ADVANCED PROCESS MODELLING FORUM **2014**

PSE 2014

Development & Directions

Costas Pantelides – Managing Director

Advanced Process Modelling

Getting the most out of past investment

Targeting future investment

Managing innovation

Managing risk in an uncertain world

PSE's belief

Advanced Process Modelling

has the power to radically transform the Process Industries

…*all* sectors of the Process Industries

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

PSE's mission

fresh thinking, new ideas
powerful tools

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

gPROMS product family – 5 years ago

General mathematical modelling

Model Builder

Advanced process modelling environment

Advanced model libraries for reaction & separation

gPROMS

The gPROMS platform

Equation-oriented modelling & solution engine

Model deployment tools

gPROMS product family – 2014

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Advanced process modelling environment

Sector-focused modelling tools

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 optimisation

gCRYSTAL

Crystallization process optimisation

gCOAS

Oral absorption

Power & CCS

gCCS

CCS system modelling

Fuel Cells & Batteries

gFUELCELL

Fuel cell stack & system design

Oil & Gas

gFLARE

Flare networks & depressurisation

Wastewater Treatment

gWATER

Wastewater systems optimisation

gPROMS

The gPROMS platform

Equation-oriented modelling & solution engine

Materials modelling

gSAFT

INFOCHEM Multiflash

OLI

Model deployment tools

gO:Run, gO:Run XML, gO:MATLAB, gO:CAPE-OPEN, gO:CFD

PSE developments – 2013-2014

A Year of Growth

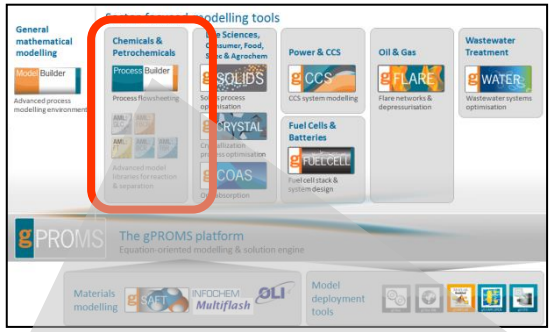
2013: +21% year-on-year revenue increase

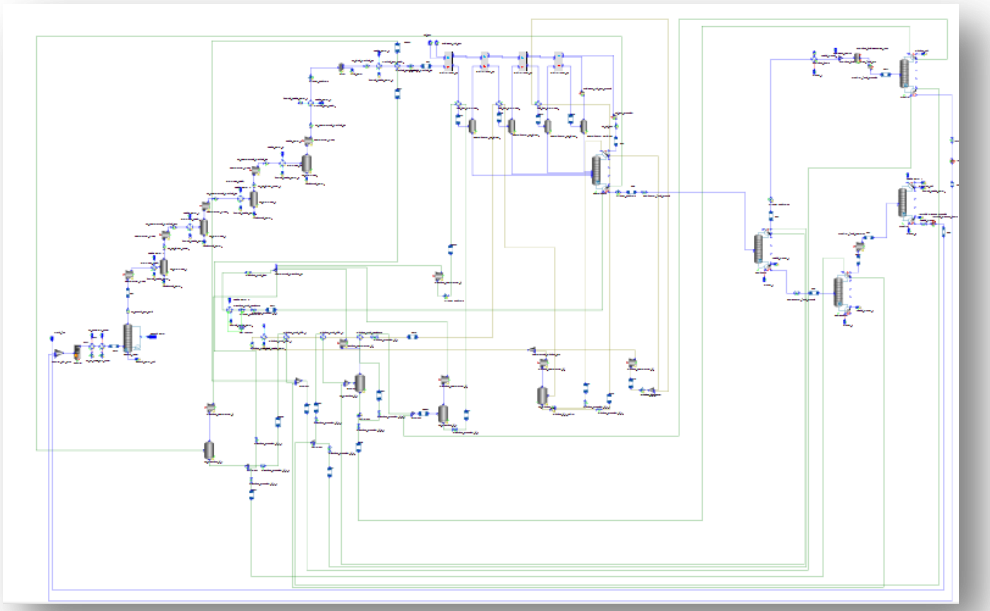
+99.2% over 3 years

R&D expenditure

- 2013: 35% of revenue
- 2014: 33% of revenue

Chemicals & Petrochemicals





Ongoing evaluation by selected users
Dedicated session tomorrow morning

- Comprehensive tool for process flowsheeting
- Steady-state & dynamic simulation & optimisation
- Equation-oriented power coupled with usability & robustness

