1 hour

Tip: Use the “Pause at” option from the run menu

11. At time 0.1 h, invoke the Script and continue the run.

12. Observe and compare the response of the product outlet concentrations of the different reactor types.

Is this the response you would expect? Can you explain the differences?

Workshop: Scripts *(6)*

Which reactor type would you expect to return to steady-state the quickest?

What is the effect of the level controller on the CSTR mode reactor?.

What other variables are worth observing for the response to a

change in the feed concentrations ?

What other variables are worth manipulating? Try adding new

Scripts for these variables and running the simulation.

13. Create a Flowsheet Script called MyUOM.

14. Use the text editor RMB popup menu “Insert File...” to insert the file ScriptsMyUOM.txt from your working directory)

15. Invoke the Script MyUOM to create your own Units of Measure (UOM) set called MyUOM.

Workshop: Scripts *(7/7)*

16. Bring up a stream results table.

17. Under the Tools menu, go to “Units of Measure” and tick MyUOM.

18. View the simulation results table in the customized UOM.

Tip: The file OnNewDocumentScript.vb containing the full UOM set

exists as part of the Aspen Dynamics system installation under the

Your_Installation_Drive_Name:/…../AMSystem/Bin directory.

Scripts

- Review

Reach Your
True
Potential

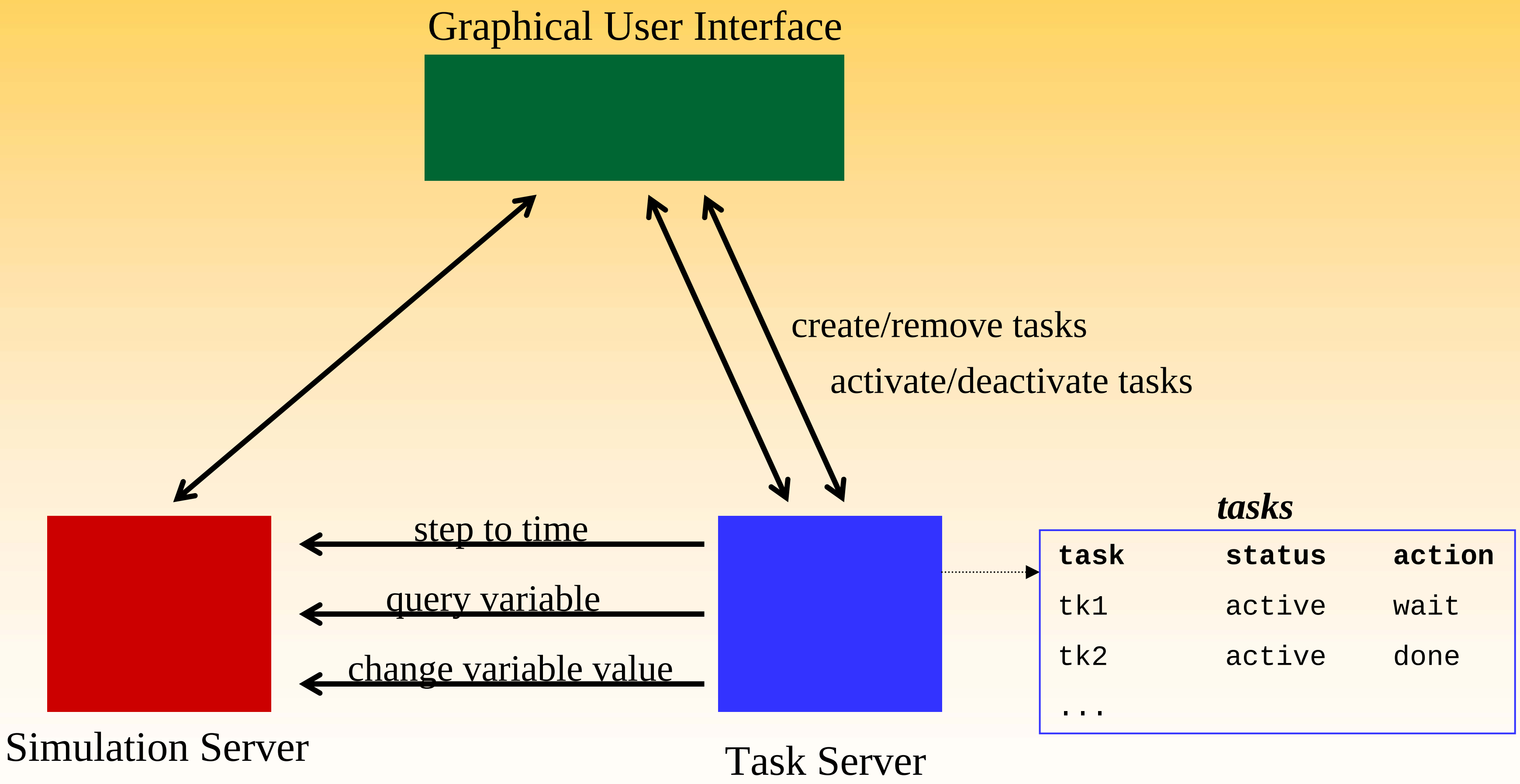
Tasks

Tasks

- Defines Sequence of Discrete Actions
  - Tasks can be event-driven actions
    - Responds to an event or condition
  - Tasks can be callable - subtasks
    - Subtasks are called by other tasks - not triggered by an event
    - Subtasks can be called in parallel

Tasks

- Overall picture



Tasks

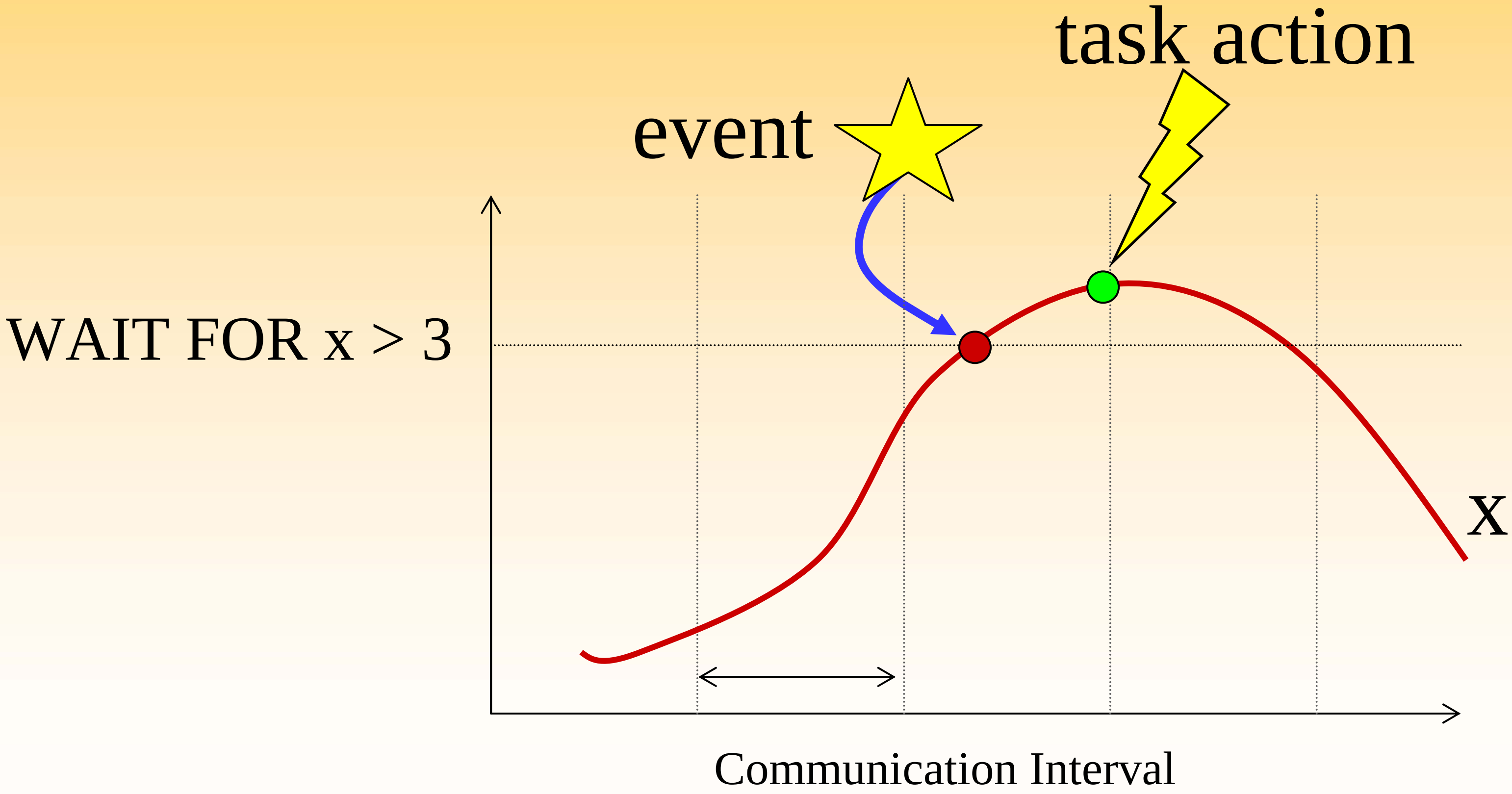
- Use Tasks to Schedule Changes to Values of (Fixed) Variables
  - Instantaneous change
  - Linear ramp
    - Predefined RAMP function
  - Sinusoidal/S-curve ramp
    - Predefined SRAMP function
- Restart other Tasks
- Take Snapshots
- IF THEN ELSE Statements allowed

Tasks

- Tasks must have Active Status to Run
  - Double (default action) click or RMB on task to activate a task
- Tasks assume system base units
  - SI/METRIC

Tasks

- Task state is checked at communication interval
  - special case for explicit events: WAIT FOR time == 1



Tasks

- Event driven task syntax:

