ADVANCED PROCESS MODELING FORUM 2014

Advanced Process Modeling

Development & Directions

Costas Pantelides – Managing Director

Advanced Process Modeling

Getting the most out of past investment

Targeting future investment

Managing innovation

Managing risk in an uncertain world

Advanced Process Modeling

has the power to radically transform the Process Industries

…*all* sectors of the Process Industries

…*all* areas of activity: R&D, Engineering, Operations

fresh thinking, new ideas
powerful tools

Realise APM's potential
from R&D to real-time operations
in every sector

The gPROMS Product Family

PSE annual expenditure on product R&D >30% of revenue

gPROMS product family – 5 years ago

General mathematical modeling

gMODEL

gPROMS ModelBuilder
Advanced process modeling environment

AML: GLC, AML: FBCR, AML: FT, AML: BCR, AML: TBR

Advanced model libraries for reaction & separation

gPROMS

The gPROMS platform

Equation-oriented modeling & solution engine

Materials modeling

INFOCHEM Multiflash
OLI

Model deployment tools

Objects

Deploy models in common engineering software

gPROMS product family – 2014

General mathematical modeling

gMODEL

gPROMS ModelBuilder
Advanced process modeling environment

Sector-focused modeling tools

Chemicals & Petrochemicals

gPROCESS

gPROMS ProcessBuilder
Advanced process simulation

AML: GLC
AML: FBCR
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Advanced model libraries for reaction & separation

Life Sciences, Consumer, Food, Spec & Agrochem

gSOLIDS

Solids process optimization

gCRYSTAL

Crystallization process optimization

gCOAS

Oral absorption

Power & CCS

gCCS

CCS system modeling

Fuel Cells & Batteries

gFUELCELL

Fuel cell stack & system design

Oil & Gas

gFLARE

Flare networks & depressurization

Wastewater Treatment

gWATER

Wastewater systems optimization

gPROMS

The gPROMS platform

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Materials modeling

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Enterprise
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Deploy models in common engineering software

Chemicals & Petrochemicals

Provide

1. All the power of the gPROMS platform and first-principles modeling
   - *without the need to write models*
2. Custom modeling capability *where necessary*
   - maximize competitive advantage

→ **Ease-of-use** combined with **equation-oriented power**
   - solve full problem scope – rapidly

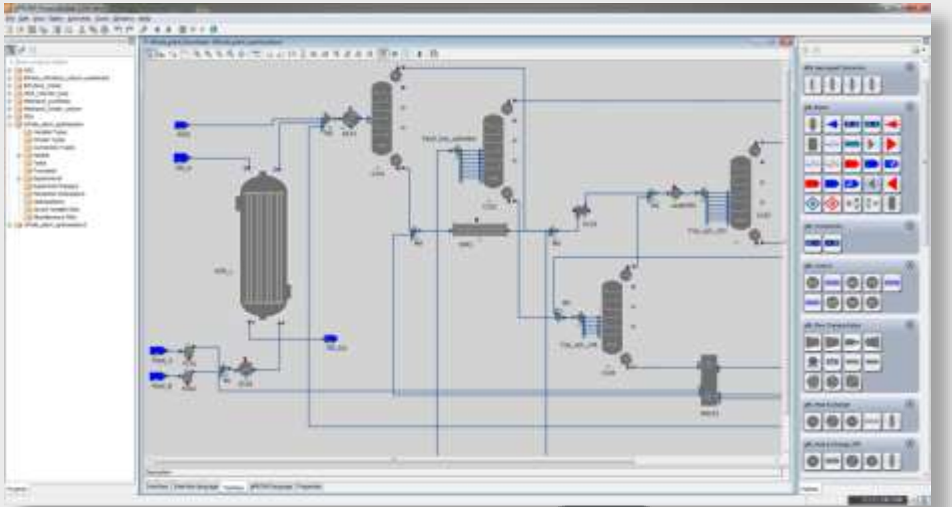
→ Full **rigorous optimization**
   - find optima directly – no need for trial & error simulation

→ gPROCESS

gPROMS ProcessBuilder

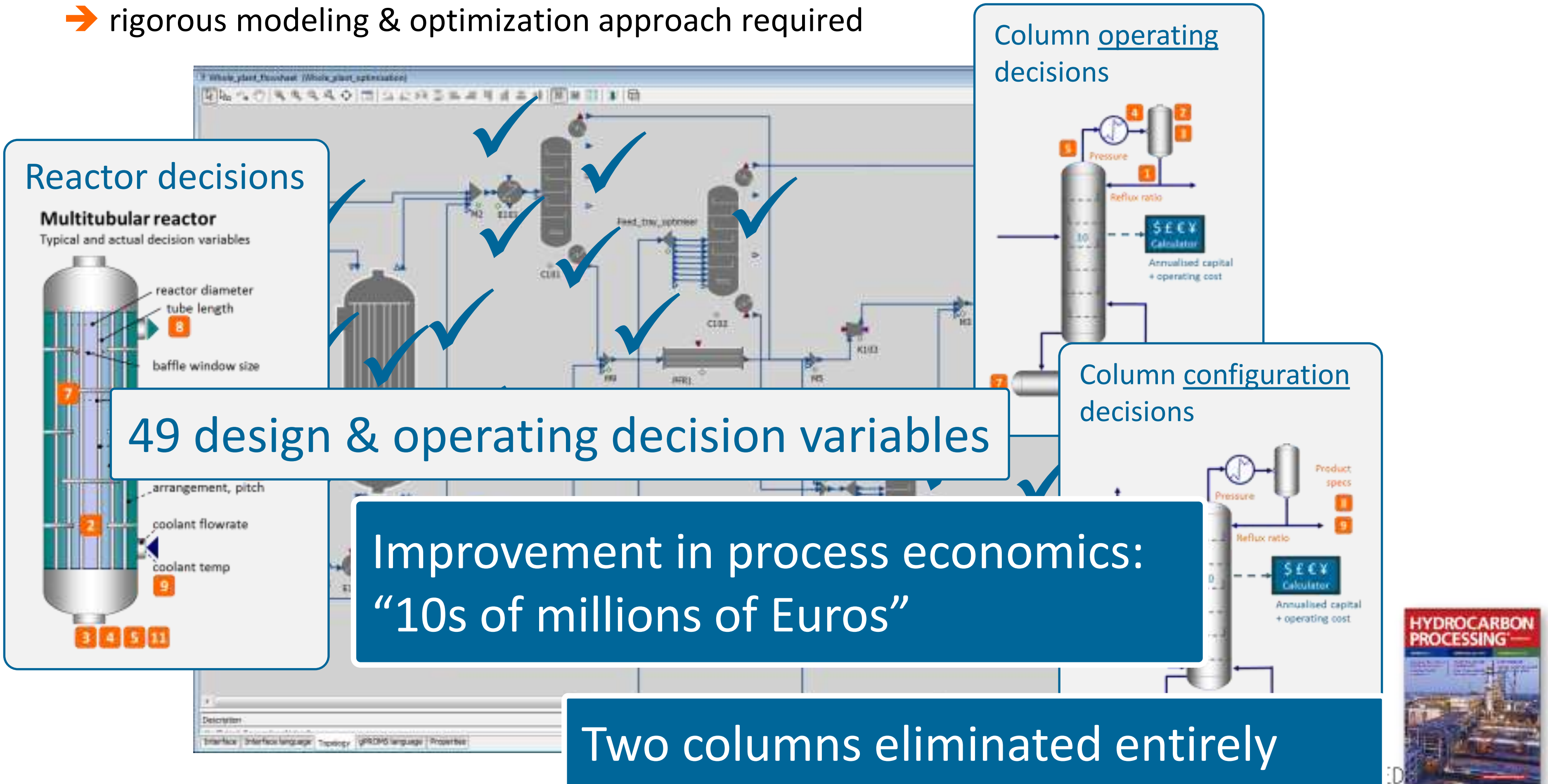
“Advanced Process Simulation”

A next-generation process modeling tool for chemicals & petrochemicals



Value creation: the vision

- New petrochemical process
- Design ‘already optimized’ using traditional simulation software
  - … but process economics poor
  - ➔ rigorous modeling & optimization approach required



49 design & operating decision variables

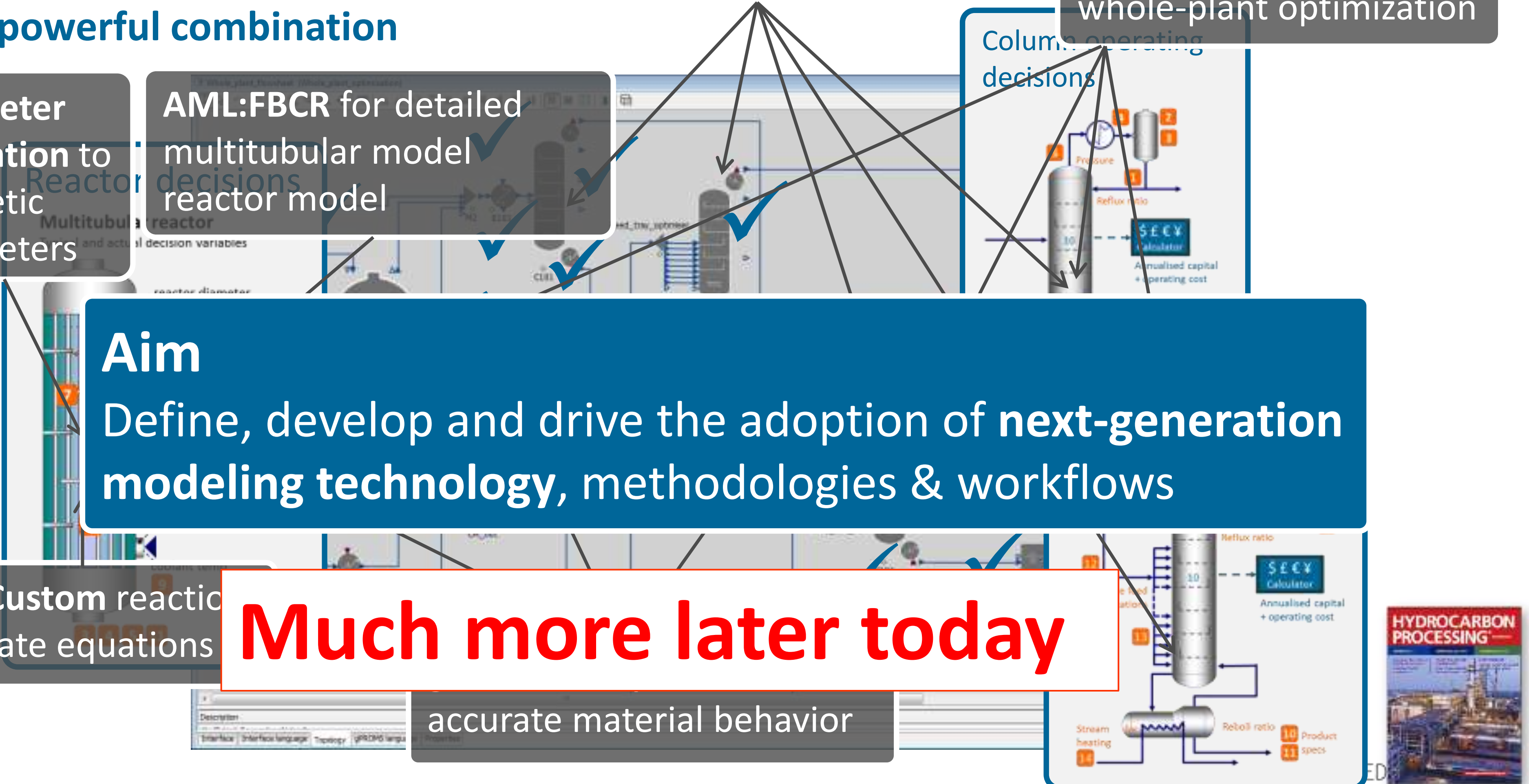
Improvement in process economics: “10s of millions of Euros”

