APM 2013

The Advanced Process Modelling Forum

17-18 April 2013, London

gPROMS Product Family

Costas Pantelides – Managing Director

gPROMS Product Family

General Mathematical Modelling

Model Builder

Sector-focused Modelling Tools

Chemicals & Petrochemicals

Process Builder

AML: GLC

ML: BCR

ML: T

ML: BR

ML: CR

Life Sciences & Fine Chemicals

gCRYSTAL

gSOLIDS

gCOAS

Power & CCS

gCCS

gFUELCELL

Oil & Gas

gFLARE

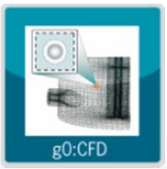
Materials Modelling

Multiflash

OLI

gSAFT

Model Deployment Tools



gPROMS

The gPROMS platform

Equation-oriented modelling & solution engine

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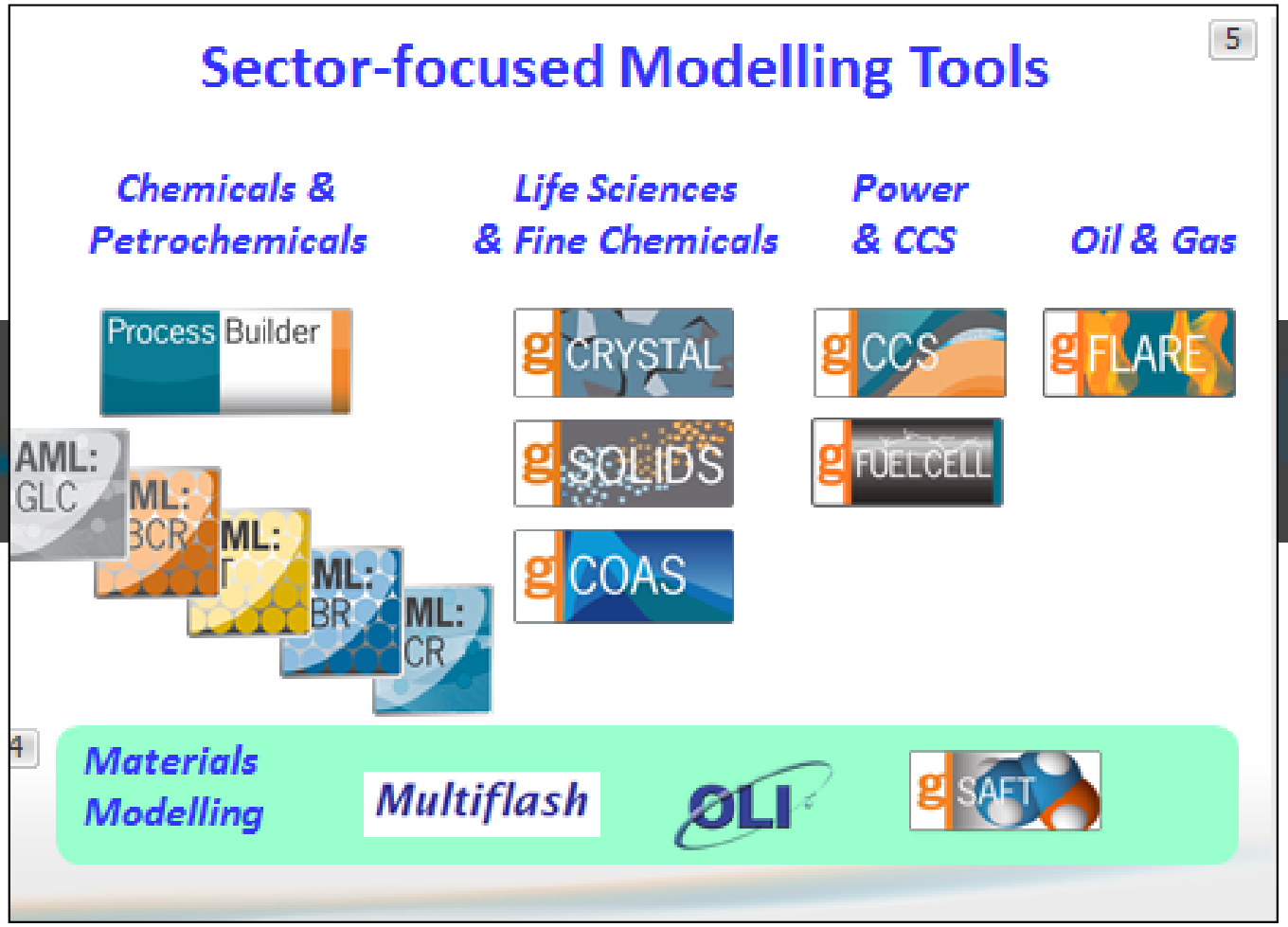
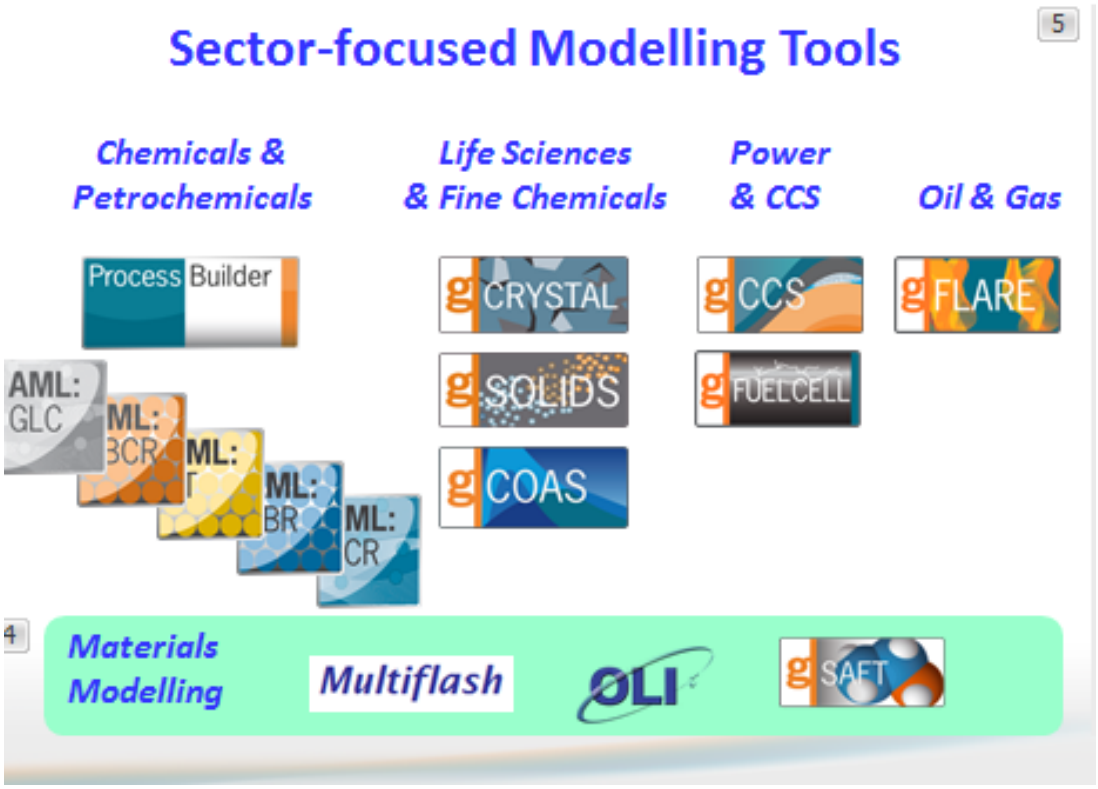
Sector-focused modelling tools