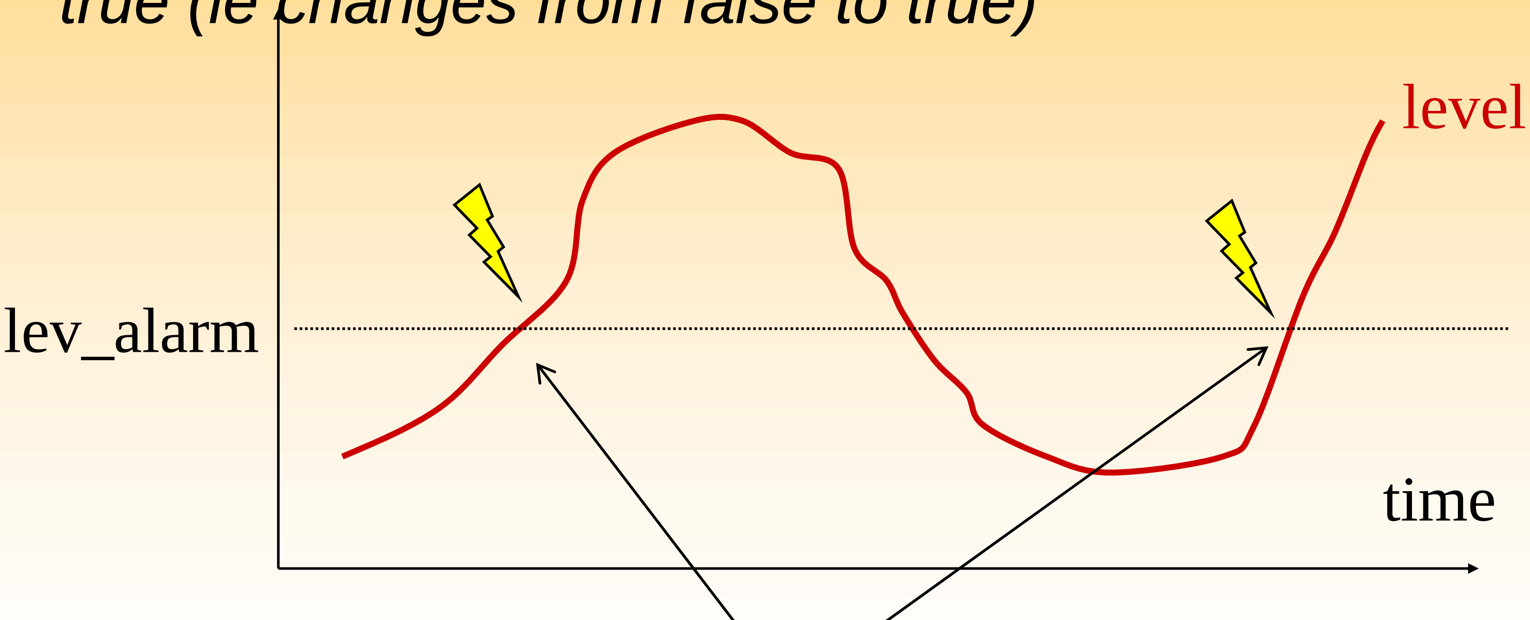
```
TASK TaskName RUNS [ONCE] WHEN Condition
  TaskStatements;
END
```

- Condition is defined by a logical statement such as
  - time == value
  - expression1 >, <, ==, <>, >=, <= expression2

Tasks

- Event-driven task status is checked at communication intervals

- *Tasks are executed whenever the condition **becomes** true (ie changes from false to true)*



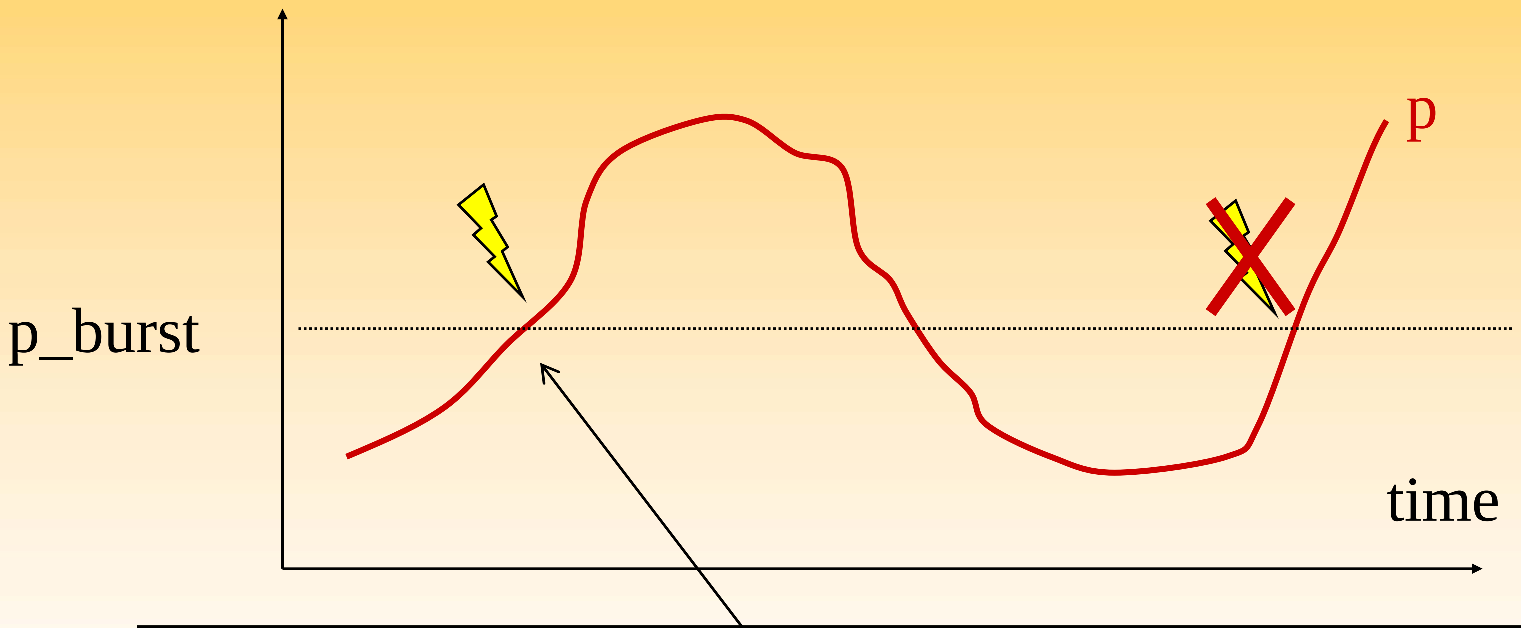

```
task xmp runs when level > lev_alarm
```

Tasks

- Tasks run whenever the start condition changes from false to true by default
- Can define task to run “Once” and never again during simulation
  - Use the ONCE qualifier for bursting disks

Tasks

- "ONCE" qualifier



Task bursting_disk runs once when p > p_burst
Blocks("Valve").Cv : 1000.0;
END

Tasks

- Step Changes in Tasks

```
Task Shutdown Runs when Time == 5.0
//Set the feed flowrate to zero
  Streams(“Feed”).FmR: 0.0;
End
```

```
Task Startup Runs When Blocks(“D101”).Level <= 0.01
//Set the feed flowrate to 10.0
  Streams(“Feed”).FmR: 10.0;
End
```

Tasks

- Parameters in Tasks

```
Task Shutdown Runs when Time == 5.0
LowFlow as Realparameter(0.0);
HighFlow as RealParameter (10.0);
//Set the feed flowrate to zero
  Streams(“Feed”).FmR: LowFlow;
Wait For Blocks(“D101”).Level <= 0.01;
//Set the feed flowrate to 10.0
  Streams(“Feed”).FmR: HiFlow;
End
```

Tasks

- Ramping functions (RAMP and SRAMP)
  - RAMP(variable, final_value, ramp_duration);
  - SRAMP(variable, final_value, ramp_duration);

```
TASK Task4 RUNS WHEN TIME == 4.0
 // Flow changes to 5.0 linearly
  // over a period of 2 time units
  RAMP (Streams("Feed").FmR, 5.0, 2.0);
END
```

```
TASK Task4 RUNS WHEN TIME == 4.0
// Temperature changes with an S-shaped curve
  // to 15.0 over a period of 3 time units
  SRAMP (Streams("Feed").T, 15.0, 3.0);
END
```

Tasks

- Callable Tasks
  - Tasks can be called within tasks

```
TASK TaskName ( ParameterList )
  Call TaskName (ParameterList);
End
```

- Task can be called in parallel or in sequence
- Parameters can be passed between callable tasks

Tasks

- Parameters in Callable Tasks

```
Task MainTask Runs when Time == 0.5
var as realparameter;
Var: Time;
Call SubTask(Var*Var+8.4*Var, Var, 4);
End
```

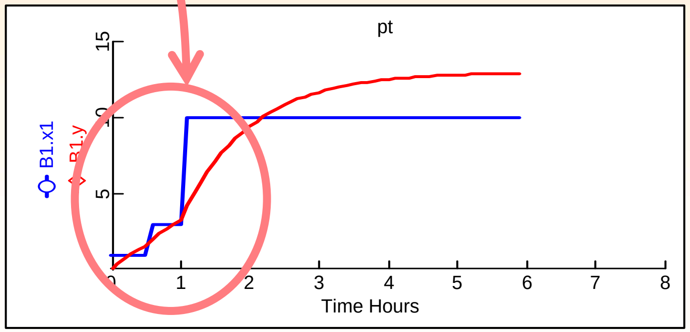
```
Task SubTask (Arg1 AS RealParameter;
              Arg2 As RealParameter;
              Arg3 As RealParameter;)
Print “Calculate function”;
Arg2: (Arg1 + 0.2)*Arg3;
End
```

Tasks

- Parameters in Callable Tasks

```
Task dorecipe runs when time == 0.5
tx as realparameter;
tx : 10;
call recipe (tx);
End
```

```
Task recipe (tx as realparameter)
  B1.x1.value : 3;
  wait for time == 1;
  B1.x1.value : tx;
End
```



Tasks

- Callable Tasks

```
Task MainTask Runs WHEN TIME == 1.0
Streams(“FEED”).FR: 4;
Call SubTaskA;
Call SubTaskB;
End
```

```
Task SubTaskA
      RAMP(Blocks(“FV101”).CV, 2.5, 3.0);
End
```

```
Task SubTaskB
 SRAMP(Streams(“FEED”).X(“H2O”),0.5, 2.0;
End
```

Tasks

- Parallel Tasks
  - Group together CALL statements within a task and execute the task calls in parallel using the PARALLEL and ENDPARALLEL construct
  - Each action is executed until it completes
  - Parallel section completes when all actions in it are complete.

```
TASK Task1 RUNS WHEN TIME == 1.25
  PARALLEL
    CALL P1; // ramp with duration=2
    CALL P2; // another ramp with duration=1
  ENDPARALLEL;
  Input4.Flow : 0.0;
END
```

Tasks

- Holding Execution - wait for an event or condition

```
WAIT FOR condition;
```

- Hint for implementing delay:
  - create a realparameter
  - use an assignment to evaluate the time of the end of the delay

```
nexttime as RealParameter;

nexttime : TIME + 2.0; // wait for 2 hours
WAIT FOR TIME == nexttime;
// some tasks
nexttime : TIME + 1.0; // wait now for 1 hour
WAIT FOR TIME == nextime;
// etc...
```