PSE developments – 2013-2014

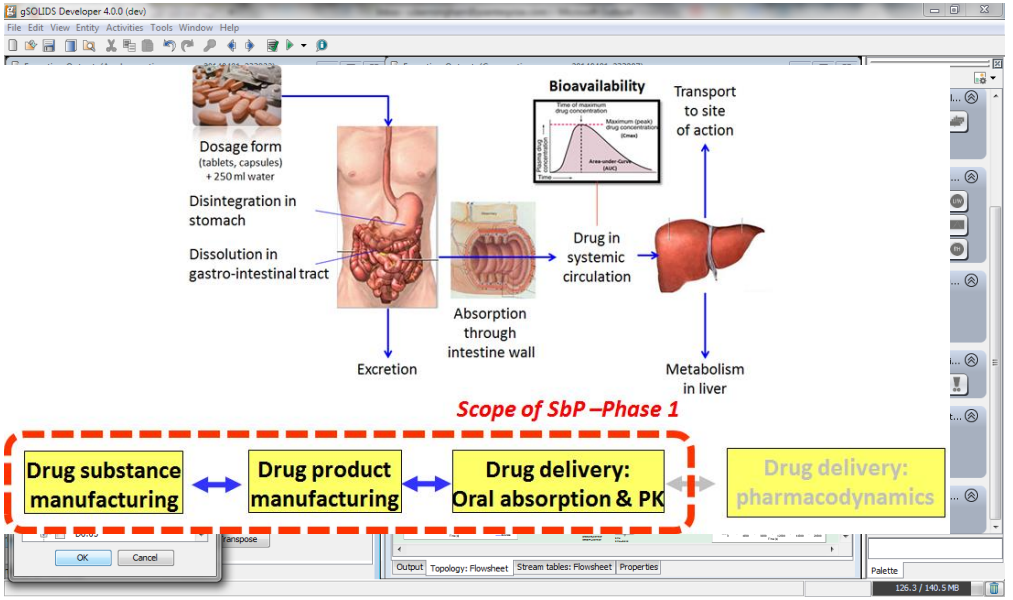
Life Sciences, Consumer Goods, Specialty & Agrochemicals

gCRYSTAL gSOLIDS gCOAS

Q4 '13: gCRYSTAL 4.0, gSOLIDS 3.1, gCOAS 1.0
Q2 '14: gCRYSTAL 4.1, gSOLIDS 4.0, gCOAS 1.1

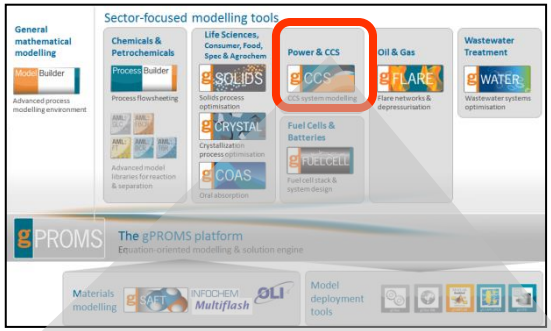
Presentations today

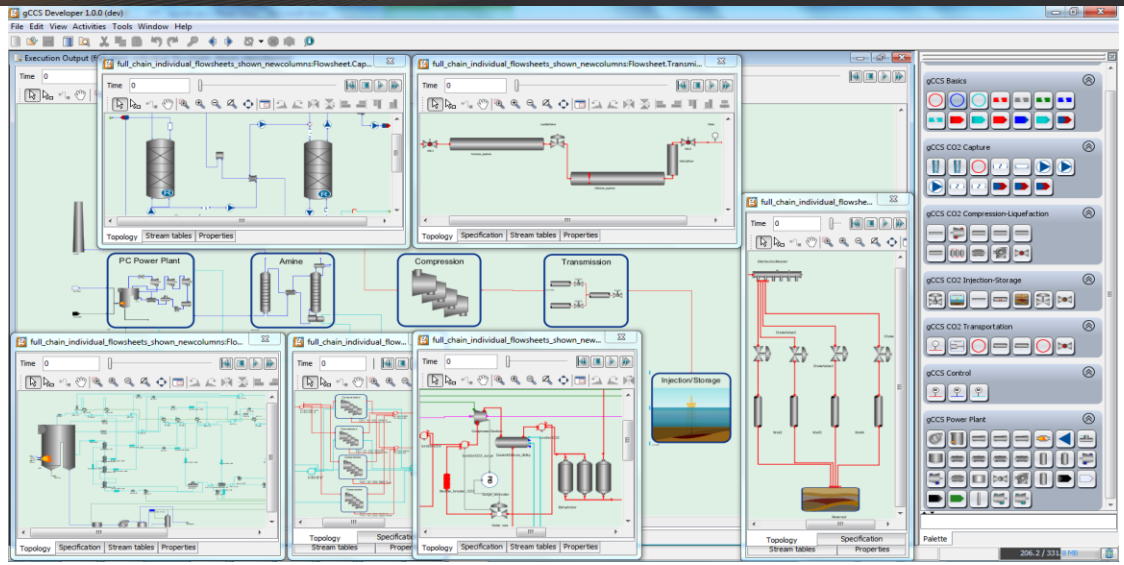
Solvay: optimise industrial crystallization operations
P&G: multi-scale spray dryer modelling
Nestlé: Continuous fluid bed agglomeration
Pfizer: Discrete element method
Rutgers: Linking DEM to PBE models
Vivo Drug Delivery: Challenges in pharma development
Pfizer: Predictive oral absorption tool for formulators