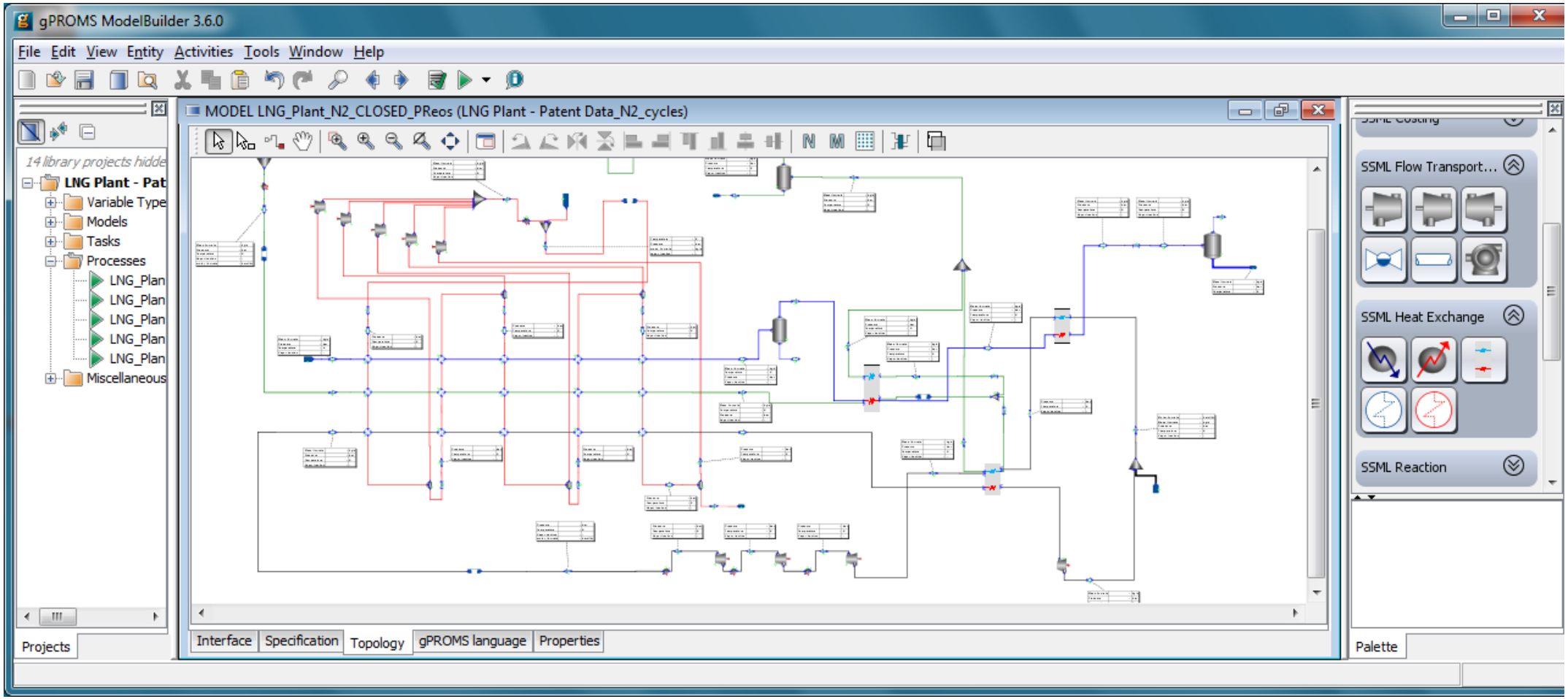


Each modelling tool comprises…

- gPROMS Platform
- Model Libraries
- Physical properties
- Workflows
- Documentation
- Training material
- Demos & examples