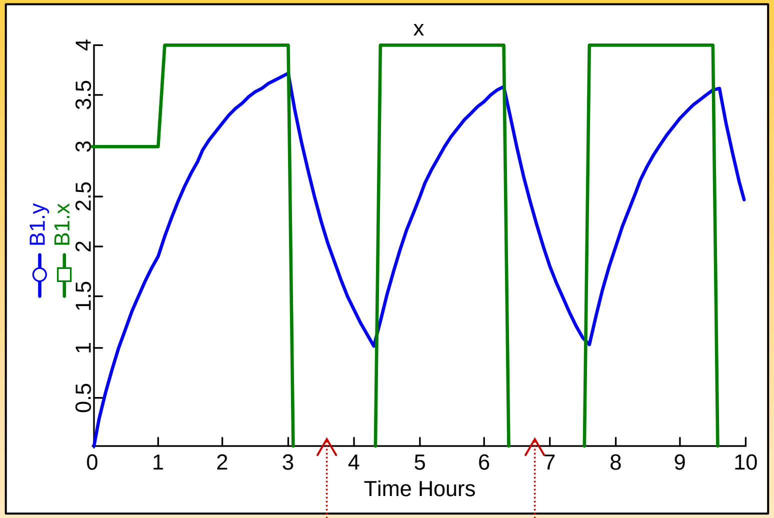
Tasks

- Conditionals in Tasks

```
Task Condition RUNS WHEN Blocks(“D101”).Level < 0.01;
IF Streams(“S101”).FmR <= 0.1 THEN
      Streams(”S101”).FmR : 10.0;
ELSE
      Streams(“S101”).FmR : 1.0;
ENDIF
END
```

Tasks

- Cyclic Events
  - RESTART WHEN condition;
    - Example: $y = x - y



RESTART makes the task execution to jump back to the first line

```
Task res runs when time == 1
  timenext as realparameter;
  B1.x : 4;
  timenext : time + 2;
  wait for time == timenext;
  B1.x : 0;
  restart when B1.y < 1;
End
```

Tasks

- Create a Snapshot

```
TASK Snapshot RUNS WHEN Time == 10.0
  CREATE SNAPSHOT "Task-Created Snapshot #1";
END
```

- Print a message and Pause the simulation

```
TASK Debug RUNS WHEN Time == 1.0
   PRINT "Start Task Test3";
   RAMP (Input1.Flow, 2.5, 5.0);
   PRINT "Task Test3 Finished";
   PAUSE;
END
```

Tasks

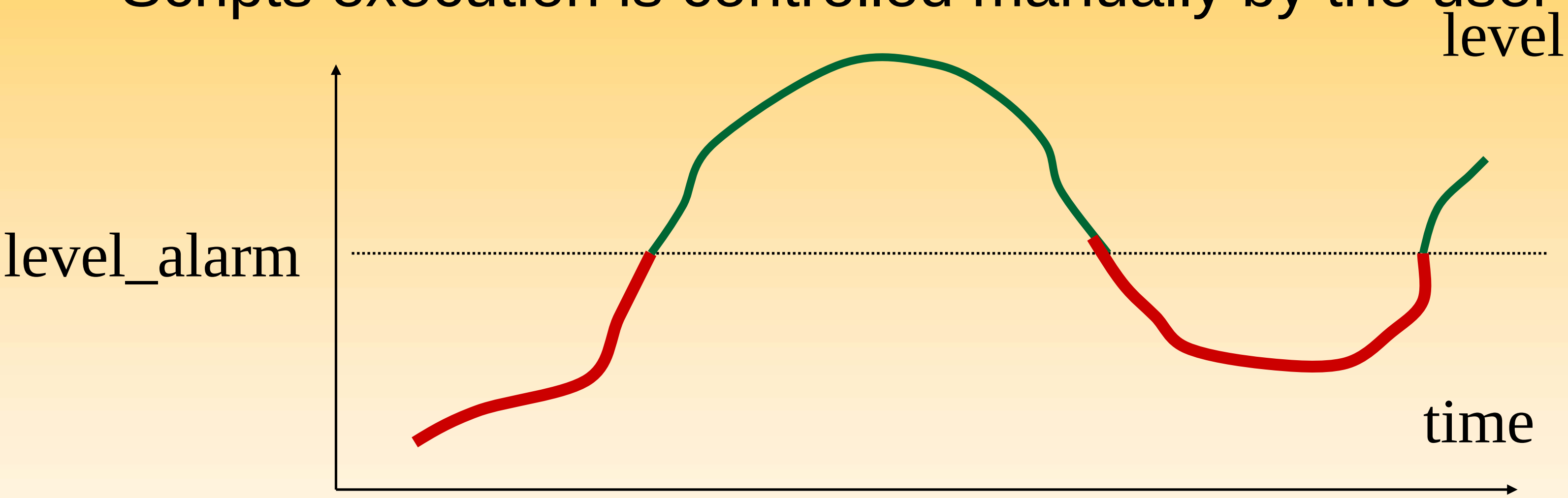
- Conflicting Tasks
  - Task RampFlow will override task Stepflow

```
TASK RampFlow RUNS WHEN TIME == 1.0
  Ramp(Streams(“FEED”).FmR, 4.0, 3.0);
END
```

```
TASK StepFlow RUNS WHEN TIME == 3.0
  Streams(“FEED”).FmR: 2.0;
END
```

Task or Script?

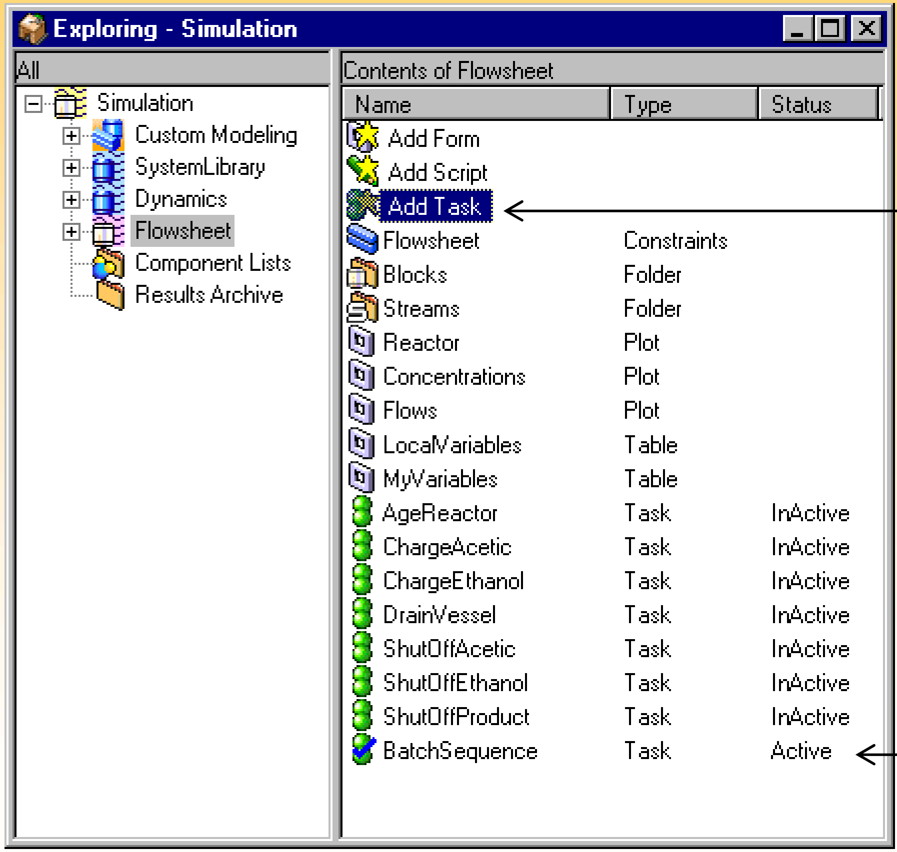
- Tasks are executed at the condition switchover
- Scripts execution is controlled manually by the user




```
if (level > level_alarm) then
        statements1
else    statements2
endif;
```

Tasks

- Creating a Task
  - Flowsheet
  - Dynamics Library Tasks folder



Add Task Icon in Flowsheet folder

Active Task with checkmark

Tasks

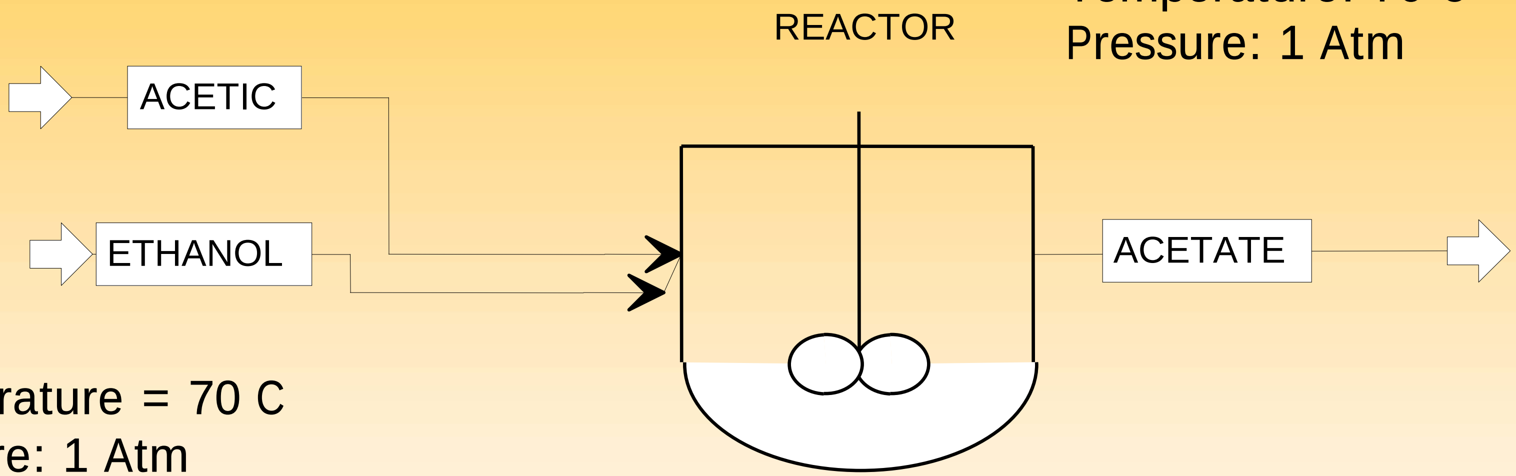
For more information and examples on the Task language, visit the Online Help.