- Tools to characterise and optimise 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

Power & CCS



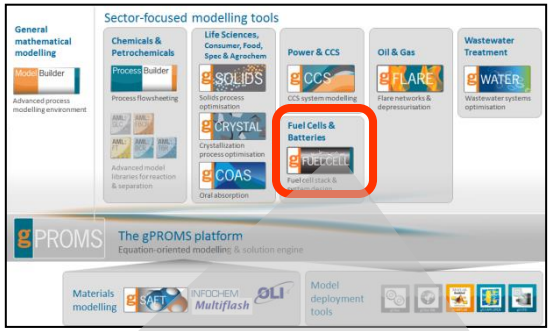


- End-to-end modelling of CCS chains
  - and their individual sub-systems
- £3m product development project
  - co-funded by Energy Technologies Institute
  - PSE, E.On, EdF, Rolls-Royce, CO2DeepStore
  - concluding in May 2014
- Significant interest in related areas
  - power generation, gas treating, EOR, …

v1.0 to be released early summer 2014

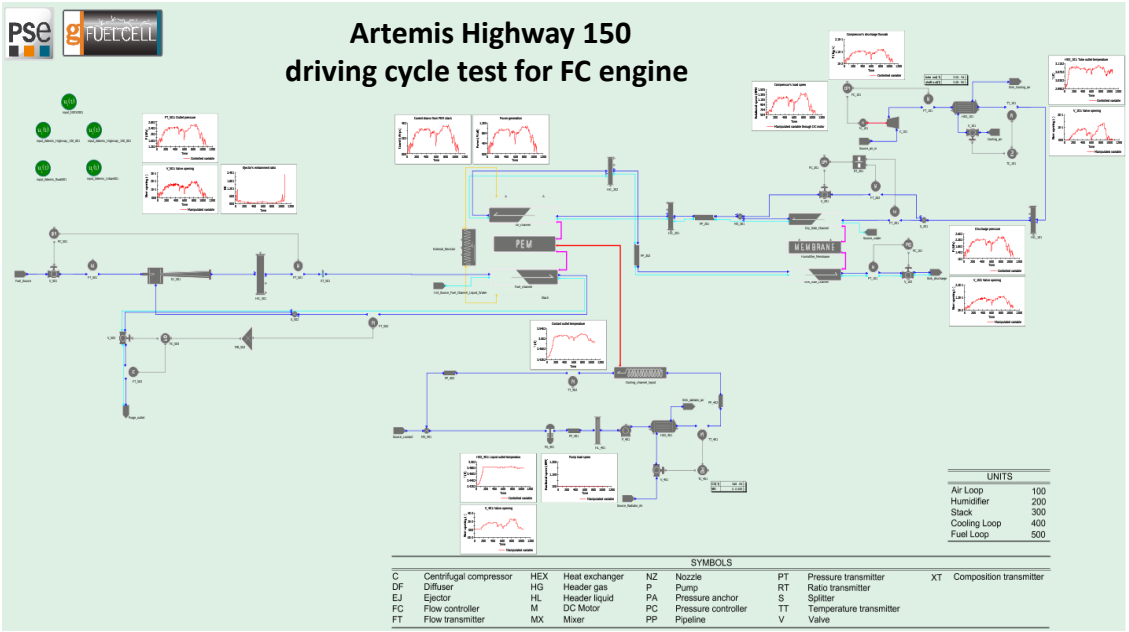
Presentations this afternoon
E.ON: whole-chain CCS study
Shell: CO_2 capture dynamics

Fuel Cells



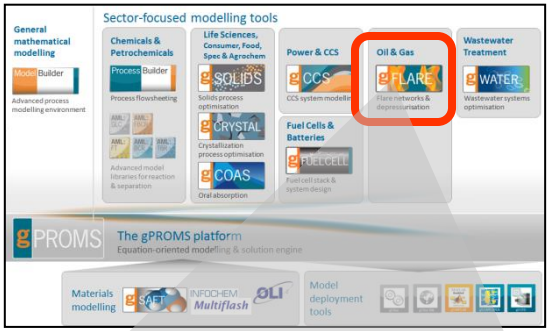
v1.0 available now

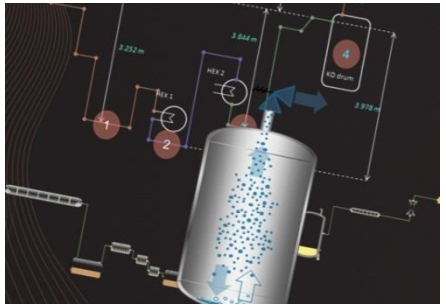
Fuel Cells & Batteries team presentation this afternoon