ProcessBuilder – C3-MR Liquefied Natural Gas process



Maarten Nauta's presentation at 14:00 today

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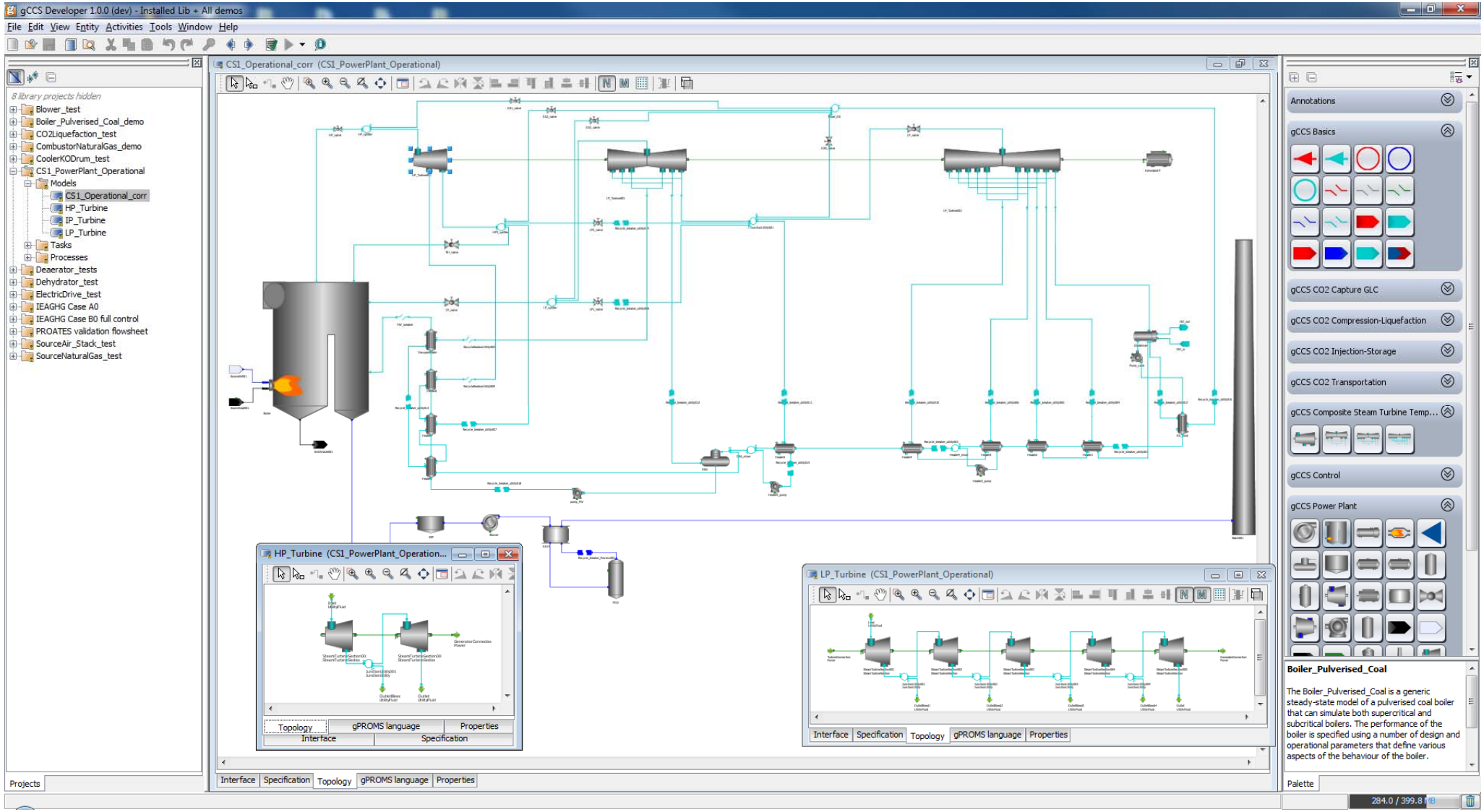