Workshop: Tasks (60 minutes)

- Use Task language to drive events.
- Use Task language for batch sequencing

Workshop: Tasks *(1)*

Volume: 5 m3
Temperature: 70 C
Pressure: 1 Atm



Temperature = 70 C
Pressure: 1 Atm
Stream Acetic: 2300 kg/h
 Acetic Acid = 2300 Kg/h
Stream Ethanol: 1700 Kg/h
 Water = 100 Kg/h
 Ethanol = 1600 Kg/h

Workshop: Tasks *(2)*

The objective of this workshop is to complete a task to sequence a batch reactor operation, starting from a RCSTR unit operation in Aspen Plus

You are provided with the file: Start-Tasks_Sequence.txt

This file contains the completed sequence of events to simulate the batch reactor schedule. Furthermore you are provided with the files listed below

The files listed below contains completed tasks called by the main batch sequence task - these correspond to the first four events in the batch schedule

Start-Tasks_ShutOffFeed.txt

Start-Tasks_DrainVessel.txt

Start-Task_ShutOffProduct.txt

Start-Tasks_ChargeReactor.txt

Workshop: Tasks *(3)*

You are to create the remaining tasks which are called by the main batch sequence task

1. Open the steady state problem in Aspen Plus and browse through the input - note that the specified reactor volume is 5 m3

2. Run the steady state problem and browse the results - note the steady state molar concentration of the ethyl acetate in the product stream

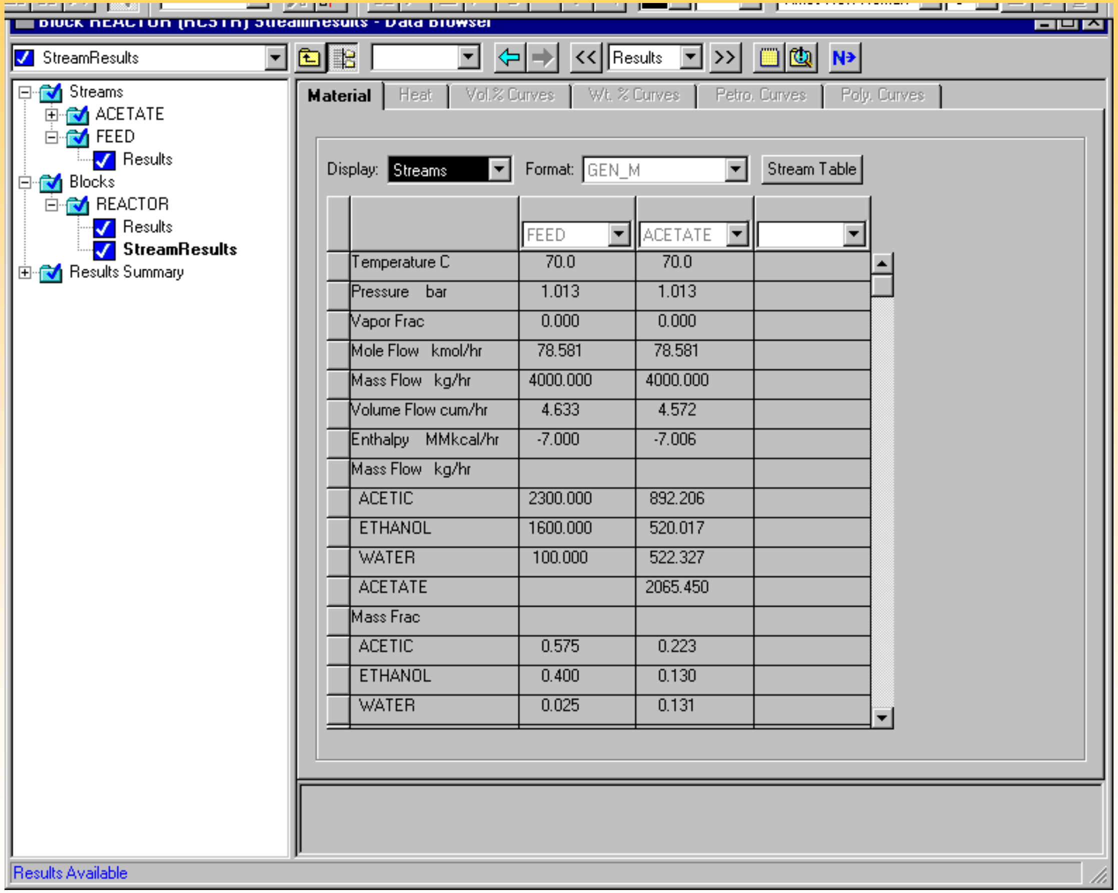
3. Modify the input with the dynamic data provided to set up the batch

Reaction (liquid holdup) volume = 2.5 m3
Vessel Length : 2 m
Heat Transfer Option: Constant temperature medium at 20 C
Initial Liquid holdup fraction: 0.5

What will Aspen Dynamics calculate as the reactor geometric volume? Why are you not required to specify a vessel diameter?

Workshop: Tasks *(4)*

Streams Summary for the 2.5 m3 Reactor



	FEED	ACETATE
Temperature C	70.0	70.0
Pressure bar	1.013	1.013
Vapor Frac	0.000	0.000
Mole Flow kmol/hr	78.581	78.581
Mass Flow kg/hr	4000.000	4000.000
Volume Flow cum/hr	4.633	4.572
Enthalpy MMkcal/hr	-7.000	-7.006
Mass Flow kg/hr		
ACETIC	2300.000	892.206
ETHANOL	1600.000	520.017
WATER	100.000	522.327
ACETATE		2065.450
Mass Frac		
ACETIC	0.575	0.223
ETHANOL	0.400	0.130
WATER	0.025	0.131

Workshop: Tasks *(5)*

4. Export the Aspen Dynamics problem definition as a flow driven simulation file.

5. Start Aspen Dynamics and open the exported problem file.

6. Delete the auto-generated level controller and associated control signal connections

9. Change the run mode to Initialization and perform an Initialization mode run.

What is the reactor geometric volume? What is the liquid volume?

10. Create separate new plots to observe the following;

10.1. Reactor liquid volume, liquid level and temperature
10.3. Reactants and products concentrations in the reactor - use one axis for the concentrations

Workshop: Tasks *(6)*

10.3 Feed and product stream mass flows - use one axis for both variables

11. Create a batch sequence main task which runs at time 0.1 hours - use the Edit/Insert menu to insert the partially completed file Start-Tasks_Sequence.txt

Tip: Do not compile the main task until all the called tasks have been successfully compiled

Workshop: Tasks *(7)*

13. The following sequence of events defines the batch schedule

13.1 Shut off the feed
13.2 Drain the vessel by emptying the product at a rate of 60 kmol/hr till the reactor liquid level falls below 0.1 m
13.3 Shut off the ethyl acetate product liquor
13.4 Charge the reactor with feed at a mass flow rate of 4000 Kg/h for 0.7 hrs, over a period of 0.1 hours
13.5. Shut off the feed
13.6 Age the reactor till ethyl acetate concentration in the reactor becomes greater than 7 Kmol/m3.
13.7 Drain the vessel of the product liquor at a rate of 60 kmol/h until the reactor liquid level falls below 0.1 m3

Workshop: Tasks *(8)*

14. Create the (sub)tasks to be called by the main batch sequence task. The first 4 events have been predefined as tasks in the text files. Use the RMB popup menu Insert/Files.... to insert these as separate tasks. Compile each task before moving on

15. Add the remaining 3 tasks (events 13.5 to 13.7 inclusive) to schedule the last 3 events. Include a Pause statement to use to stop the simulation at the end of the cycle.

Tip: Tasks which are called must be compiled before the task which does the calling

11. Activate the batch sequence main task - make sure all subtasks are compile ok first

Note: Tasks which are called CANNOT be activated

Workshop: Tasks *(9/9)*

12. Run the simulation in dynamic mode and observe the plots.

What is the volume of the reactor at the end of the charge stage?

How long does it take for the ethyl acetate concentration to reach the desired value from the the time the charge stops?

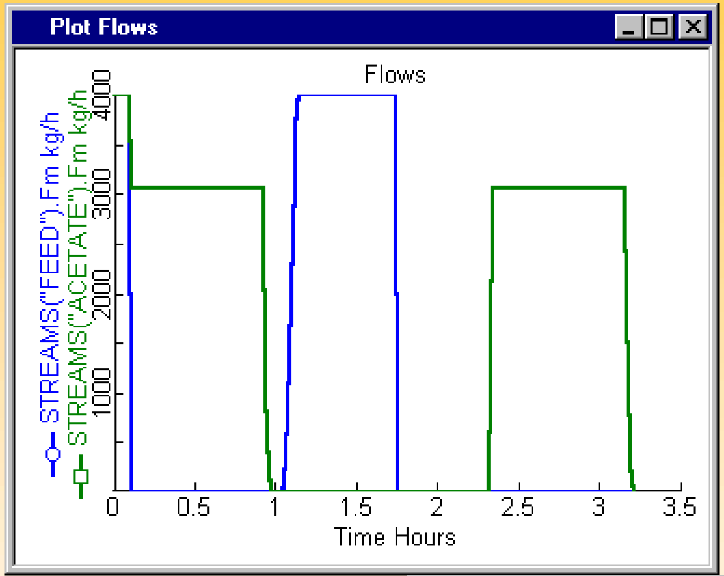
What are the concentrations of the reactants and products at the end of the cycle?

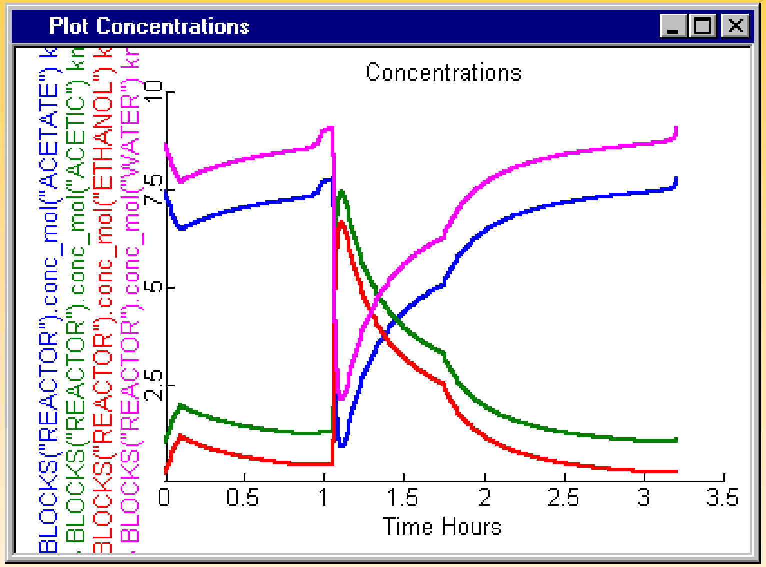
How long does it take to discharge the product liquor?