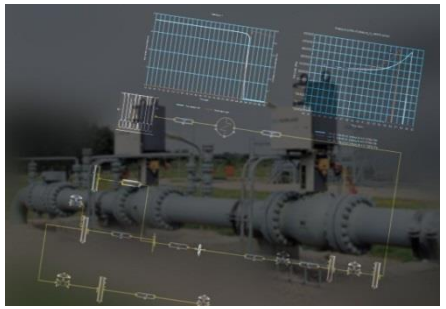


- Comprehensive modelling environment
  - fuel cell stack & fuel cell system
- Underpins FC engine development by major automotive manufacturers
  - strong demand for very high levels of modelling detail & predictive accuracy
  - …coupled with usability by engineering teams
- Focus on productisation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

Oil & Gas



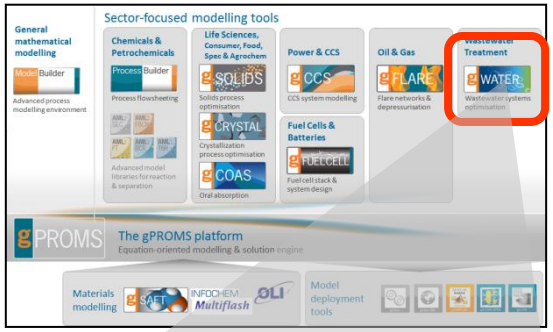


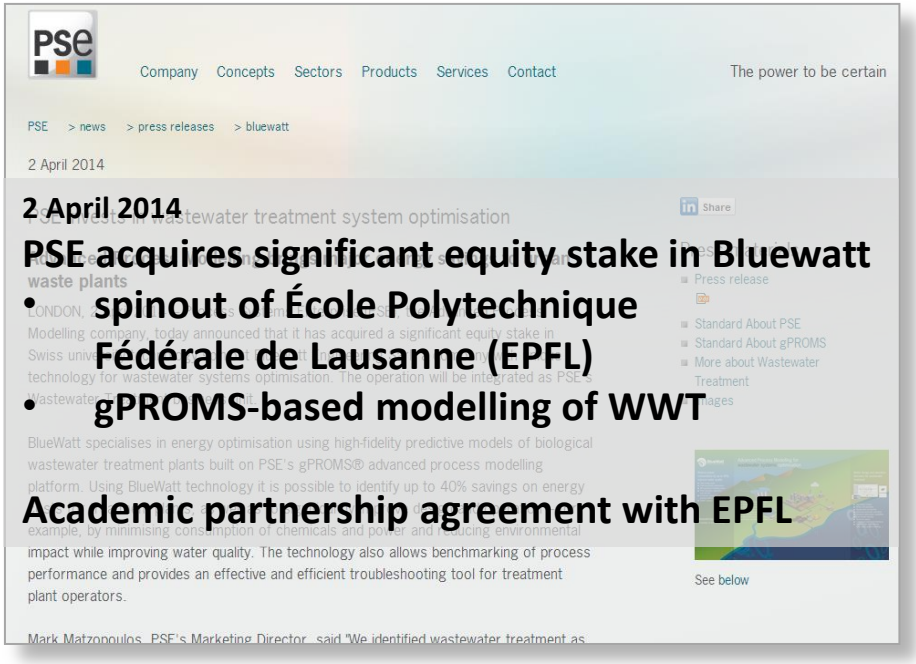


- **Focus: Safety in upstream oil & gas industry**
- High-fidelity modelling of depressurisation, flare networks, topside start-up, HIPPS
- Change the way industry approaches safety
  - recognised in latest revision of API 521 standard (6th edition – 1 January 2014)
  - 840 registrations for PSE webinar two weeks ago
- Large, highly skilled project delivery teams
  - London & Houston

- **Seminar tomorrow morning**
- **Session tomorrow afternoon**

Wastewater treatment





- Urban wastewater treatment
  - tightening regulations
  - excessive energy consumption
  - urban growth pressures – people ↑ space ↓
  - new treatment technologies
- Major opportunity for system-level modelling & optimisation