gCCS – Pulverised coal power plant



Alfredo Ramos' presentation at 15:30 today

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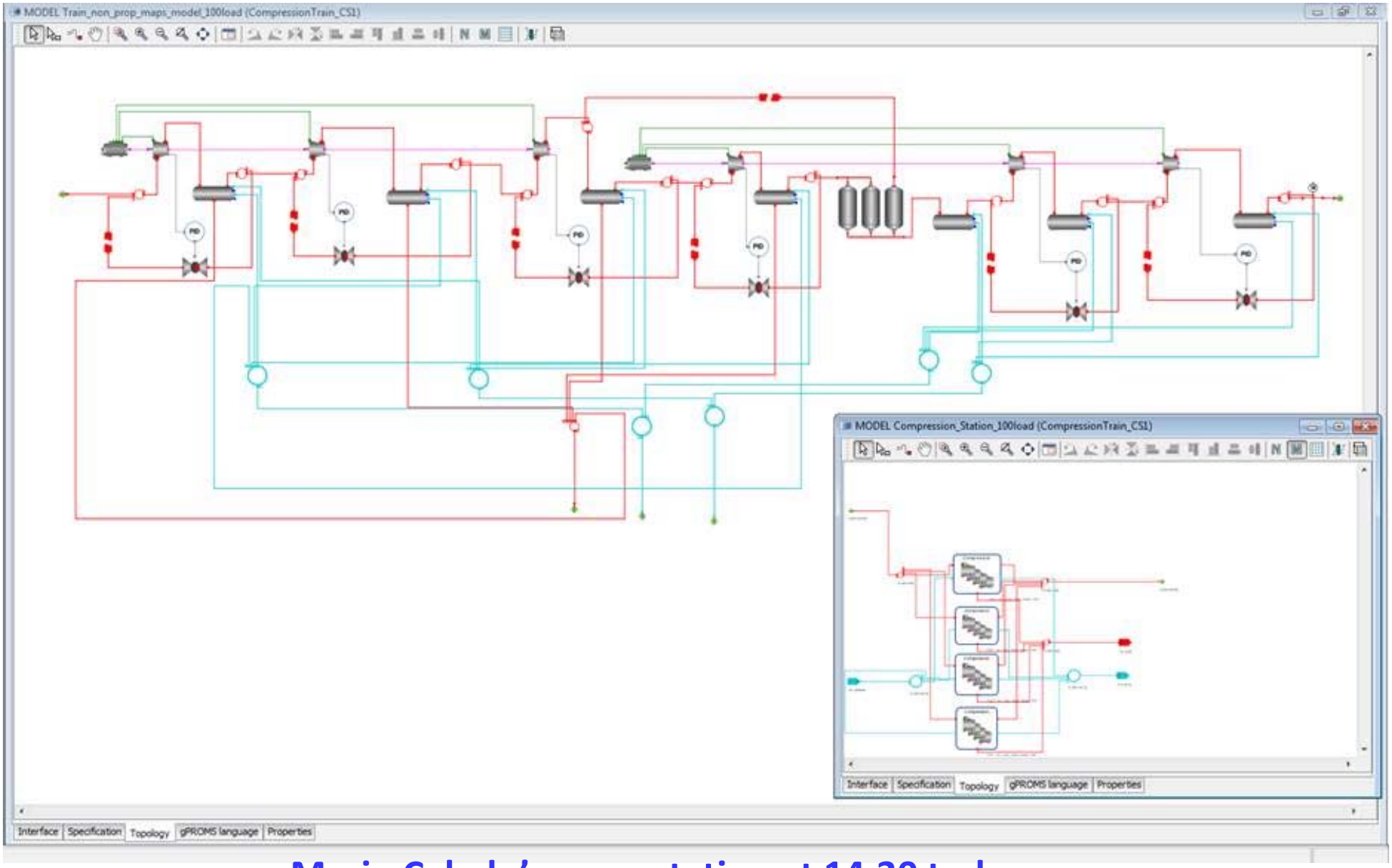
gCCS – CO_2 compression station