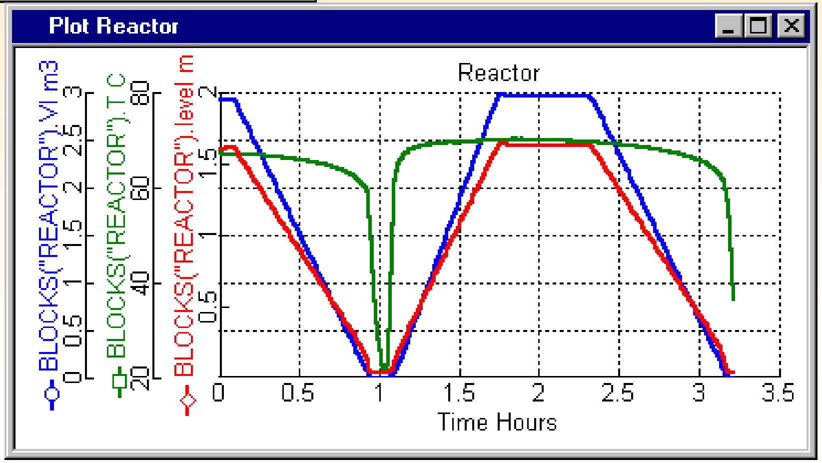
What is the volume of the reactor at the end of the product discharge step?
How and where can the batch cycle time be reduced?

Workshop: Tasks

Time Series Profiles







Workshop: Tasks

- Review

Reach Your
True
Potential

Pressure Driven Simulations

Objective:

Learn how to implement pressure-driven simulations in Aspen Dynamics.

Pressure Driven Simulations

- What is a Flow Driven Simulation?
- What is a Pressure Driven simulation?
- Configuring a Pressure Driven Simulation
  - Use of the Pressure Checker

Pressure Driven Simulations

- What is a Flow Driven Simulation?
  - Outlet stream pressure determined from inlet conditions and block specifications
  - Outlet flow rates determined from inlet conditions and block specifications
  - Outlet stream pressures unaffected by downstream pressure
  - Outlet flow rates unaffected by downstream pressures
  - Assumes perfect flow and pressure control

Pressure Driven Simulations

- What is a Pressure Driven Simulation?
  - Downstream pressures influence flowrates
  - Flowrates are determined by pressure/flow relationship between upstream and downstream blocks
    - Line or system resistance forces a pressure drop between units

Pressure Driven Simulations

- Steam Heated Reboiler Example

Steam_Duty = Steam_Flow * Latent_Heat_of_Vaporization

- Reboiler imposes constraint;
  Reboiler_Duty = UA * Temperature_Difference

- If Reboiler area (UA) is fixed, then;
  Reboiler_Duty =function(Temperature_Driving_Force)

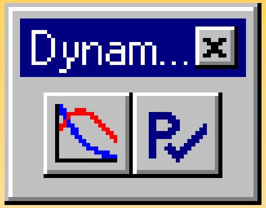
- Control reboiler duty by stream pressure (steam flow) at reboiler inlet with control valve;
  Steam_Flow = function(Valve_Pressure_Drop)

Configuring a Pressure Driven Simulation

- Configuring a Pressure Driven Simulation
  - Use the pressure checker
  - Remove unsupported models
  - Add blocks for pressure/flow relationships
    - Units which determine pressure must not be connected directly together
  - Ensure block pressures are consistent
    - Equal upstream and downstream block pressures
    - Inlet pressures greater than outlet pressure
  - Use the “Pressure Checker”
  - Export “P Driven Dyn Simulation” file

Pressure Driven Simulations

- The Pressure Checker

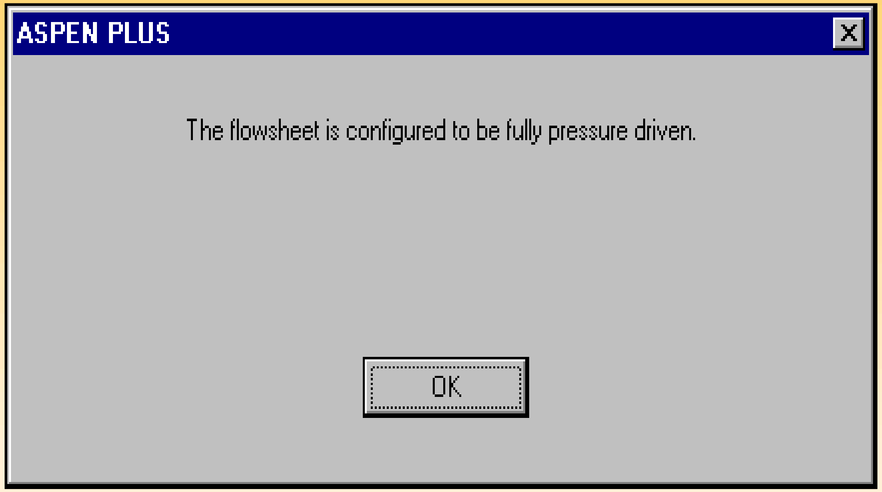


Pressure Checker tool button

  - Checks flowsheet for consistency
    - Consistency of interconnecting blocks
    - Consistency of pressures
  - Advises on required changes to flowsheet
  - Warns of potential problems in dynamic simulations

Pressure Driven Simulations

- The Pressure Checker OK Message



Flowsheet is fully configured for a
Pressure Driven Dynamic Simulation
- OK to export “P Driven Dyn Simulation” file

Workshop: (60 min): Pressure Driven Simulation

- Configure a Flow Driven Simulation Flowsheet to become a Pressure Driven Simulation

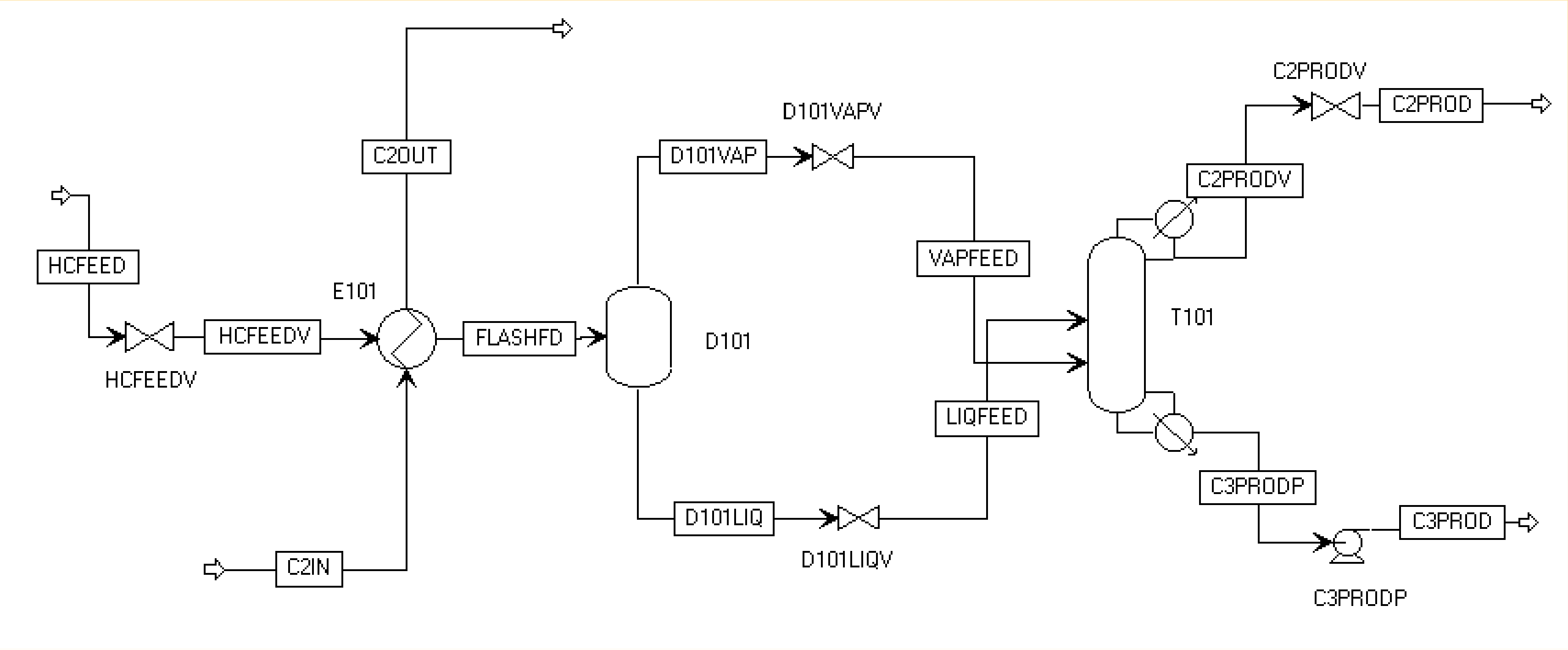
Workshop: Pressure Driven Simulation *(1)*

1. Open Aspen Plus and load the file Start-PDrivenSim.bkp
2. Use the Pressure Checker to confirm what is required to configure the flowsheet to be pressure driven
3. Following the pressure checker directive modify the flowsheet to configure the deethanizer flowsheet to be FULLY pressure driven - see the diagram following
4. Use the data supplied to complete and run the flowsheet

Note: Pressure/flow relationship blocks are not necessary in streams connected to unit operations (e.g. HEATER and HEATX) modeled with a pressure/flow equation.