Two columns eliminated entirely

REPSOL

Value creation: the tool – gPROMS ProcessBuilder

Detailed customizable models of key units, within a flowsheeting and optimization framework
➔ **a powerful combination**



Standard library models for separation section

Optimization (including mixed-integer) for whole-plant optimization

Parameter estimation to fit kinetic parameters

AML:FBCR for detailed multitubular model reactor model

Custom reactio… rate equations

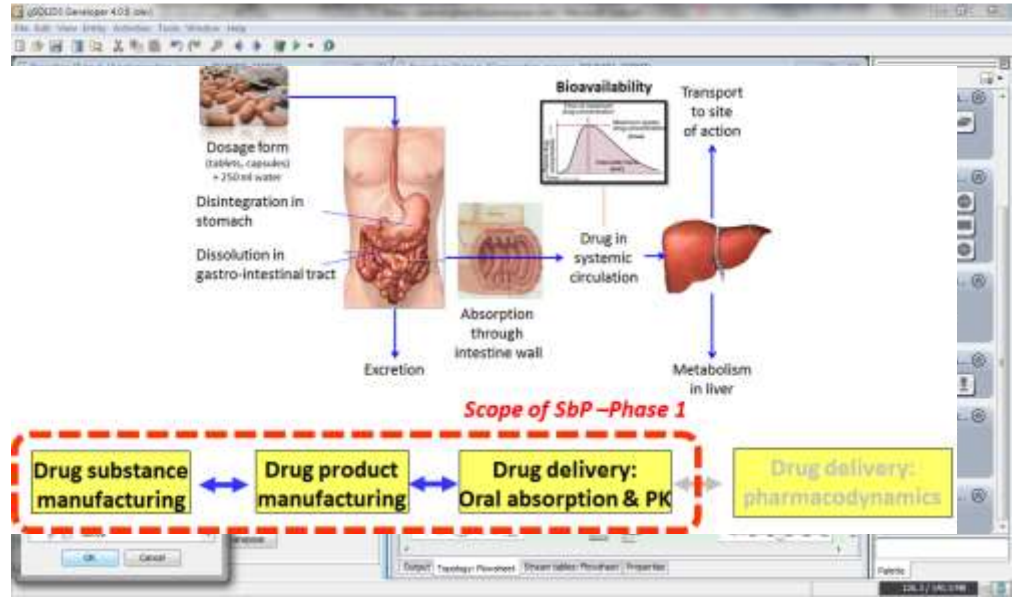
… accurate material behavior

Aim

Define, develop and drive the adoption of **next-generation modeling technology**, methodologies & workflows

Much more later today

Life Sciences, Consumer Goods, Specialty & Agrochemicals



Q4 '13: gCRYSTAL 4.0, gSOLIDS 3.1, gCOAS 1.0
Q3 '14: gCRYSTAL 4.1, gSOLIDS 4.0, gCOAS 1.1

Presentations today

P&G: Role of modeling in consumer goods innovation
Pfizer: Predictive oral absorption tool for formulators
PSE: progress made on Systems-based Pharmaceutics
Rutgers: Linking DEM to PBE models

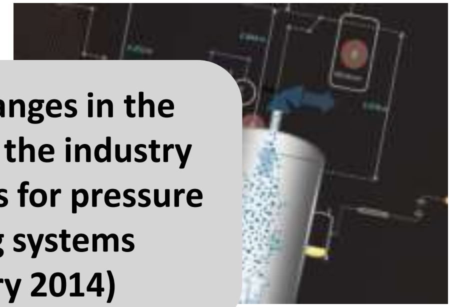
Presentations @ London APMF (April 2014)

Solvay, P&G, Nestlé, Pfizer (2), Rutgers, Vivo Drug Delivery
Available in customer area of PSE website

- Tools to characterise and optimize batch and continuous manufacture and delivery of particulate products
- **Advisory Board**: AstraZeneca, BASF, DuPont, Lilly, GSK, Nestlé, Pfizer, P&G, Purdue U, Sheffield U, Solvay, TU Delft
- **Systems-based Pharmaceutics**
  - A new vision for the pharmaceutical industry
  - Industrial Alliance established in October 2013
    - 2-year development programme under way

Oil & Gas

gFLARE has facilitated changes in the recently revised edition of the industry standard API 521 guidelines for pressure relief and depressuring systems (6th edition – 1 January 2014)



- **Main Focus: Safe process and flare system design for the upstream oil & gas industry**
- Large, highly skilled project delivery teams
- New projects
  - Supporting *Major Project* business units on large capital projects; working collaboratively with their engineering partners

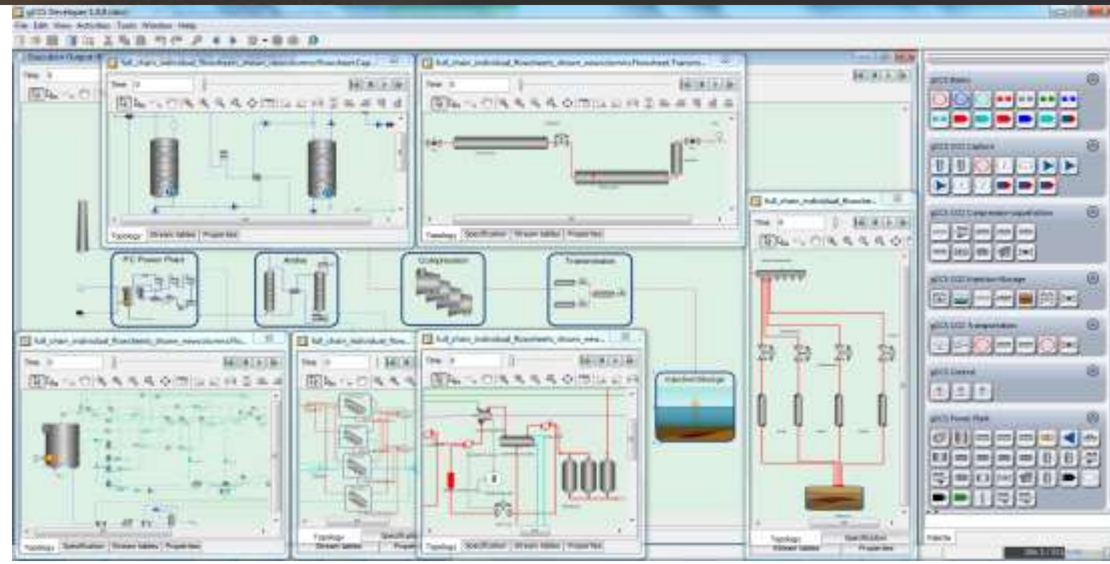
Example: Recently saved an operating company several hundred million dollars demonstrating that a facility could be made out of carbon-steel (rather than stainless steel).

- Existing infrastructure and operations
  - Supporting maintenance programmes and asset reviews; including how to screen and identify risks for detailed investigation
  - Operational decisions that can minimize start-up delays and reduce turnaround times

Best practice pressure relief, blowdown and flare system assessment

Seminar in Houston – September 17th

Power & CCS



- End-to-end modeling of CCS chains
  - and their individual sub-systems
- £3.6m product development project
  - co-funded by Energy Technologies Institute
  - PSE, E.On, EdF, Rolls-Royce, CO2DeepStore
  - original scope completed in June 2014
- Significant interest in related areas
  - power generation, gas treating, EOR, …

v1.0 to be released September 2014

Presentation tomorrow

Power & CCS

Carbon Capture Journal

News | Events | Magazine | Social Network | Videos

gCCS system modelling technology used for Shell Peterhead project

Aug 10 2014

Shell Peterhead CCS project will be the first commercial UK user of PSE's gCCS systems modelling environment for whole-chain CCS design and operation.

gCCS is the world's first process modelling environment for support of design and operating decisions across the full CCS chain, from power generation through CO2 capture, compression and transport to injection. It is specifically designed to allow developers across the chain to address issues of interaction and interoperability between different chain components.

The gCCS software will be used during the Front-End Engineering Design (FEED) study phase of Shell's Peterhead CCS demonstration project to provide insight into the transient behaviour of the amine-based capture unit, and its effect on operations when integrated within the full system. In particular it will help to demonstrate the flexibility of the capture process design within the wider CCS chain through simulation of normal and off-design operational scenarios, and thus help reduce technology risks in this first-of-a-kind CCS project.

Alfredo Ramos, PSE's head of Power & CCS and leader of the development, said, "this is precisely the type of large-scale CCS application that gCCS was developed to support. For the first UK commercial use, we are very pleased to see it being used on such an important development."

gCCS is the commercially-supported product resulting from the £3m Energy Technologies Institute (ETI) funded CCS Systems Modelling Tool-kit project. The project was established to support the future design, operation and roll-out of cost-effective CCS systems in the UK and involved E.ON, EDF, Rolls-Royce, CO2DeepStore, PSE and E4tech.

Process Systems Modelling

CARBON COUNTS

PSE

Imperial College London

The University Of Sheffield.

Demonstrating CO_2 capture in the UK cement, chemicals, iron and steel and oil refining sectors by 2025: A Techno-economic Study

Final report

for

DECC and BIS

30/04/14

Element Energy Limited
20 Station Road
Cambridge CB1 2JD
Tel: 01223 852 496

CCS FLEXIBILITY

amine-based CO2 capture unit dynamics for CCGT applications

Nicola Ceccarelli
Modeling & Optimization Engineer

ELSEVIER

Avail

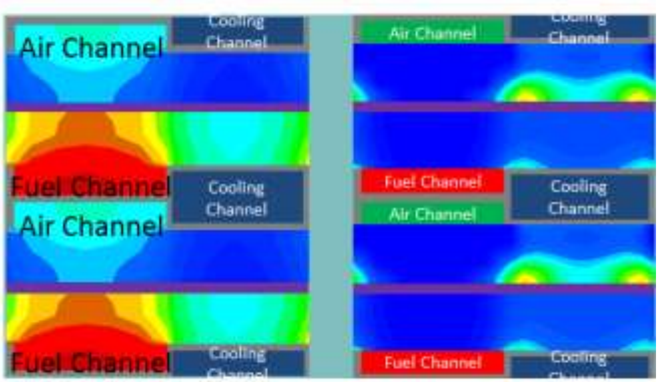
Flexibility of low- cap

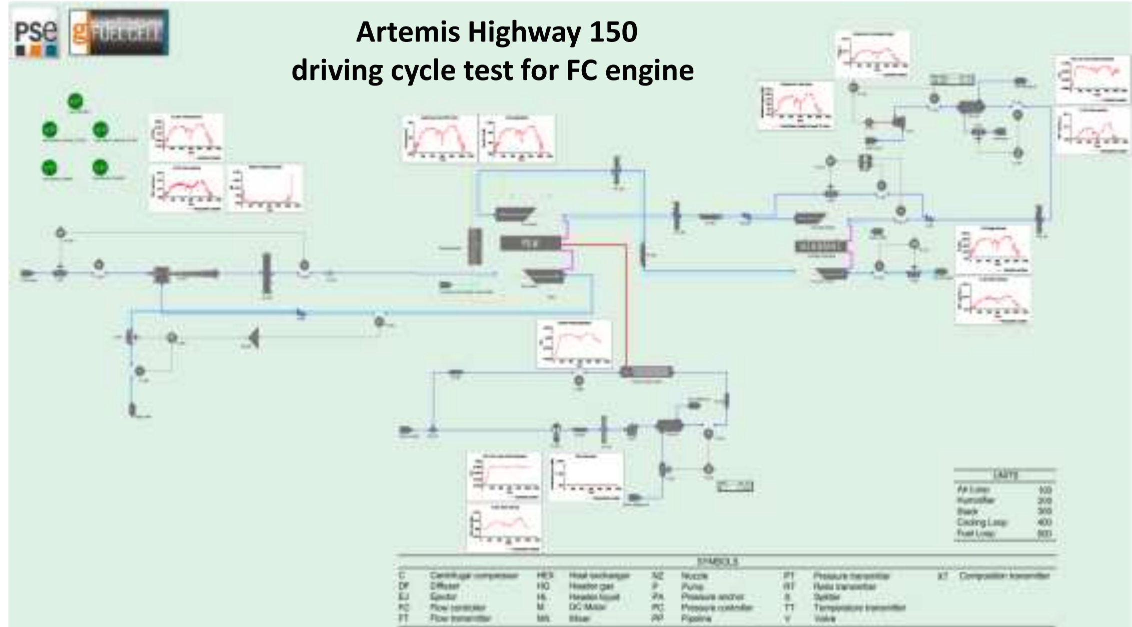
Nicola Ceccarelli, Monica van Leeuwen, Tanja Wolf, Peter van Leeuwen, Rick van der Vaart, Wilfried Maas[a], Alfredo Ramos[b]