Presentation by Nicolas Descoins this afternoon

gPROMS product family – 2014

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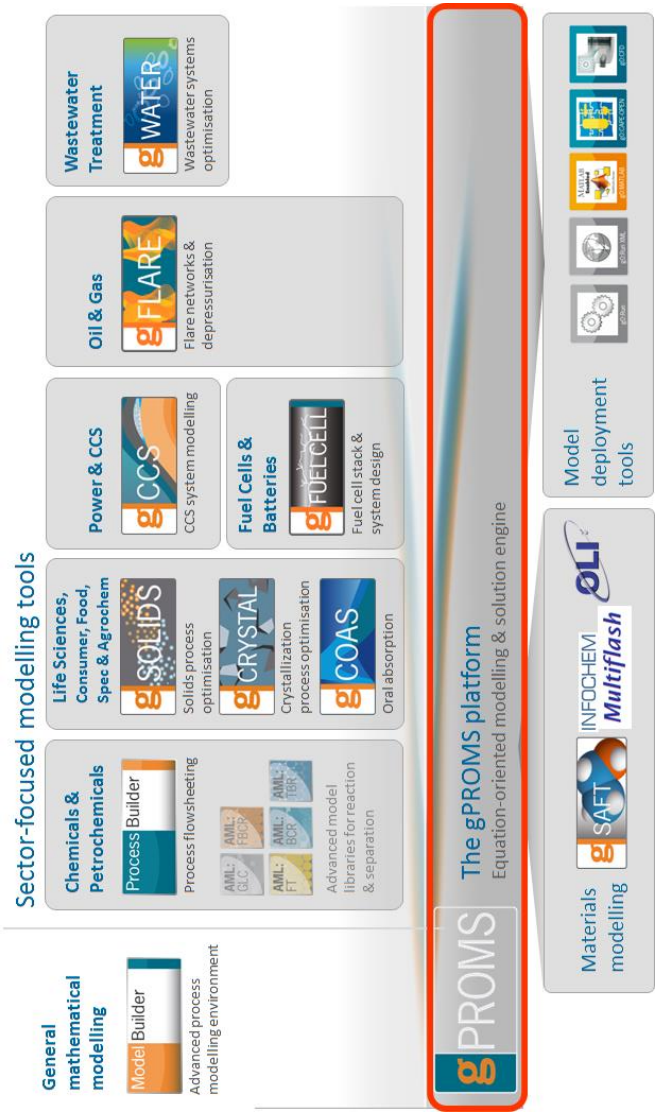
The gPROMS Platform – 2013-2014

The gPROMS Platform

PSE product development principles



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

gPROMS Platform

Overview of developments in v4.0

Usability

Tier I: "Model Developer"

- Model versioning
- Topology connection rules
- Units of measurement – input specification
- FOR loops in SET & TOPOLOGY sections
- Conditional reports