Workshop: Pressure Driven Simulation *(2)*

Note: Valve HCFEEDV is not mandatory for a pressure driven simulation.
The valve is included so to enable control of the hydrocarbon feed flow



Workshop: Pressure Driven Simulation *(3)*

Valves Data

	HCFEEDV	C2PRODV	D101LIQV	D101VAPV
Calculation Type	Valve flow coefficient	Valve flow coefficient	Valve flow coefficient	Valve flow coefficient
Pressure Specification	Outlet pressure	Pressure drop	Outlet pressure	Outlet pressure
Pressure Value	21 (bar)	0.5 (bar)	20.1279 (bar)	20.1412 (bar)
Flash Options	Vapor-Liquid	Liquid-Only	Liquid-Only	Vapor-Only
Type	Ball	Ball	Ball	
Manufacturer	Neles-Jamesbury	Neles-Jamesbury	Neles-Jamesbury	Neles-Jamesbury
Series/Style	5000_ reduced_ port_ flanged	5000_ reduced_ port_ flanged	5000_ reduced_ port_ flanged	Ansi_ class_ 150_
Size	8-IN	6-IN	6-IN	3-IN

Workshop: Pressure Driven Simulation *(4)*

Other Data

Pump C3PRODP

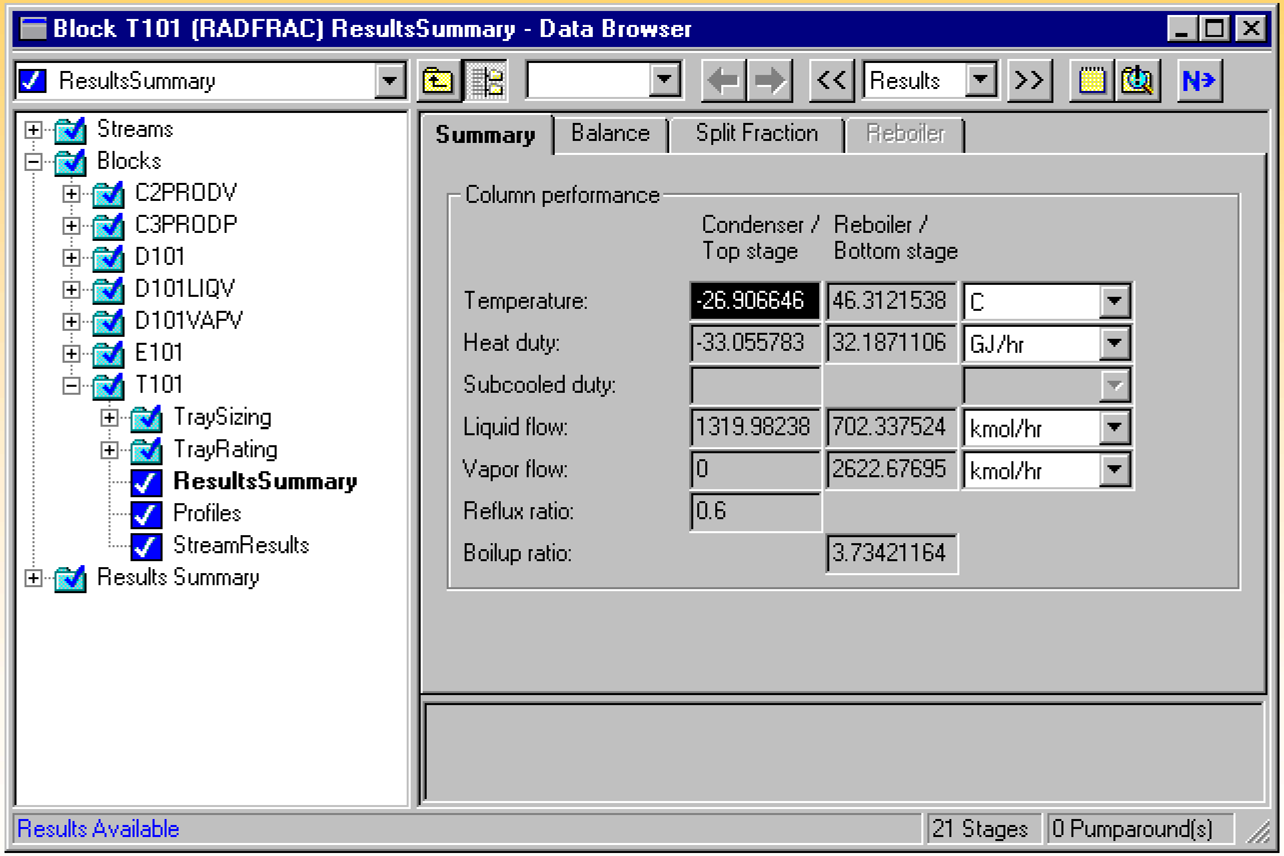
Outlet Specification	Pressure increase
Pressure	1 (bar)

Column T101

Feed Stream	Feed Stage
VAPFEED	17
LIQFEED	13

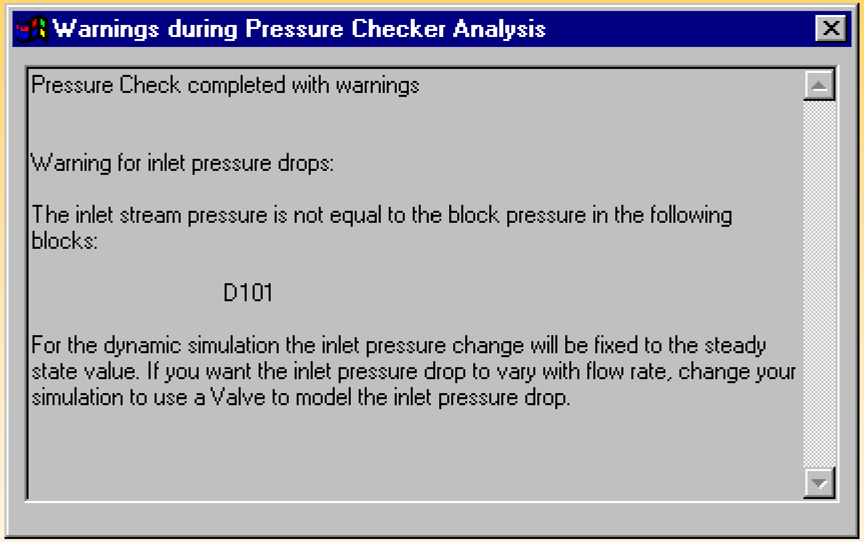
Workshop: Pressure Driven Simulation *(5)*

5. When the run completes, check the column summary results to make sure you have inputted the data correctly - the results should be as below



Workshop: Pressure Driven Simulation *(6)*

6. Once you are happy with the results, use the Pressure Checker to confirm that the simulation is indeed fully pressure-driven - you should get the following message



To correct this problem, edit the flash block to enter a pressure drop of 0.0. The the inlet stream FLASHFD pressure thus becomes equal to the flash block D101 operating pressure. This allows the flash block feed flowrate to vary with the inlet pressure and the flash operating pressure - a pressure driven flow! - in the dynamic simulation.

Workshop: Pressure Driven Simulation *(7)*

7. Run the modified flowsheet

8. When the run completes with status Results Available, use the Pressure Checker to confirm that the simulation is indeed pressure-driven. You should get the following message

Workshop: Pressure Driven Simulation *(8)*

9. Export the simulation as a pressure driven simulation
10. Save the backup file and exit Aspen Plus
11. Load the new problem file into Aspen Dynamics
12. Reconnect the output of controller LC5 (controls the reboiler liquid sump level) to manipulate the product pump power
13. Use the controller LC5 configure form to initialize the controller variables - the operator set point should be 2.2, the bias should be 2.9588 and the gain and integral time will remain at 10.0 and 6000 respectively
14. Change the LC5 controller action to be Direct
15. Open the product stream C2PROD and C3PROD predefined TPF plots and set the time axis range to 0.5 hours
16. Set the simulation to pause at time 0.1 hours and run the simulation in dynamic mode

Workshop: Pressure Driven Simulation *(9)*

17. At time 0.1, set the simulation to pause again at time 0.5 hours

18. Create a new plot to observe both the HCFEEDV valve position and the hydrocarbon feed stream mass flowrate. Set the time axis range to 0.5 hours

19. From the valve HCFEEDV manipulate table, change the HCFEEDV valve position to 50% and observe the open plots

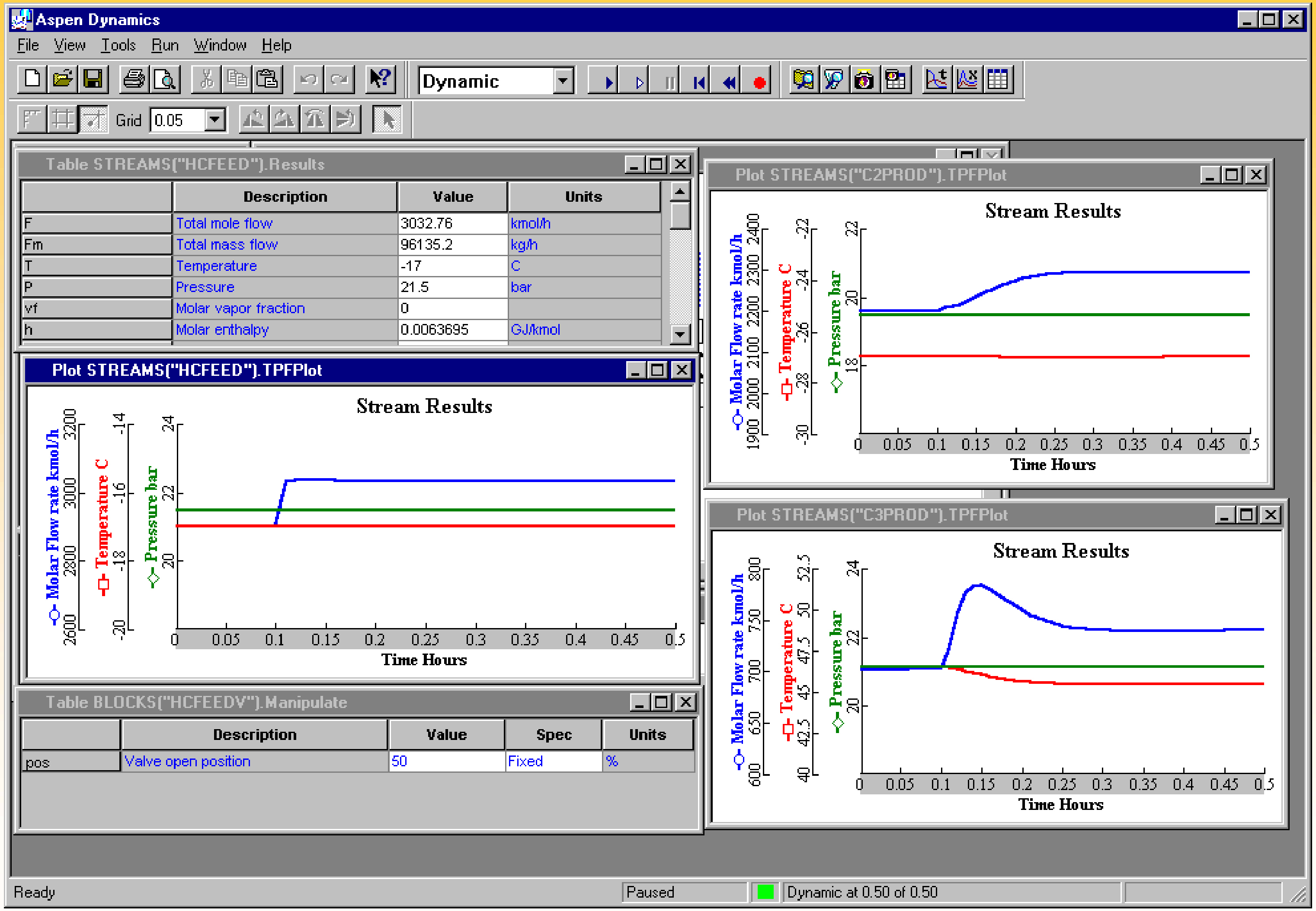
Can you reproduce the following plots for the predefined product and feed streams?