[a]Shell Global Solutions, Carel van Bylandtlaan 23, 2596 HP The Hague, The Netherlands
[b]Process Systems Enterprise, 26-28 Hammersmith Gr, London W6 7HA, United Kingdom

Fuel Cells & Batteries

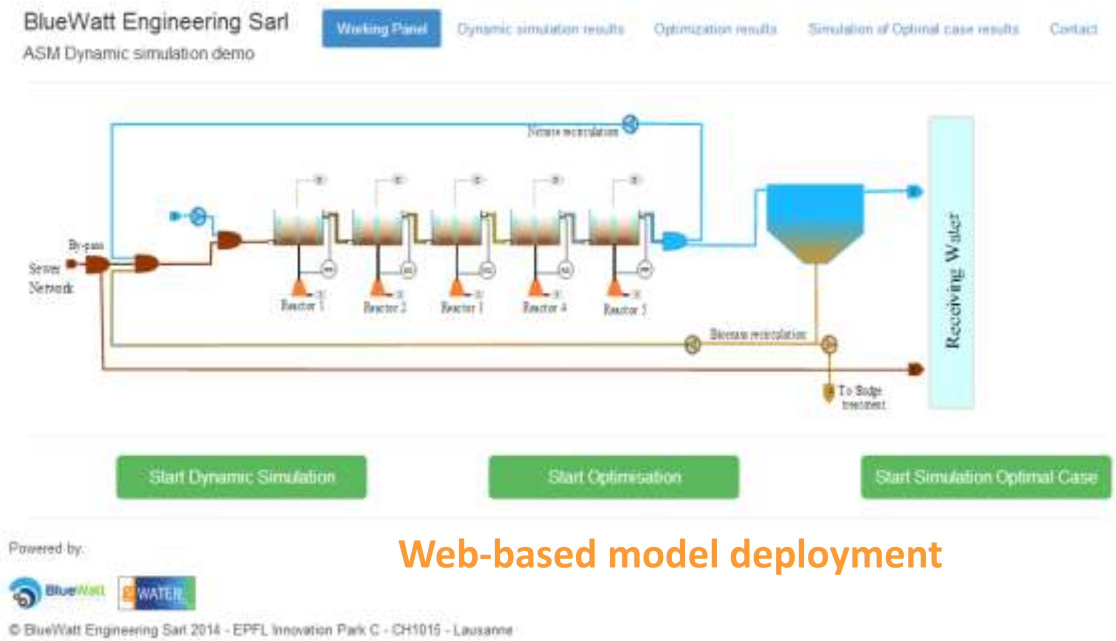
v1.0 available now





- Comprehensive modeling environment
  - fuel cell stack & fuel cell system
  - data-based model validation
  - model-based data interpretation
- Focus on productization
  - significantly increased PSE resource
- Underpins FC engine development by major automotive manufacturers
  - strong demand for very high levels of modeling detail & predictive accuracy
  - …coupled with usability by engineering teams

Wastewater treatment



Web-based model deployment

April 2014

PSE acquires significant equity stake in Bluewatt

- **spinout of École Polytechnique Fédérale de Lausanne (EPFL)**
- **gPROMS-based modeling of WWT**

Academic partnership agreement with EPFL

Presentation tomorrow

- Urban and industrial wastewater treatment system modeling & optimization
  - tightening regulations
  - excessive energy and chemicals consumption
- Ongoing development
  - high-fidelity models library
  - web deployment technology

gPROMS product family – 2014

General mathematical modeling

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Advanced process modeling environment

Sector-focused modeling tools

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Solids process optimization

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Power & CCS

CCS system modeling

Fuel Cells & Batteries

Fuel cell stack & system design

Oil & Gas

Flare networks & depressurization

Wastewater Treatment

Wastewater systems optimization

The gPROMS platform

Equation-oriented modeling & solution engine

Materials modeling

INFOCHEM *Multiflash*

Model deployment tools

Enterprise

Objects

Deploy models in common engineering software

The gPROMS Platform v4.0

Released June 6th, 2014

ADVANCED PROCESS MODELING FORUM 2014

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Fuel Cells & Batteries

gFUELCELL: Fuel cell stack & system design

Oil & Gas

gFLARE: Flare networks & depressurization

Wastewater Treatment

gWATER: Wastewater systems optimization

The gPROMS platform

Equation-oriented modeling & solution engine

Advanced modeling & solution engine
Simulation, Optimization,
Parameter Estimation, Experiment Design
~2m lines of code, ~25 computer scientists & mathematicians

Materials modeling

gSAFT, INFOCHEM Multiflash, OLI

Model deployment tools

Enterprise — Objects

Deploy models in common engineering software

The gPROMS Platform

PSE product development principles

- 100% <u>commonality of computer code</u> among gPROMS-family products
- Platform supports <u>product customization</u>
  - look-and-feel, content, workflow
  - project files
  - documentation…
- …and <u>product inter-operability</u>
- Key priorities (<u>not</u> in order of importance)
  - Modeling power
  - Robustness & efficiency of solution
  - Usability

gPROMS Platform

Overview of developments in v4.0

Usability

Tier I: "Model Developer"

Tier II: "Flowsheeting" User

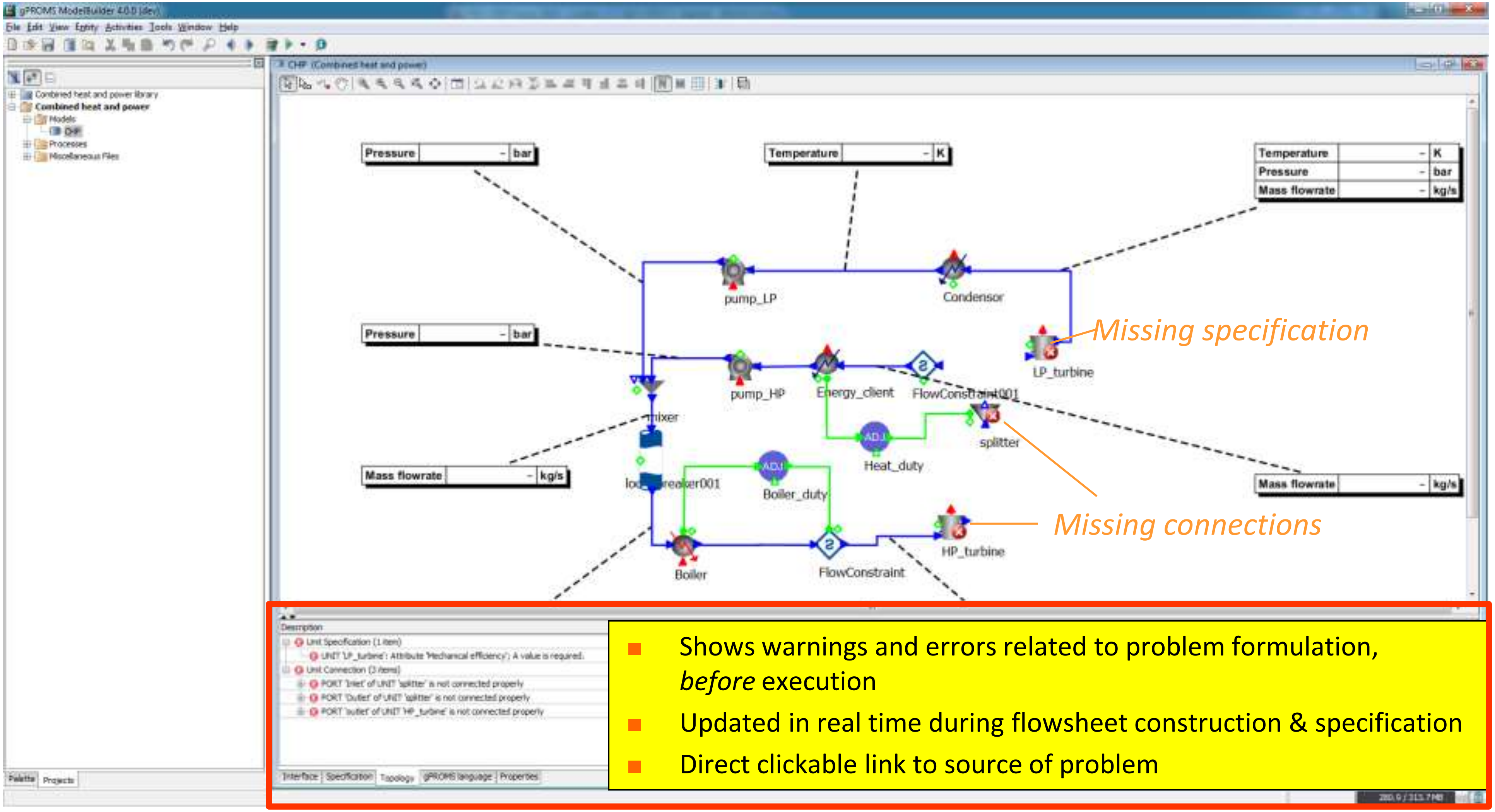
- Flowsheet diagnostics panel
- Model versioning
- Early warnings for wrong specifications
- Topology connection rules
- Units of measurement – input specification
- FOR loops in SET & TOPOLOGY sections
- Full interoperability between gPRODUCTS
- Conditional reports
- Faster model construction

Solution power

- Model Initialization Procedures – Unit Operations
- Model pruning
- New NLPSQP optimization solver

gPROMS Platform v4.0 – usability

Flowsheet diagnostics panel

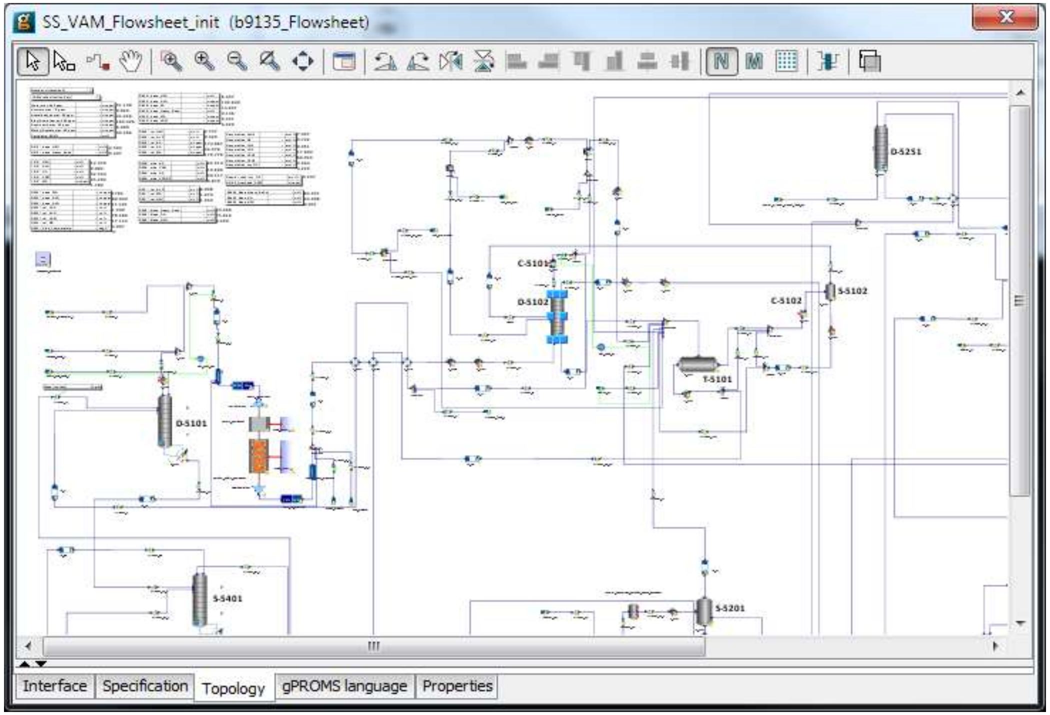


- Shows warnings and errors related to problem formulation, *before* execution
- Updated in real time during flowsheet construction & specification
- Direct clickable link to source of problem