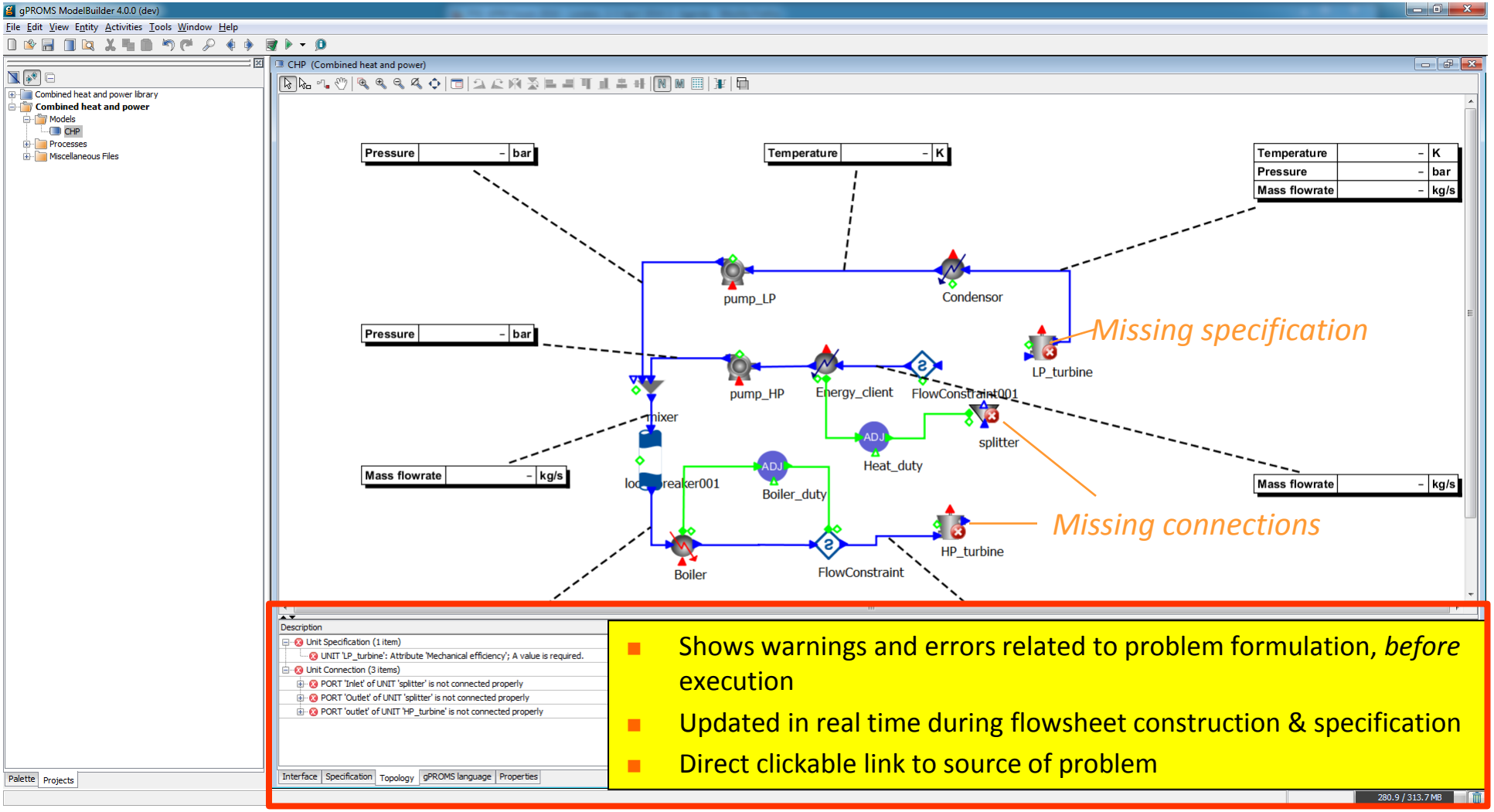
Tier II: "Flowsheeting" User

- Flowsheet diagnostics panel
- Early warnings for wrong specifications
- Full interoperability between gPRODUCTS
- Faster model construction

Solution power

- Model Initialisation Procedures – Unit Operations
- Model pruning
- New optimisation solver

Flowsheet diagnostics panel

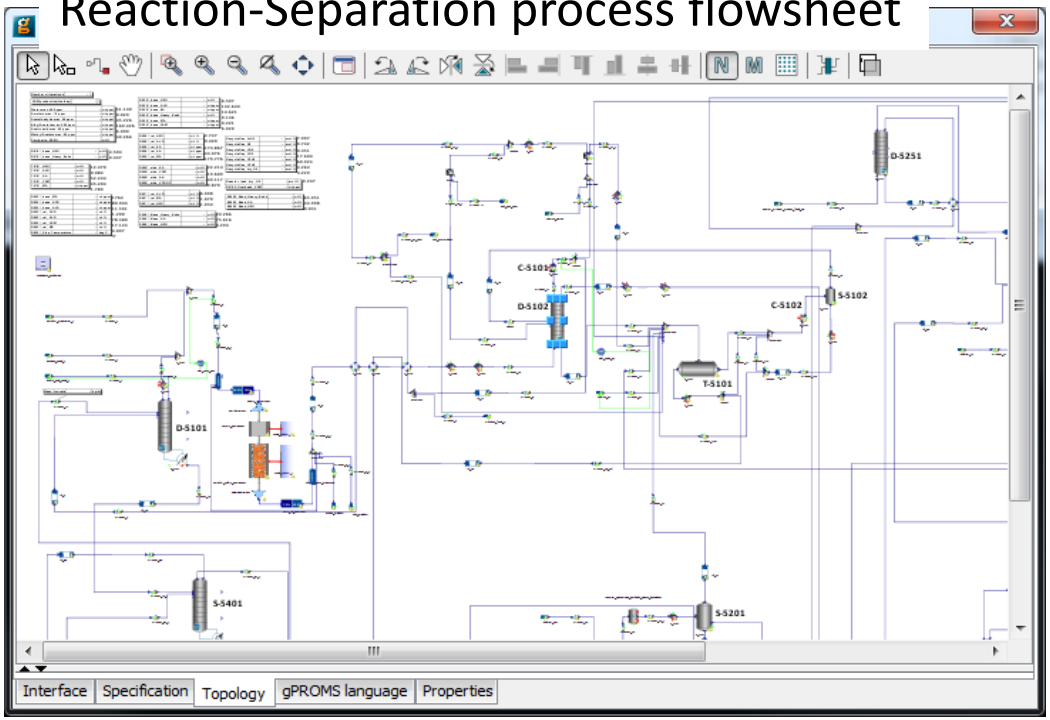


- Shows warnings and errors related to problem formulation, *before* execution
- Updated in real time during flowsheet construction & specification
- Direct clickable link to source of problem

Higher interactivity

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

Reaction-Separation process flowsheet



- 290,000 parameter elements
- 330ms model construction time
  - Down from 680ms

Model Pruning – key concepts

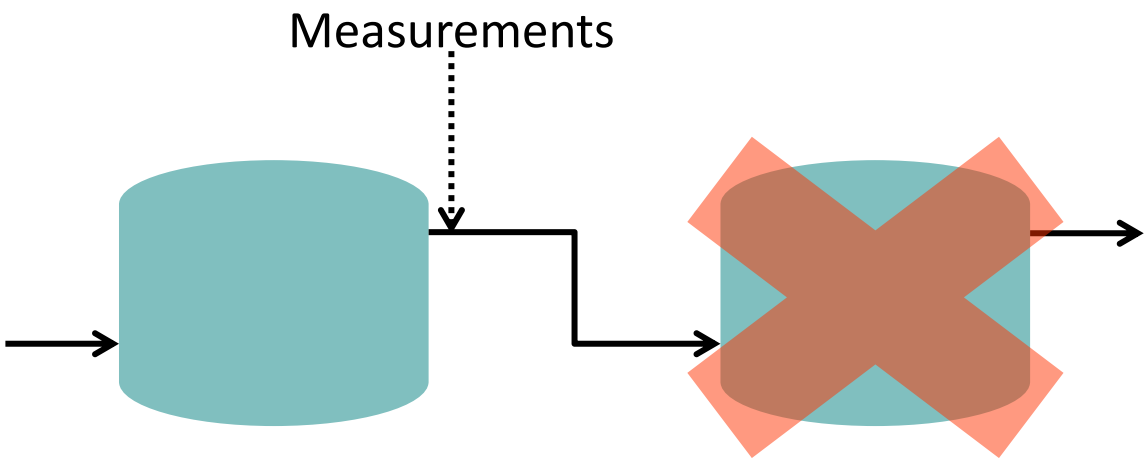
- Automatically reduce model to minimum required to produce information requested by the user