What is the effect of increasing the hydrocarbon feed flow to the deethanizer?

What happens to the C3PROD stream temperature ?

How can the C3PROD stream temperature be maintained?

Workshop: Pressure Driven Simulation *(10)*



Pressure Driven Simulation

- Review

Reach Your
True
Potential

Process Control

Objective:

Learn about the Aspen Dynamics process control models and become familiar with the PID controller

Process Control

- Auto-generated PID Controllers
  - Pressure
  - Level
  - Temperature
- Modify Control Scheme with GUI
- Import Existing Control Scheme
  - Select blocks to import
- Comprehensive Control Model Library

Process Control Models

Model	Description
Comparator	Calculates the difference between two input signals
Dead_time	Delays a signal by a specified time
IAE	Calculates the integral of the absolute value of the error between a process variable and its desired value
ISE	Calculates the integral of the squared error between a process variable and its desired value
Lag_1	Models a first order lag between the input and output
Lead_lag	Models a lead-lag element
Multiply	Calculates the product of two input signals
PID	A three mode proportional integral derivative controller
PRBS	Generates a pseudo-random binary signal
Ratio	Calculates the ratio of two input signals
Scale	Scales an input signal
Sum	Calculates the sum of two input signals
Valve_dyn	Models the dynamics of a valve actuator

Auto-Generated Controllers

Controller added	**When**	**Measured variable**	**Manipulated variable**
Pressure	Vapor holdup is modeled	Pressure in vessel	Vapor outlet flow rate
Level	Liquid holdup is modeled	Liquid level	Liquid outlet flow rate
Temperature	CSTR block	Temperature	Duty

Auto-Generated Controllers

- MAXIMUM CONTROL ACTION: 2 * BIAS
- SET POINT: steady state value of measured variable
- BIAS: steady state value of manipulated variable

Auto-Generated Pressure Controller

- Pressure Controller where Vapor Holdup is Modeled
- Proportional with Integral Control
  - GAIN = 100%/%
  - INTEGRAL TIME = 12 minutes

Auto-Generated Level Controller

- Level Controller where Liquid Holdup is Modeled
- Proportional only control
  - GAIN: 10 %/%

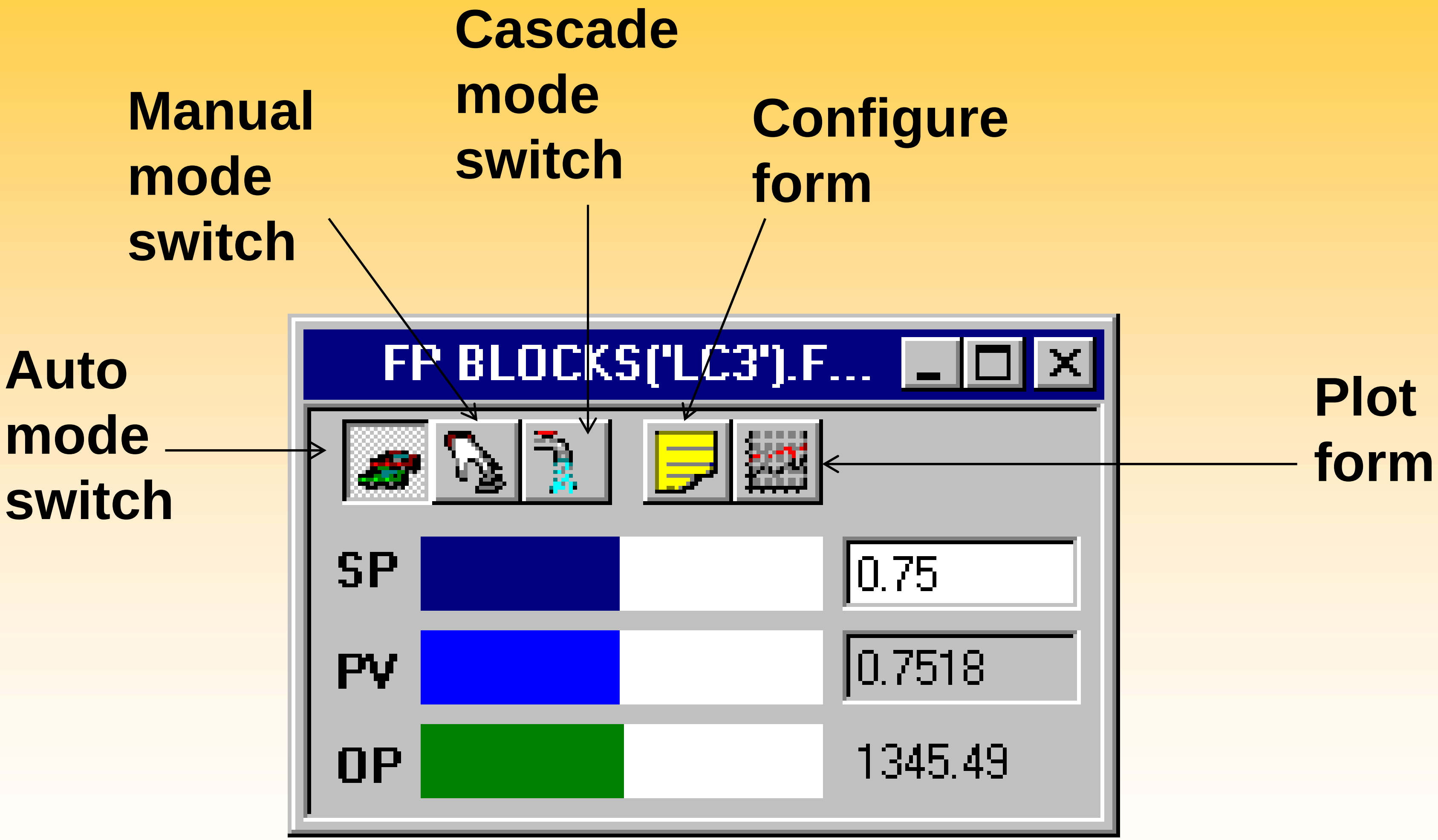
Auto-Generated Temperature Controller

- Temperature Control for RCSTR
  - Constant duty heat transfer option
- Proportional with Integral Control
  - GAIN: 100%/%
  - INTEGRAL TIME: 12 minutes

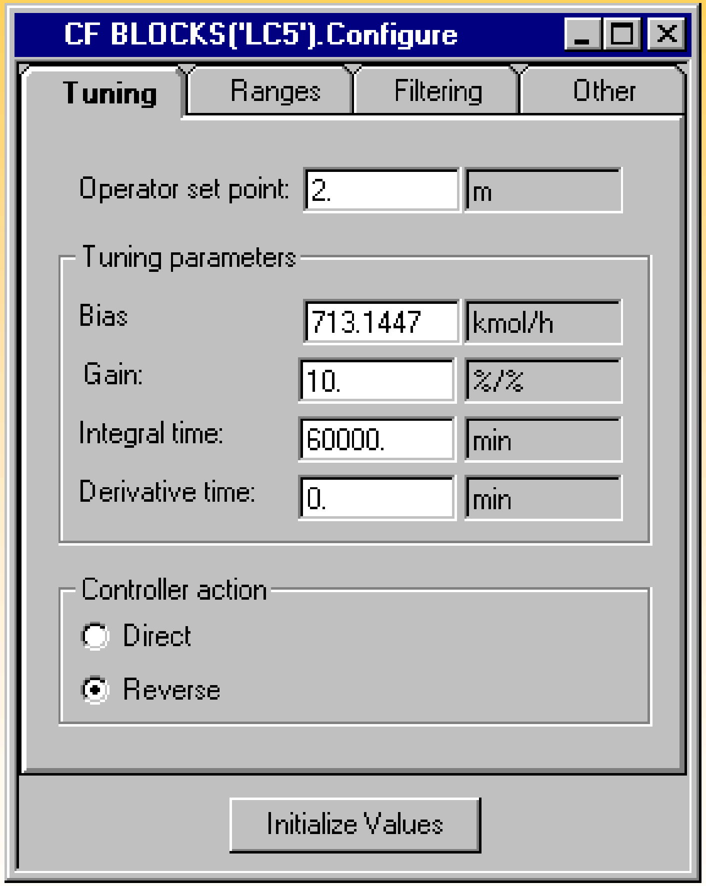
PID Control Block - Default Forms

- AllVariables
- Configure
- Faceplate
  - Set point
  - Process variable
  - Controller output
- Plot
  - Set point
  - Process variable
  - Controller output
- Results