Higher interactivity

- Much faster construction time for large models
- 25% smaller memory footprint

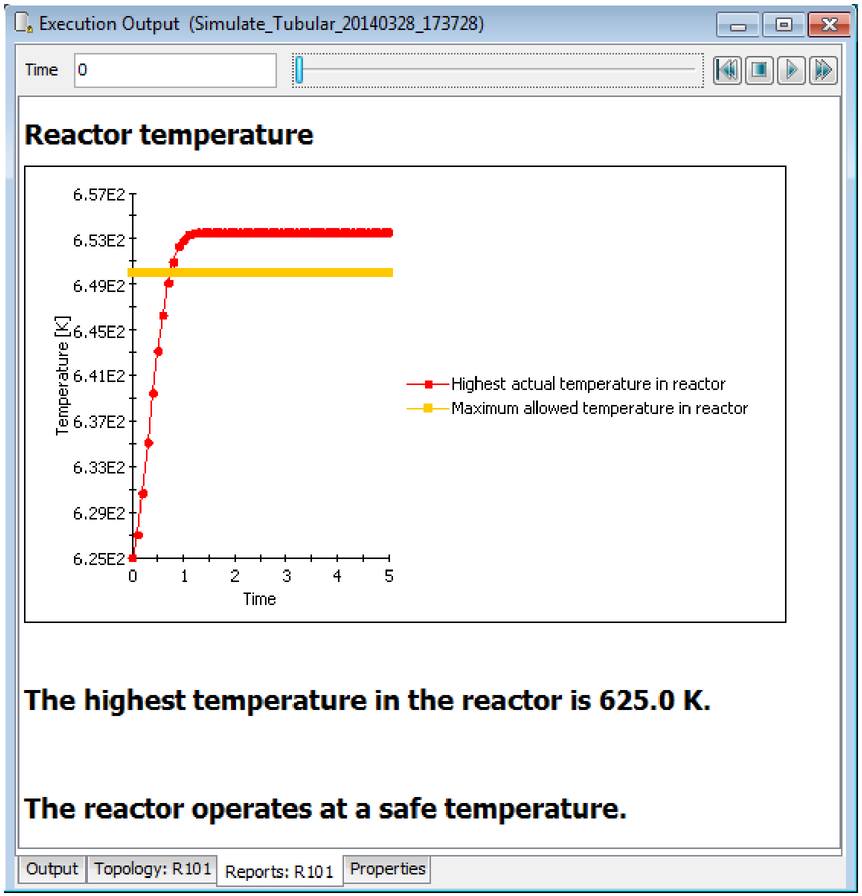
Reaction-Separation process flowsheet

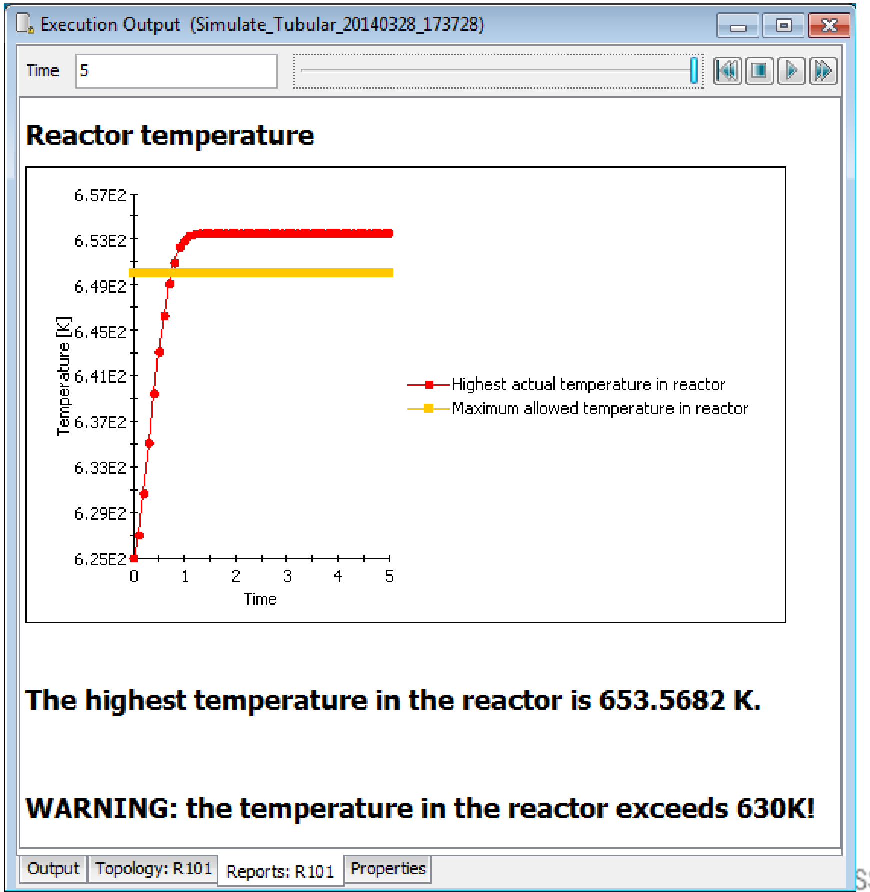


- 290,000 parameter elements
- 330ms live parameter resolution
  - Down from 680ms

Conditional model reports

- Make report elements dependent on model variables
  - e.g. display warning message if temperature exceeds safety threshold