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

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

Model Pruning – example #1

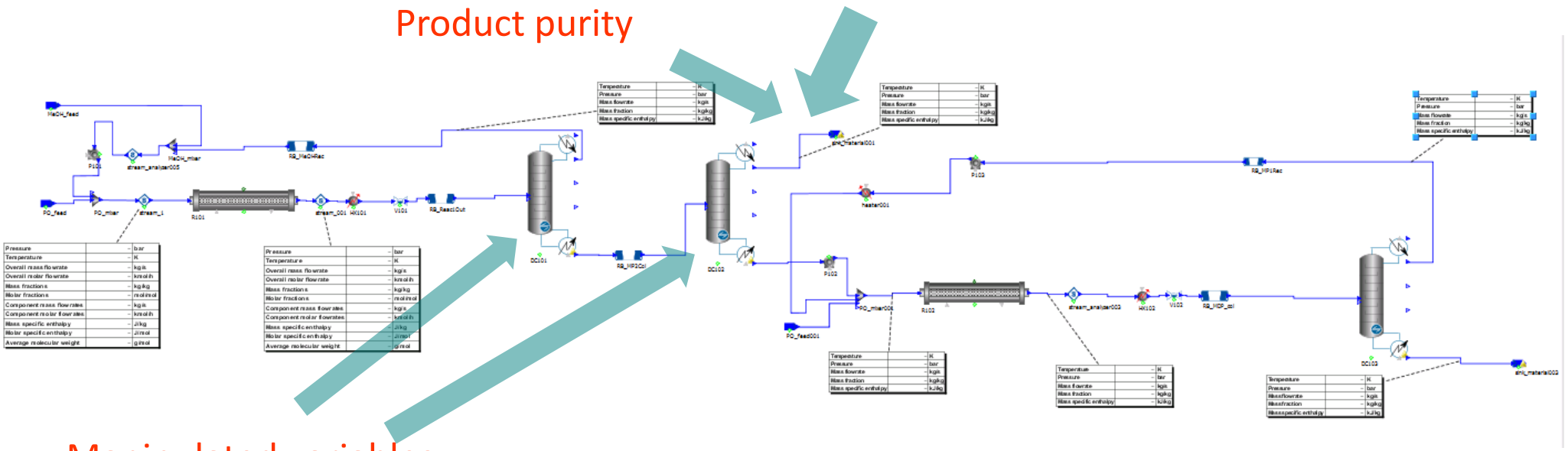
- Two reactors in series
  - Model typically used for dynamic simulation
  - Use model to perform parameter estimation
  - Model Pruning: eliminate all variables/equations in 2nd reactor



Model Pruning – example #2

Constraint:
Product purity

Objective: maximise product flow



Manipulated variables:
Reboiler duties

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

Post-calculated variables hidden from solvers

Model Pruning – example #2

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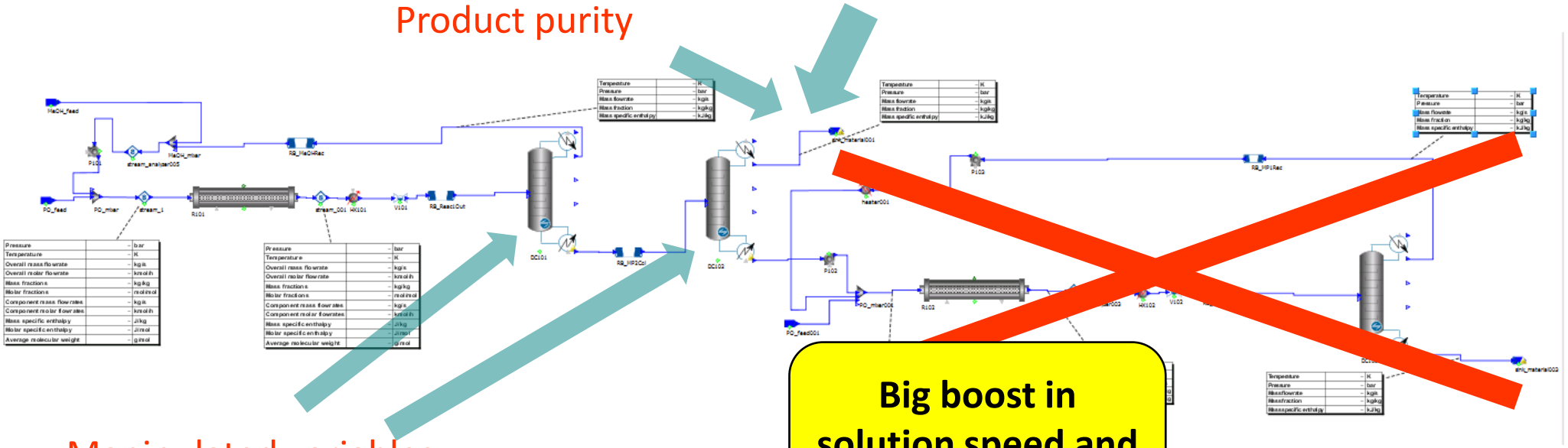
Objective: maximise product flow