PID Controller FacePlate



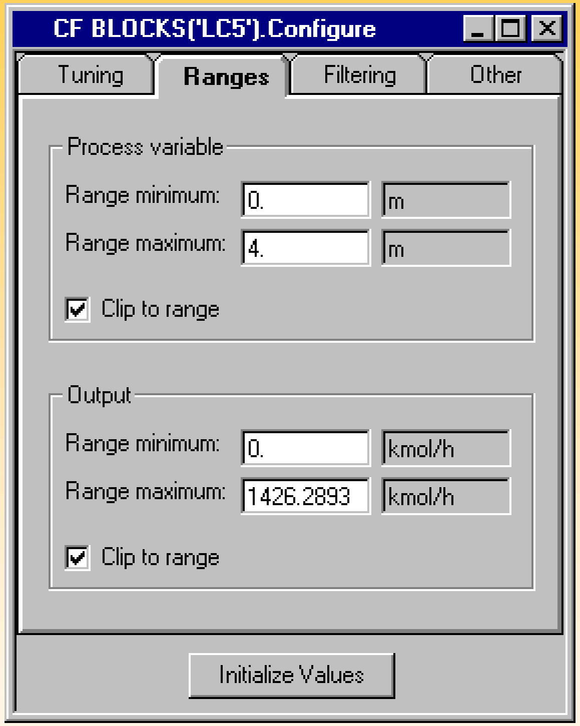
PID Block Configure Form -Tuning



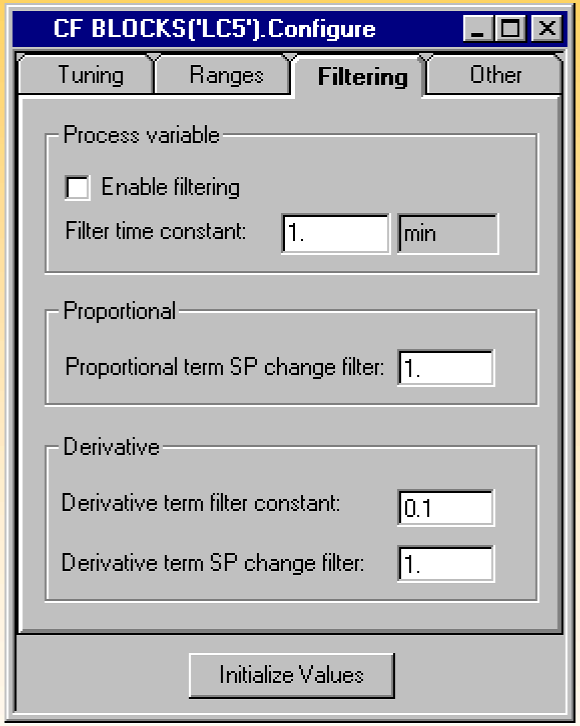
PID Controller Action

When the action is	And the measured variable	Then the manipulated variable
Direct	Increases	Increased
Direct	Decreases	Decreased
Reverse	Increases	Decreased
Reverse	Decreases	Increased

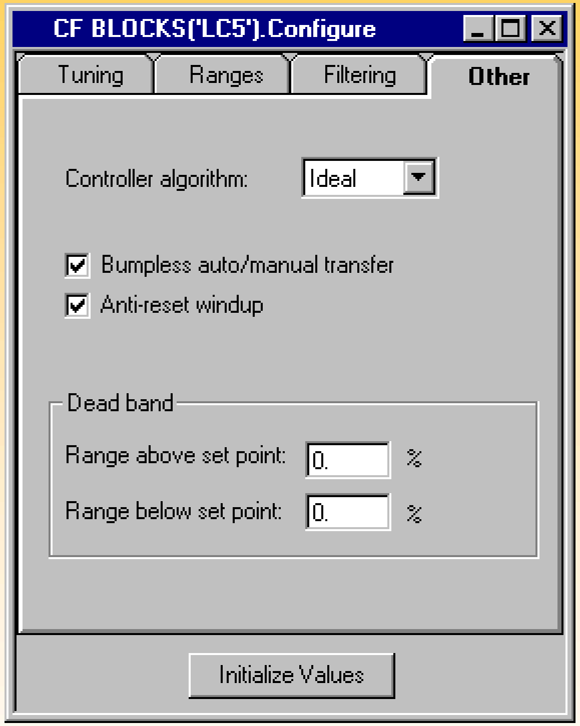
PID Block Configure Form - Ranges



PID Block Configure Form- Filtering



PID Block Configure Form - Other



PID Configure Parameters

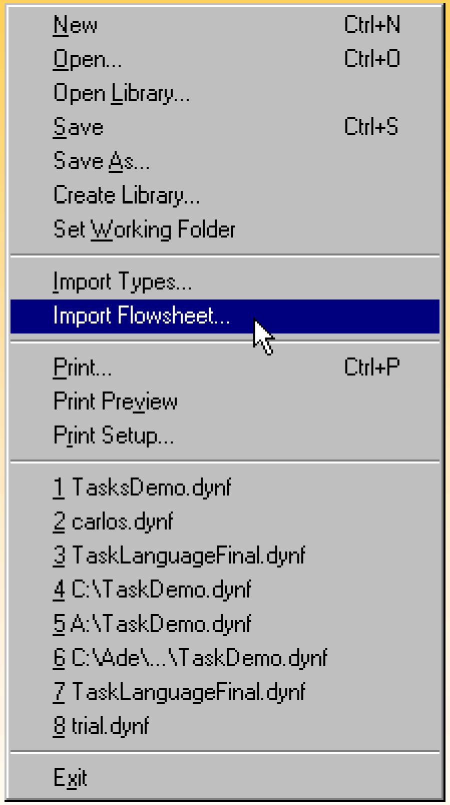
Parameter	Description	Units	Valid values	Default Value
Algorithm	Controller algorithm	–	IdealParallelSeries	Ideal
SPo	Operator set point	–	-1E9 -> 1E9	50
Action	Controller action	–	DirectReverse	Direct
Bias	Bias	–	-1E9 -> 1E9	0
Gain	Controller proportional gain	–	-1E9 -> 1E9	1
IntegralTime	Integral time	min	1E-3 -> 1E6	20
DerivTime	Derivative time	min	0 -> 1E6	0
PVmin	PV range minimum	–	-1E9 -> 1E9	0
PVmax	PV range maximum	–	-1E9 -> 1E9	100
OPmin	OP range minimum	–	-1E9 -> 1E9	0
Opmax	OP range maximum	–	-1E9 -> 1E9	100
OPClipping	Clip output between min and max	–	YesNo	Yes
PVFiltering	PV filtering	–	YesNo	No
PVFilter	PV filter time constant	min	1E-3 -> 1E6	1
ARWindup	Anti-reset windup	–	YesNo	Yes
Alpha	Derivative term filter constant	–	0.03 -> 1	0.1
Beta	Proportional term SP change filter	–	0. -> 1	1.0
Gamma	Derivative term SP change filter	–	0 £ x £ 1	1
Bumpless	Bumpless auto/manual transfer	–	YesNo	Yes
DBlo	Lower dead band as % of PV range	%	0 -> 100	0
DBhi	Upper dead band as % of PV range	%	0 -> 100	0

PID Controller Equation

- Ideal (classical)
  - Default
- Series (interacting or analog)
- Parallel (ideal parallel or non-interacting)

Importing a Flowsheet

Import Existing Control Scheme



Workshop (45 min): PID Controller Tuning

- Tune a single loop PID control loop
- Import an existing flowsheet (control scheme)

Workshop: PID Controller Tuning *(1)*

The objective of this workshop is to modify the deethanizer flowsheet control scheme by adding a PID temperature controller, with a sensor dead-time. You will then tune the PID controller.

1. Load your previously saved deethanizer flowsheet into Aspen Dynamics

2. Set the simulation to pause at 0.5 hour.

2. Run the problem in Dynamic mode for 0.5 hours to make sure that the column is operating in steady state (effectively)

3. Take a manual snapshot of the simulation at time 0.5 hours

4. Use the column's predefined TemperatureProfile results form to determine the stage 18 column temperature (26.8663 C)

Workshop: PID Controller Tuning *(2)*

5. From the ControlModels folder in the Dynamics library, drag and drop a dead-time block unto the flowsheet. The dead-time block models the temperature controller sensor dead time.

6. Specify a dead time of 18 seconds (0.3 minutes)

7. Use a ControlSignal from the Stream Types folder in the Dynamics library to connect the input of the dead-time block to stage 18 of the column. Why is stage 18 suitable for measuring/controlling the column temperature - how can this be verified?

8. From the ControlModels folder in the Dynamics library, drag and drop a PID model unto the flowsheet. The PID block models the temperature controller.

9. Connect the PV (InputSignal) of your new PID controller block to the output signal of the dead-time block using the ControlSignal stream type.

Workshop: PID Controller Tuning *(3)*

10. Using the ControlSignal stream type, connect the MV (OutputSignal) of the new controller to manipulate the reboiler heating medium flow (variable name T101.Fl_medReb)

11. Go to the Tools menu and bring up the Use dialogue box. Use the previously saved snapshot to initialize the new flowsheet by selecting the snapshot and then clicking the Copy button.

12. Open the PID controller configure form and use the Initialize Values button to initialize the controller (set point = 1.0, bias = 267085 Kg/h).

13. Specify an operator set-point of 27 C (the starting operator set point of 1.0 is taken directly from the default value of the dead-time block output).

14. As a starting estimate, for the tuning, specify a gain of 1 %/% and an integral time of 20 minutes

15. Make sure the controller action is set to be reverse

Workshop: PID Controller Tuning *(4)*

16. Change the run mode to Initialization and run the simulation

17. Tune the controller by following the steps outlined below

Tip: The steps described below will require the use of the **Ziegler-Nichols** (i.e. Z-N) controller tuning technique. Please read the online help on Z-N controller tuning before attempting the following.

a) Change the run mode to dynamic and run the simulation to “steady state” (effectively).

b) Pause the simulation at “steady state”.

c) Introduce a hydrocarbon feed flow disturbance by changing the flow from 92000 Kg/h to 97000 Kg/h (>5% change in feed flow rate) .

d) Continue the simulation run, whilst observing the controller response.

Workshop: PID Controller Tuning *(5)*

e) The controller response becomes oscillatory with the right **“ultimate gain”** value.

Note: For this system a gain of 50%/% is **near** the “ultimate gain”. Depending on the initial estimate of the gain, the controller response may be over-damped, under-damped or even unstable. In that situation you would need to pause the simulation, enter a new estimate of the gain, rewind the simulation and repeat steps a) to e) above.

For this system the **“ultimate period”** is about 0.01 hours. From the Z-N correlation, the required controller gain is about 22 .5 and the required integral time is about 50 minutes.

What is the value of the default controller gain and integral action ?

Is the controller direct or reverse acting ?

Are the controller output default minimum and maximum values reasonable ?

Workshop: PID Controller Tuning *(6/6)*

h) What mode should the controller operate in (P-only, PI, or PID)

What other variable(s) can be manipulated instead of the reboiler

heating medium flow?

What possible disturbances should be taken into account in

designing a control scheme to maintain the purity of the column product?

Workshop (30 min): Cascade Control *(Opt.)*

- Implement a cascade control scheme (optional workshop to be attempted only if there is time)

Workshop: Cascade Control *(1 of 2)*

1. Implement a two-level cascade control system for the temperature and bottoms product ethane composition of the de-ethanizer tower.

Tip: use the FacePlate cascade button

2. Include a sensor dead-time of 12 minutes for the composition controller.

3. Tune the controllers.

Is the composition controller direct or reverse acting?

What does the dead-time represent in this situation?

Workshop: Cascade Control *(2 of 2)*

In the cascade system, which controller is the primary or master and which the secondary or slave? Which controller should be tuned first?

What possible upsets (internal and external) to the distillation unit are we considering when a cascade system such as that described above is implemented?

Which variable(s) can be varied for an open loop test?

Process Control

- Review

Course Review

- Questions & Answers