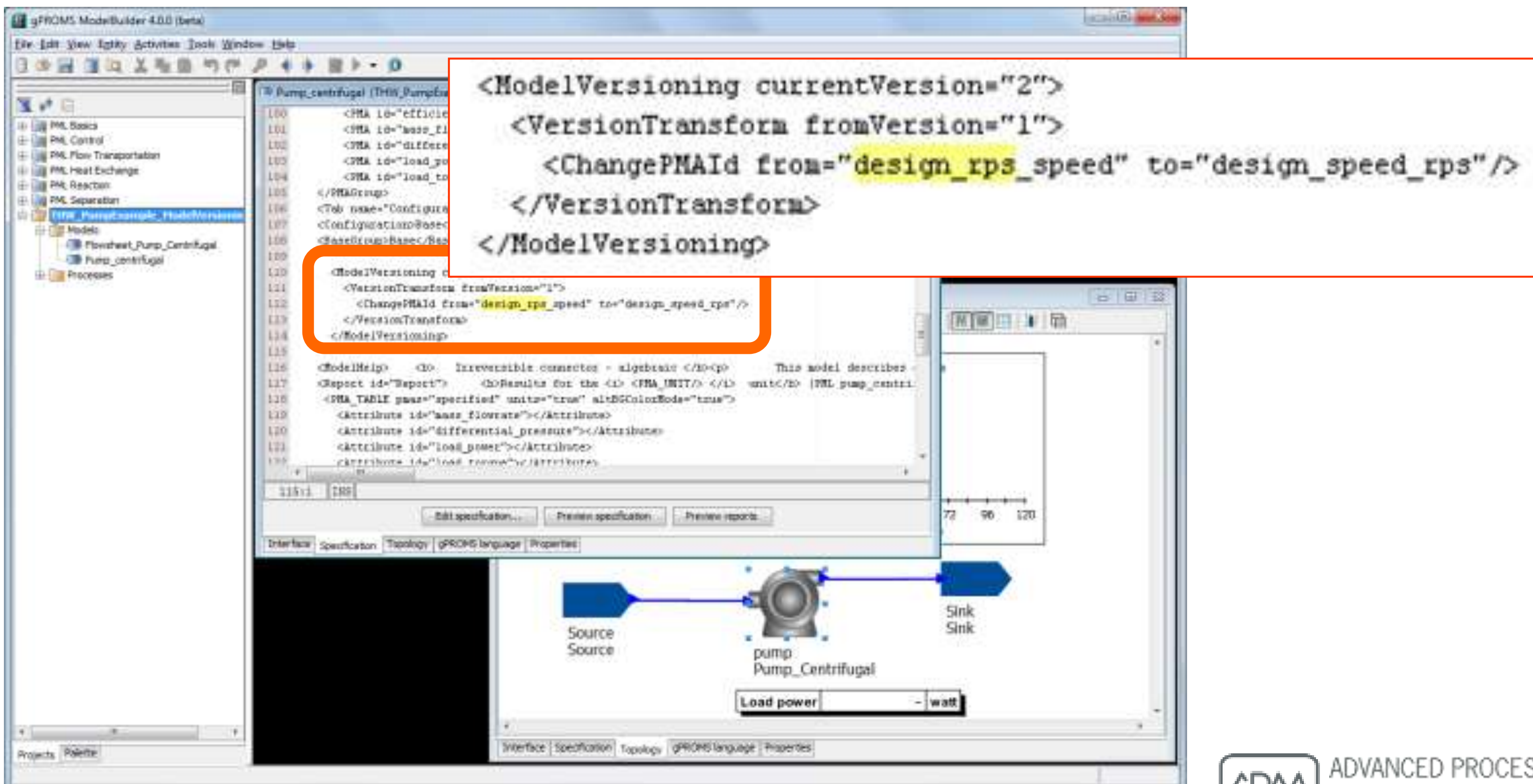




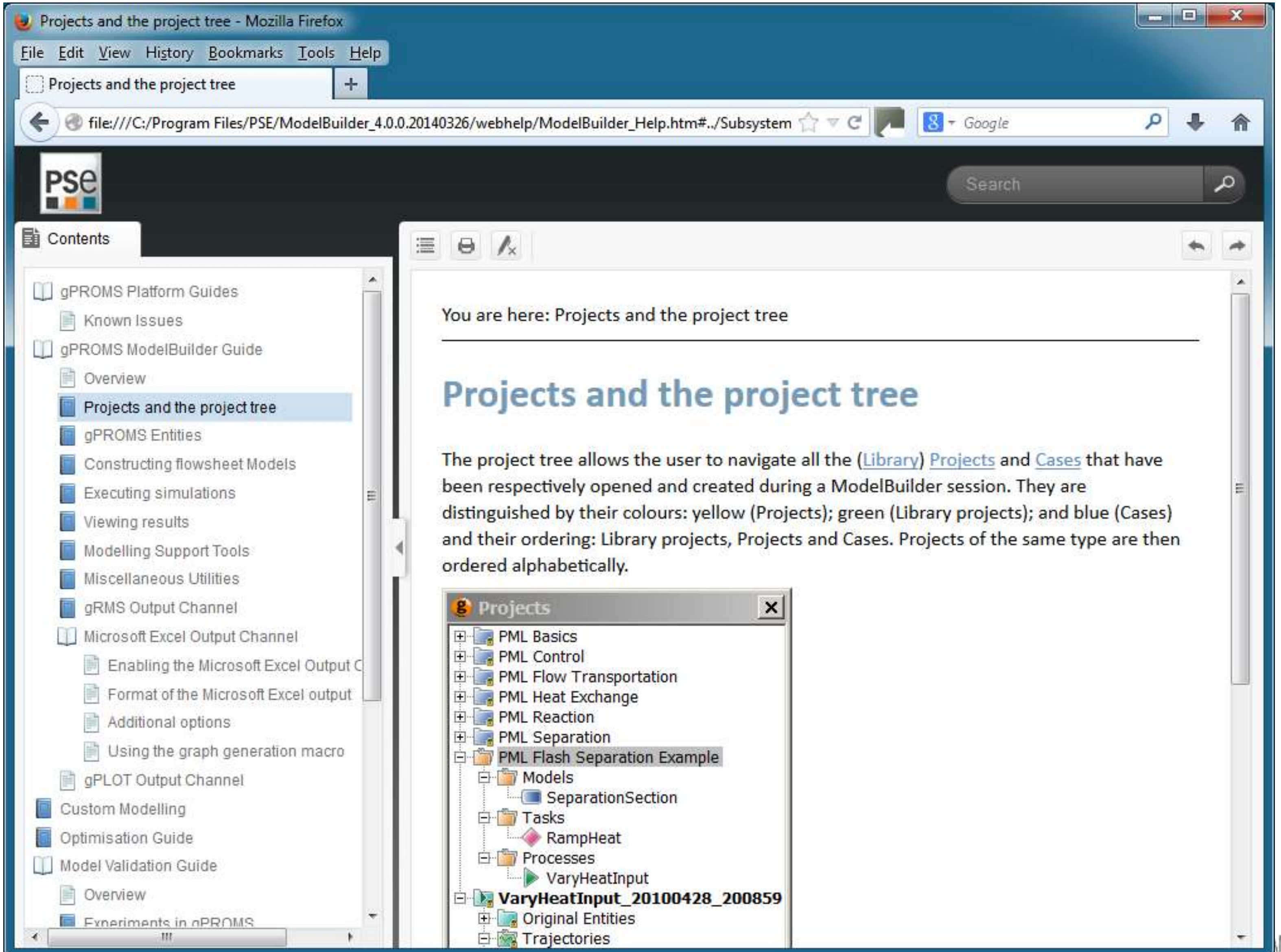
Model library versioning

Handling of Public Model Attributes

- Address issue in pre-4.0 platform
  - changing Public Model Attribute (PMA) names in MODEL entities in a new version of library…
  - …invalidated flowsheets built with older versions of the library



New documentation



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Solution power

- Model Initialization Procedures – Unit Operations
- Model pruning
- New NLPSQP optimization solver

Model Pruning – key concepts

- Automatically reduce model to minimum required to compute information requested by the user

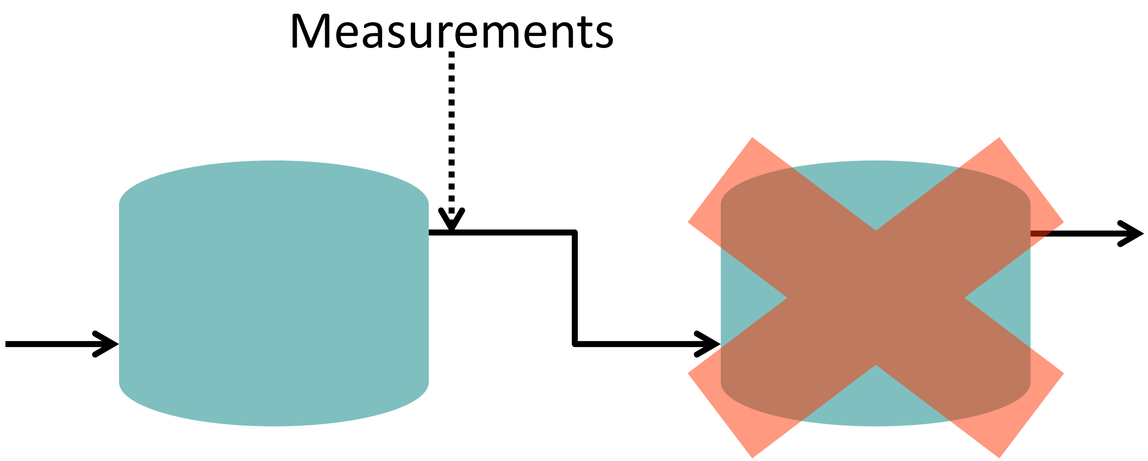
- Take account of
  - type of calculation
    - simulation, optimization, parameter estimation, experiment design
  - model specification

→ Pose smallest possible mathematical problem to numerical solver(s)

→ **Significantly improve efficiency, robustness, diagnostics**

Model Pruning – example #1

- Two reactors in series
  - Model typically used for dynamic simulation
  - Now use model to perform parameter estimation
  - Model Pruning
    - eliminate all variables/equations contributed by 2nd reactor
    - identify infeasibility of estimating *any* parameter from 2nd reactor
      - a badly-posed problem

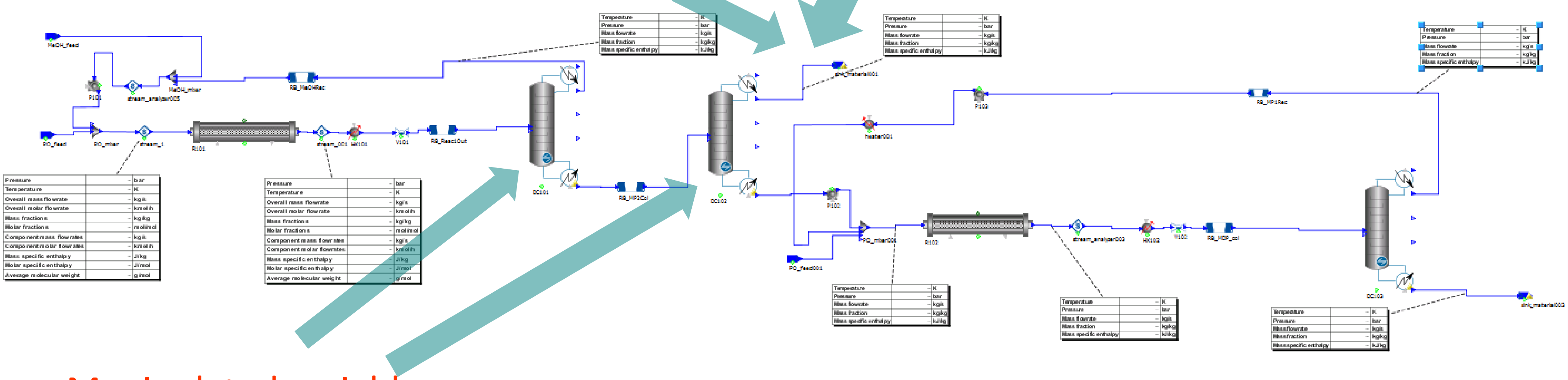


Model Pruning – example #2

PSE

Constraint:
Product purity

Objective: maximize product flow



Manipulated variables:
reboiler duties

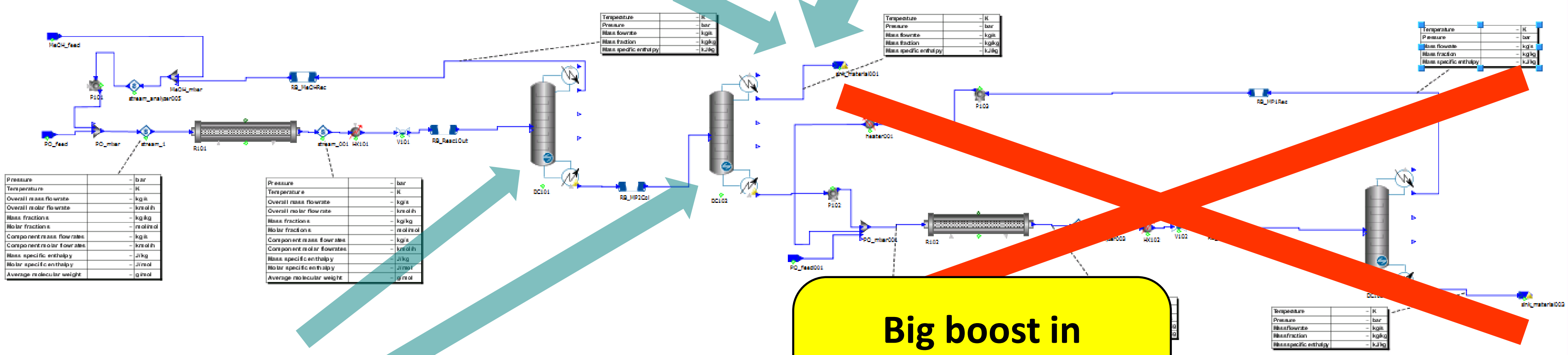
# equations	Original	+ Identity Elimination	+ Model Pruning
Simulation	48,711	25,932	23,757

Post-calculated variables automatically identified & "hidden" from equation solvers

Model Pruning – example #2

Constraint:
Product purity

Objective: maximize product flow



Manipulated variables:
reboiler duties

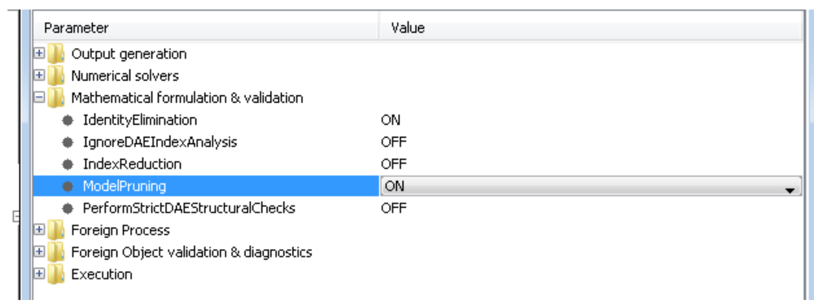
Big boost in solution speed and robustness

# equations	Original	+ Identity Elimination	+ Model Pruning
Simulation	48,711	25,932	23,757
Optimization			**8,389**

Post-calculated variables automatically identified & "hidden" from equation solvers

Model Pruning

- Benefits
  - large improvements in efficiency and robustness
  - better identification of badly-posed problems
- Enhance **model re-usability**
  - Reduce/eliminate need for manual "tailoring" of model to match specific calculation
- Side-effects: none
  - now the default option



gPROMS Platform

Overview of developments in v4.0

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Solution power

- Model Initialization Procedures – Unit Operations
- Model pruning
- New NLPSQP optimization solver

gPROMS Platform

Overview of developments in v4.0 + 4.1

Usability

Tier I: "Model Developer"

Tier II: "Flowsheeting" User

- Flowsheet diagnostics panel
- Model versioning
- Early warnings for wrong specifications
- Topology connection rules
- Units of measurement – input specification **+ results display**
- FOR loops in SET & TOPOLOGY sections
- Full interoperability between gPRODUCTS
- Conditional reports
- Faster model construction

Solution power

- Model Initialization Procedures – unit-level initialization **+ flowsheet-level initialization**
- Model pruning
- New NLPSQP optimization solver

v4.1 expected release: Q4/2014

Unit-Level Model Initialization Procedures (UL-MIPs)

gPROMS Platform v3.3+

- **MIP $\equiv$ sequence $f^{[k]}(x)=0$, $k=1,..,K$**

$$f^{[1]}(x)=0 \longrightarrow f^{[2]}(x)=0 \longrightarrow \ldots \longrightarrow f^{[k]}(x)=0 \longrightarrow f^{[k+1]}(x)=0 \longrightarrow \ldots \longrightarrow f^{[K]}(x)=0$$

System that is "easy" to solve (even from poor initial guesses)