Manipulated variables:
Reboiler duties

Big boost in solution speed and robustness

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

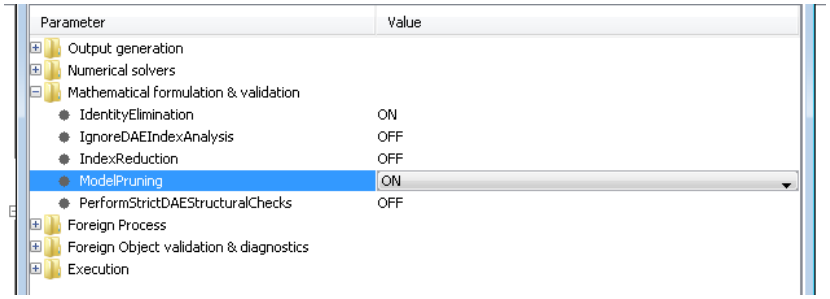
Post-calculated variables hidden from solvers

Model Pruning

- Benefits
  - Large improvements in efficiency and robustness
  - Better identification of badly-posed problems

- Enhance **model re-usability**
  - reduce need for manual “tailoring” of model to match specific calculation
  - a step towards full realisation of the “**Master Model**” concept

- Side-effects: none
  - now the default option



gPROMS Platform

Overview of developments in v4.0

Usability

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- Flowsheet diagnostics panel
- Early warnings for wrong specifications
- Full interoperability between gPRODUCTS
- Faster model construction

Solution power

- Model Initialisation Procedures – Unit Operations
- Model pruning
- New optimisation solver

v4.0 - Beta-2 version used internally in PSE
Expected release date: end of April 2014

gPROMS Platform

Overview of developments in v4.0 + 4.1

Usability

Tier I: "Model Developer"

- Model versioning
- Topology connection rules
- Units of measurement – input specification **+ results display**
- FOR loops in SET & TOPOLOGY sections
- Conditional reports

Tier II: "Flowsheeting" User

- Flowsheet diagnostics panel
- Early warnings for wrong specifications
- Full interoperability be
- Faster model c

Session on gPROMS ProcessBuilder tomorrow morning

Solution power

- Model Initialisation Procedures – unit-level initialisation **+ flowsheet-level initialisation**
- Model pruning
- New optimisation solver

v4.1 expected release: summer 2014

Materials modelling – 2013-2014

gPROMS product family – 2014

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Modelling of materials behaviour a central part of PSE's product strategy

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Objective: Unified & consistent physical properties across gPROMS-family products

Multiple phases…

gCCS	gFUELCELL	Process Builder	gFLARE	gSOLIDS	gCRYSTAL	gCOAS
Gas Liquid	Gas Liquid	Gas Liquid (Solid)	Gas Liquid Hydrate	Solid (Liquid) (Gas)	Liquid Solid	Liquid Solid Micelle

Complex materials & challenging behaviour…

strongly-associating compounds

near-critical point behaviour

acids & bases

oligomers & polymers

complex gas/liquid phase envelopes

salts & salt hydrates

ions

gPROMS materials modelling

Overview of developments in v4.0

Multiflash

- Long-term supply agreement with KBC
- Rewritten gPROMS interface
  - more extensive range of thermodynamic calculations from within gPROMS models
  - improved efficiency
    - caching & hot starting

gSAFT

- Completed acquisition of technology from Imperial College London
- Extensive developments at PSE with focus on
  - numerical efficiency & robustness
  - phase equilibrium algorithms
  - software architecture

- State-of-the-art thermodynamics

Presentation in tomorrow's gPROMS ProcessBuilder session

In conclusion…

PSE's commitment

General mathematical modelling

Model Builder

Advanced process modelling environment

Sector-focused modelling tools

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gWATER

Wastewater systems optimisation

APM

fresh thinking, new ideas, powerful tools

gPROMS

Model development platform

Equation-oriented modelling & solution engine

Pushing the boundaries of Model-based Engineering

Materials modelling

gSAFT | INFOCHEM Multiflash | OLI

Model deployment tools

gO:Run | gO:Run XML | gO:MATLAB | gO:CAPE-OPEN | gO:CFD

ADVANCED PROCESS
MODELLING FORUM **2014**

Thank you