Automatically constructed homotopy from $f^{[k]}(x)$ to $f^{[k+1]}(x)$

System of actual interest $F(x)=0$

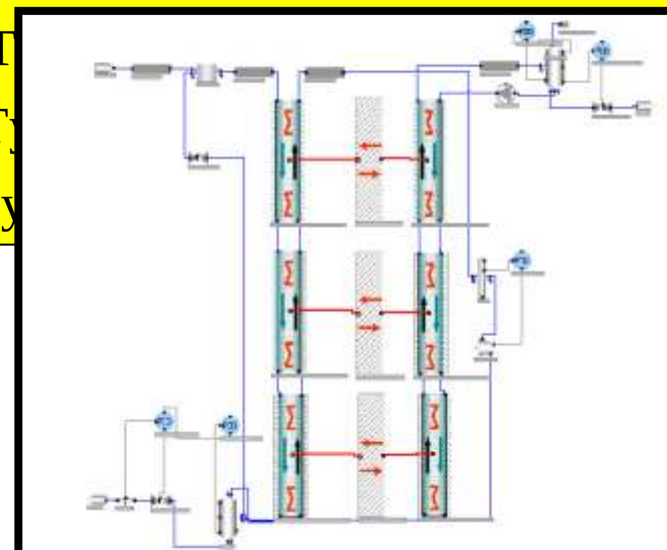
- Definition of MIPs is an **integral part of evolutionary model development** process
- gPROMS provides formal high-level mechanisms for
  - describing different types of functions $f^{[k]}(x)$ and their relations to the original model equations
  - ordering these functions in sequences
  - defining hierarchical MIPs
- MIPs become a **formal part of a re-usable model**
  - stored in model libraries
  - executed automatically as and when required

$$f^{[k]} = 0 \quad \rightarrow \quad f^{[k+1]} = 0$$

T b

Ty b

Ty 0



Model Initialization Procedures

Example: Distillation column model

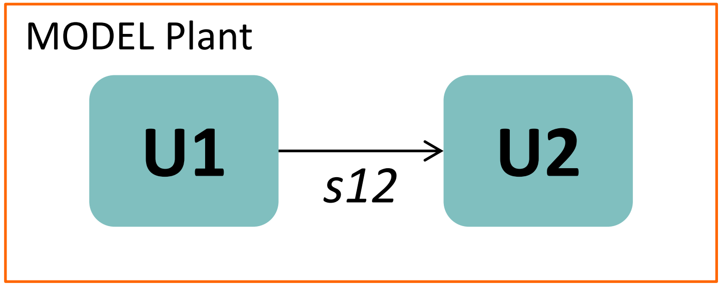
```
INITIALIZATION_PROCEDURE Init_Column DEFAULT
 USE
   q_init_model()  : DEFAULT;
   C_init_model() : DEFAULT;
   SP()                   : Init_Robust;
END

START
   M_eqs.component_balance   := M_eqs.init ;
   E_eqs.phase_equilibrium       := E_eqs.init ;
  S_eqs.summation                       := S_eqs.init ;
   H_eqs.energy_balance           := H_eqs.init ;
END
NEXT
   ADVANCE C_init_model();
END
NEXT
   JUMP_TO
      REVERT M_eqs.component_balance    ;
      REVERT E_eqs.phase_equilibrium        ;
      REVERT S_eqs.summation                      ;
      REVERT H_eqs.energy_balance            ;
   END
   COMPLETE q_init_model();
   COMPLETE C_init_model();
END
NEXT
   COMPLETE SP();
END
```

Flowsheet-level Model Initialization Procedures (FL-MIPs)

Why do we need them?

A simple flowsheet: two units in sequence, each with its own UL-MIP

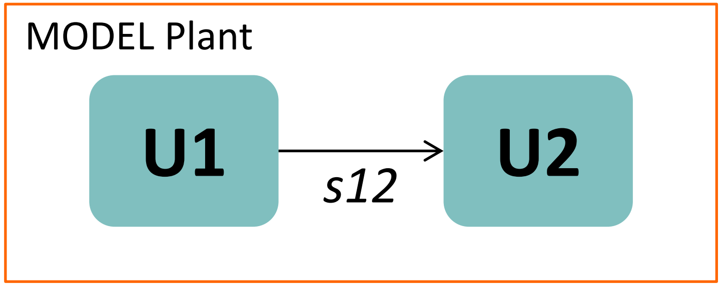


- MODEL Plant comprises variables & equations from U1 and U2
- (Obvious) MIP for MODEL Plant:
  1. Apply UL-MIP for U1
  2. Apply UL-MIP for U2
- **Issue #1**: User actually has to specify this within MODEL Plant
  - not convenient in drag-and-drop flowsheeting context
- **Issue #2**: While U1 is being initialized…
  - …variables in stream *s12* may take physically unrealistic values
  - …causing a failure in U2

Flowsheet-level Model Initialization Procedures (FL-MIPs)

How can we address these issues?

A simple flowsheet: two units in sequence, each with its own UL-MIP

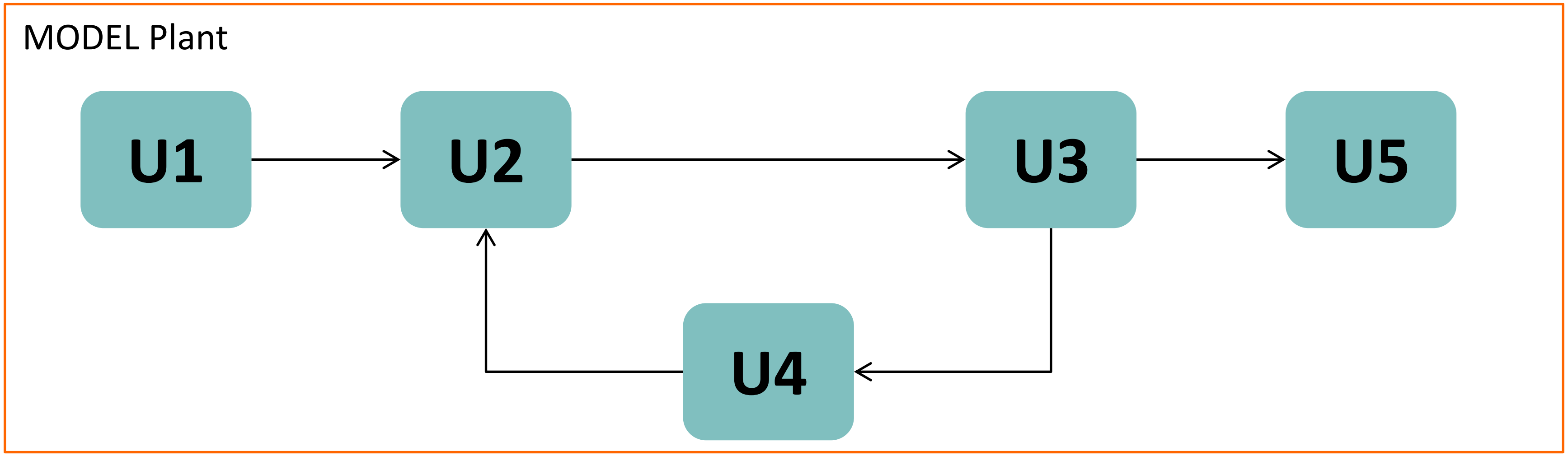


- MODEL Plant comprises variables & equations from U1 and U2
  - BUT do NOT form mathematical system for entire MODEL Plant during initialization
- Instead,
  1. Form mathematical system for U1
  2. Perform UL-MIP for U1 ➔ obtain converged values for s12; discard system U1
  3. Form mathematical system for U2
  4. Perform UL-MIP for U2; discard system U2
  5. Form mathematical system for MODEL Plant
     - already initialized!
  6. Solve MODEL plant

gPROMS Platform v4.1
forms, solves & destroys
multiple mathematical systems
on-the-fly during a single run
- all done automatically
& transparently to the user

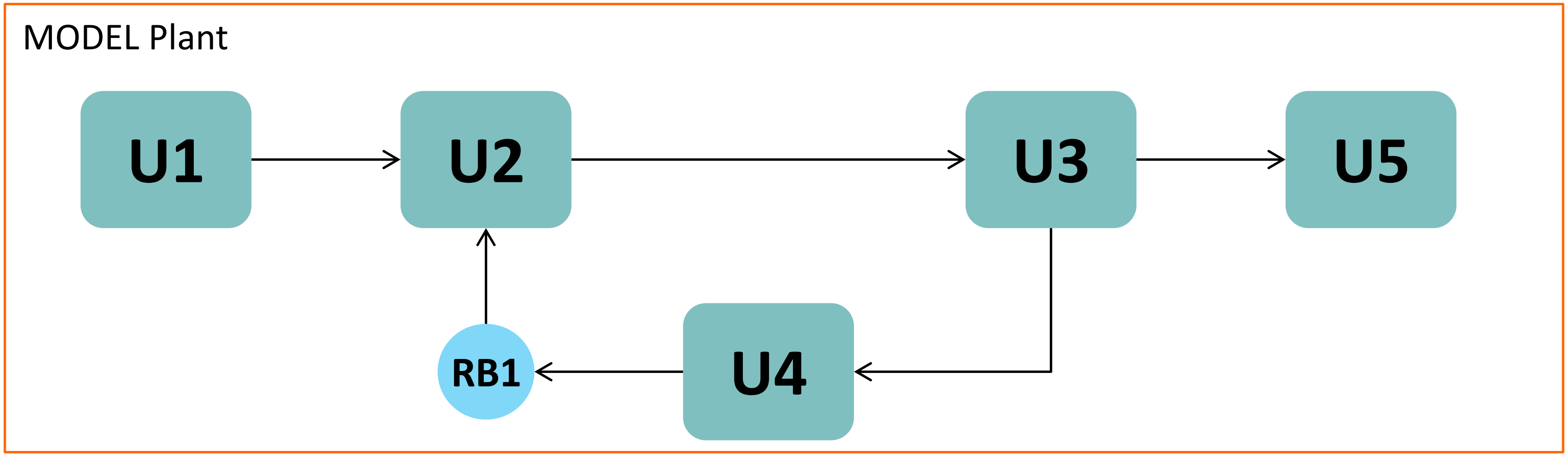
Flowsheet-level Model Initialization Procedures (FL-MIPs)

Handling recycles



Flowsheet-level Model Initialization Procedures (FL-MIPs)

Handling recycles

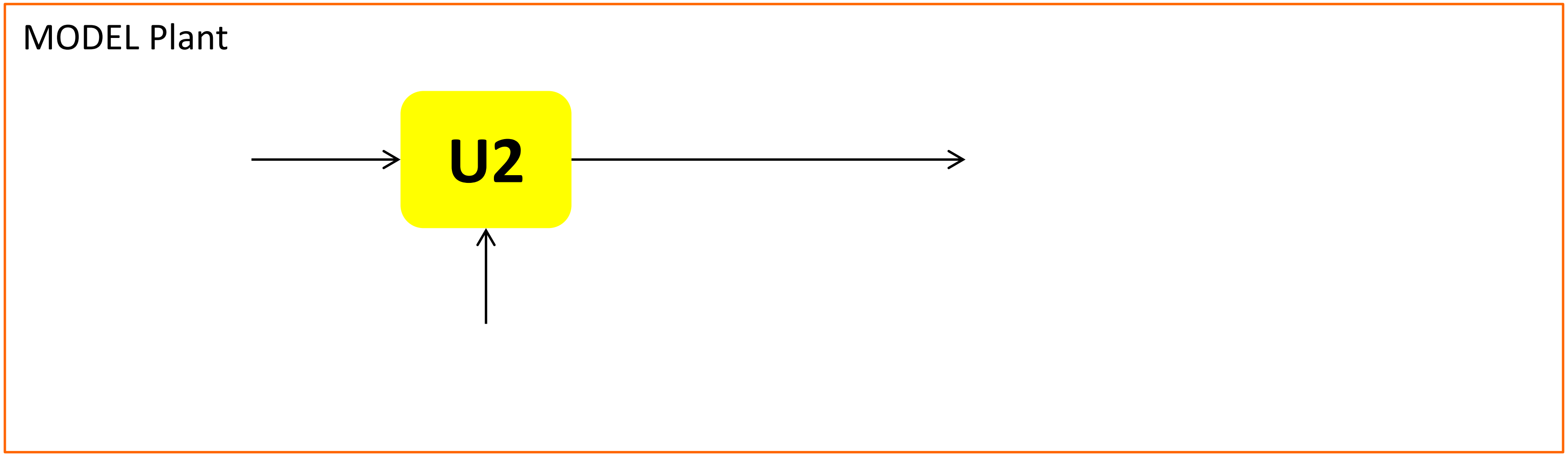


- MODEL Recycle Breaker
  - allows user to guess outlet stream
  - has its own special UL-MIP
- Recycle Breaker instances are
  - introduced by the user
  - automatically recognized by the gPROMS Platform
  - handled in a special manner during flowsheet initialization

- Initialization algorithm
  1. **Form system U1; perform UL-MIP for U1; discard system U1**

Flowsheet-level Model Initialization Procedures (FL-MIPs)

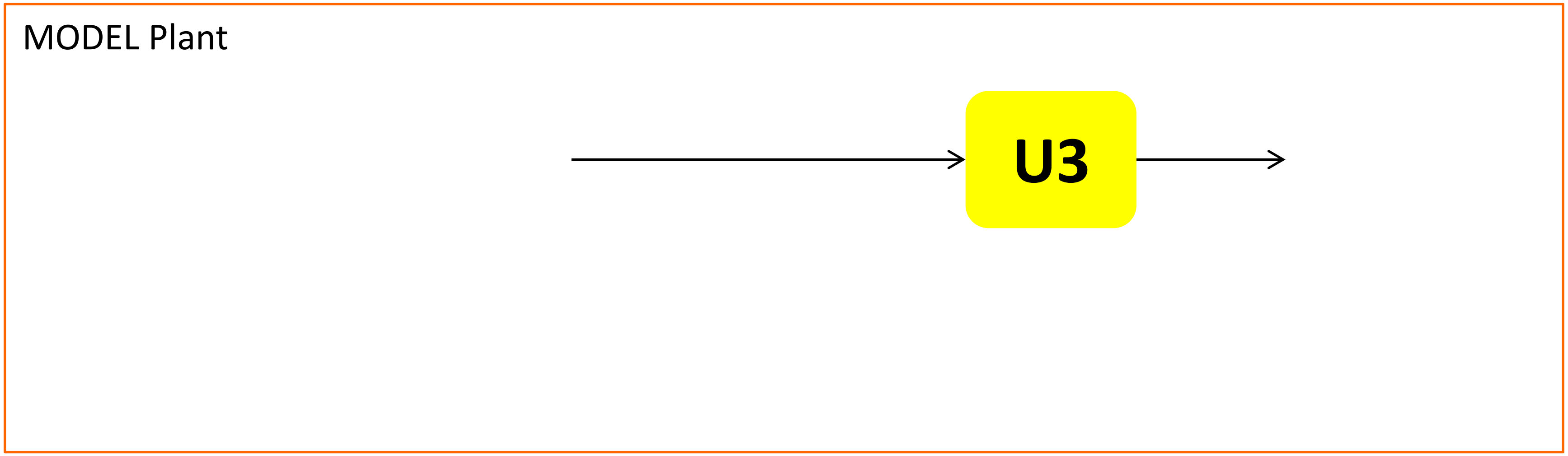
Handling recycles



- Initialization algorithm
  1. Form system U1; perform UL-MIP for U1; discard system U1
  2. **Form system U2; perform UL-MIP for U2; discard system U2**

Flowsheet-level Model Initialization Procedures (FL-MIPs)

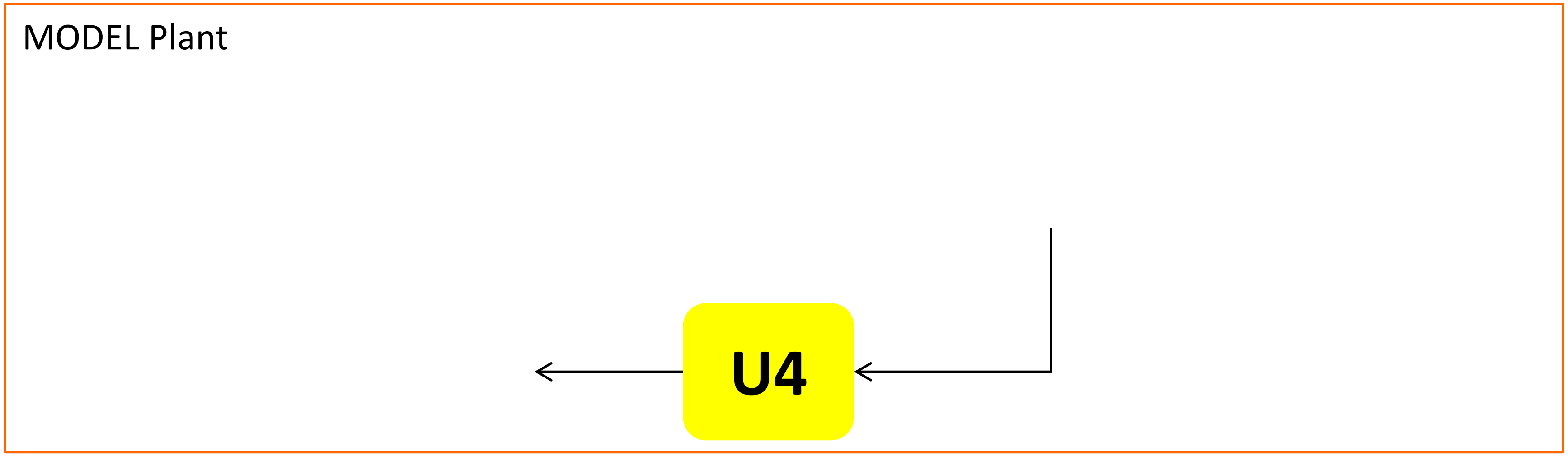
Handling recycles



- Initialization algorithm
  1. Form system U1; perform UL-MIP for U1; discard system U1
  2. Form system U2; perform UL-MIP for U2; discard system U2
  3. **Form system U3; perform UL-MIP for U3; discard system U3**

Flowsheet-level Model Initialization Procedures (FL-MIPs)

Handling recycles



- Initialization algorithm
  1. Form system U1; perform UL-MIP for U1; discard system U1
  2. Form system U2; perform UL-MIP for U2; discard system U2
  3. Form system U3; perform UL-MIP for U3; discard system U3
  4. **Form system U4; perform UL-MIP for U4; discard system U4**

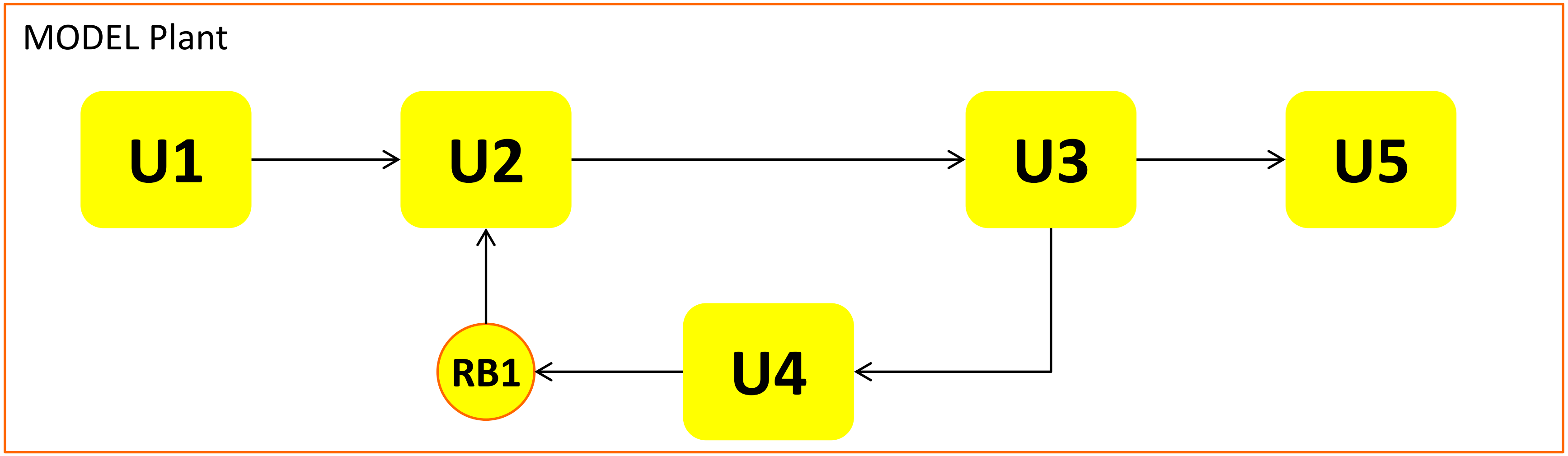
Flowsheet-level Model Initialization Procedures (FL-MIPs)

Handling recycles

- Initialization algorithm
  1. Form system U1; perform UL-MIP for U1; discard system U1
  2. Form system U2; perform UL-MIP for U2; discard system U2
  3. Form system U3; perform UL-MIP for U3; discard system U3
  4. Form system U4; perform UL-MIP for U4; discard system U4
  5. **Form system U5; perform UL-MIP for U5; discard system U5**

Flowsheet-level Model Initialization Procedures (FL-MIPs)

Handling recycles



- Initialization algorithm
  1. Form system U1; perform UL-MIP for U1; discard system U1
  2. Form system U2; perform UL-MIP for U2; discard system U2
  3. Form system U3; perform UL-MIP for U3; discard system U3
  4. Form system U4; perform UL-MIP for U4; discard system U4
  5. Form system U5; perform UL-MIP for U5; discard system U5
  6. **Form system for Model Plant including RB1;**
     perform special UL-MIP for RB1 to close recycle

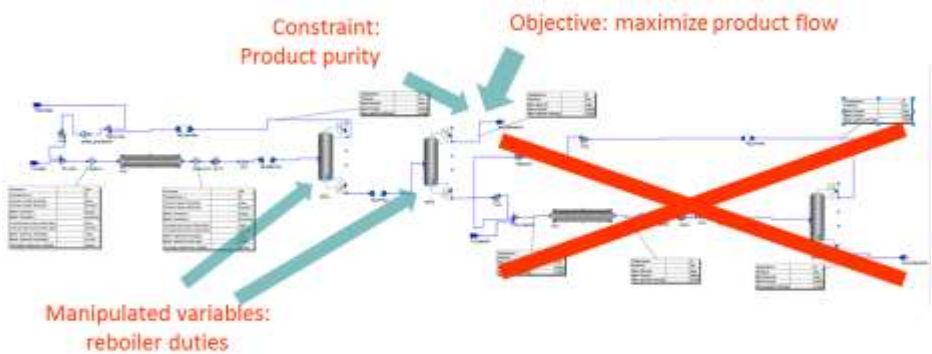
gPROMS Platform v4.1
handles all steps
automatically
& transparently to the user.

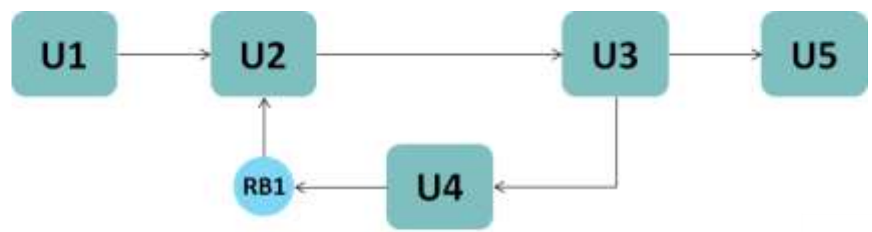
User can control how
multiple recycles
are to be handled
(default: all recycles
closed in parallel)

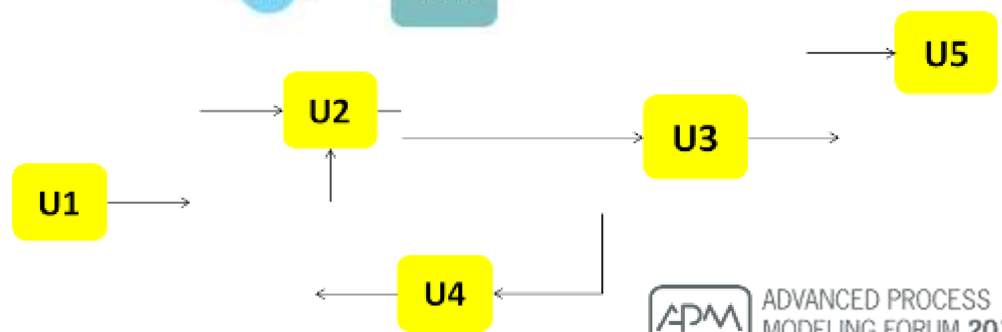
$$f^{[1]}(x)=0 \longrightarrow f^{[2]}(x)=0 \longrightarrow \ldots \longrightarrow f^{[k]}(x)=0 \longrightarrow f^{[k+1]}(x)=0 \longrightarrow \ldots \longrightarrow f^{[K]}(x)=0$$

Multipurpose Process Modeling Environments

A new architectural paradigm



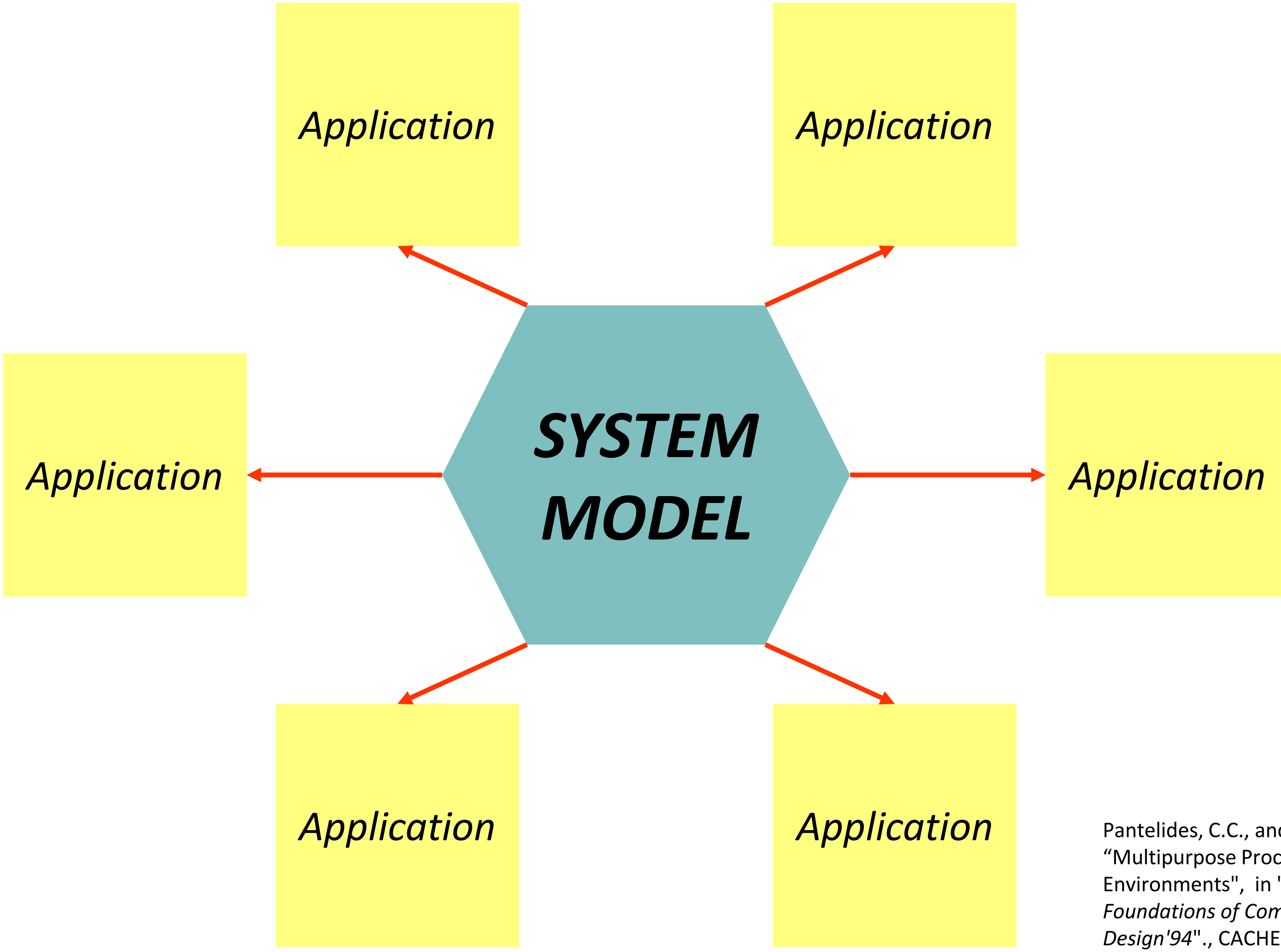




ADVANCED PROCESS MODELING FORUM 2014

Process Modeling Environments

The Original Vision (~1990s)



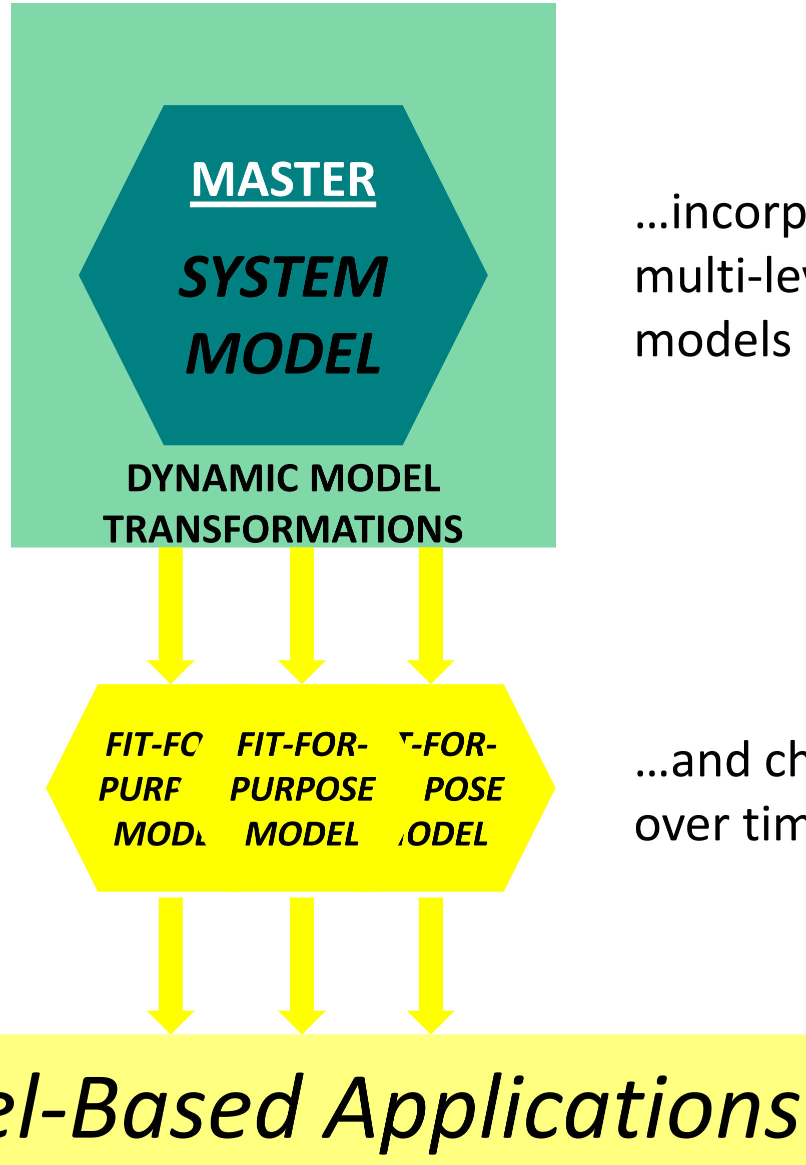
Pantelides, C.C., and Britt, H. "Multipurpose Process Modeling Environments", in "*Proc. Conf. on Foundations of Computer-Aided Process Design'94*"., CACHE Publications (1995), 128-141.

Process Modeling Environments & Model-Based Applications

A new relationship

Process Modeling Environment…

…incorporating multi-level component models



Model optimized for specific application …generated automatically from Master Model

…and changing dynamically over time

In conclusion…

PSE's commitment

Sector-focused modeling tools

General mathematical modeling

Model Builder

Advanced process modeling environment

Chemicals & Petrochemicals

Process Builder

Process flowsheeting

AML: GLC AML: FBCR AML: FT AML: BCR AML: TBR

Advanced model libraries for reaction & separation

Life Sciences, Consumer, Food, Spec & agrochem

gSOLIDS

Solids process optimization

gCRYSTAL

Crystallization process optimization

gCOAS

Oral absorption

Power & CCS

gCCS

CCS system modeling

Fuel Cells & Batteries

Fuel cell stack & system design

Oil & Gas

gFLARE

Flare networks & depressurization

Wastewater Treatment

gWATER

Wastewater systems optimization

gPROMS

The gPROMS platform

Equation-oriented modeling & solution engine

Materials modeling

gSAFT INFOCHEM Multiflash OLI

Model deployment tools

fresh thinking, new ideas, powerful tools

Pushing the boundaries of Model-based Engineering

APM ADVANCED PROCESS MODELING FORUM 2014

Roadmap 2014 – 2015

Key:
Black text – work not started Blue text – feature complete
Green text – work in progress

Version	v4.0.0	v4.1.0	v4.2.0	4.3.0+
Date	**June 2014**	**December 2014**	**June 2015**	**TBD**
Usability	[SW-1020] Units of Measurements - I [SW-0008] Unit Specification Enhancement	[SW-1020] Units of Measurements- II Stream table (display UoMs only) Trajectories (display UoMs only) Time Units support [SW-1022] PMA support throughout GUI - II (Results: plots and value-tables on topologies)	[SW-1020] Units of Measurements - III [SW-0008] Unit Specification/ UMS Enhancements [SW-1022] PMA support throughout GUI - III (Entity editors: schedule & task)	[SW-1020] Units of Measurements – IV ModelProtection: Improved diagnostics for protected models Global Sensitivity Analysis UI for External Objects
Modeling & solution power	[SW-0020] Multiflash correctness & robustness (phase 1)	Flowsheet-level Model Initialization Procedures	[SW-0016] Parameter Estimation Enhancements	[SW-0016] DAE Solver Enhancements
Tools interoperability & integration	gSAFT Enhancements – I	gSAFT Enhancements – II	gSAFT Enhancements – III Native interfaces to 3rd-party physical property tools	Unified gPROMS Properties
Software architecture & infrastructure	gIME re-architecting - II [SW-0013] Solvers: new NLPSQP code [SW-2001] Solver deCORBAfication [#9287] gPRODUCTs project file interoperabiity	Enhanced parameter estimation MXLKHD solver	[SW-2000] gIME re-architecting – III [SW-0016] Solvers: new DAE solver IME Language Engine – I	[SW-2000] gIME re-architecting – IV IME Language Engine – II

Thank you