Mario Calado's presentation at 14:30 today

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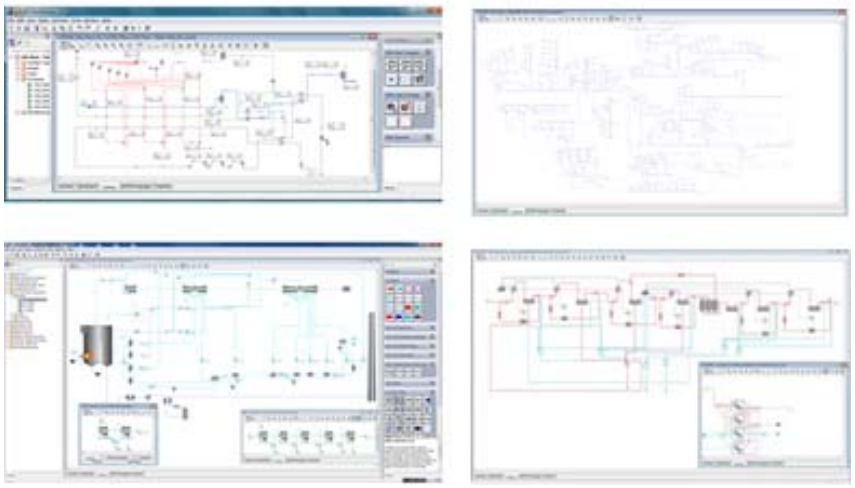
Q: What do these flowsheets have in common ?



1. Large-scale systems
   - some with complex unit operation models
2. Tightly coupled systems
   - multiple recycles of material & energy
   - backward flow of information
3. All models initialise from scratch without any user-provided initial guesses
   - all model libraries incorporate Model Initialisation Procedures

➔ **Efficient and robust solution using equation-oriented technology**

gPROMS' Model Initialisation Procedure (MIP) technology is effecting a radical change in the balance between Sequential Modular and Equation Oriented process modelling tools

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Physical properties in the gPROMS product family

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

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

Process Lifecycle

Fundamental Process R&D

Optimal selection of "auxiliary" process materials (solvents, entrainers, etc.)

Process Development

Good predictive capability with little or no experimental data

Plant Design

Accurate calculation of physical properties over wide ranges of conditions

Plant Operations

Accurate calculation of physical properties over wide ranges of conditions

Requirement:
Fundamental basis on molecular interactions

Requirement:
Information (e.g. parameter values) transferable from one compound to another

gSAFT

Javier Rodriguez's presentation at 09:30 today

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The gPROMS platform

Equation-oriented modelling & solution engine

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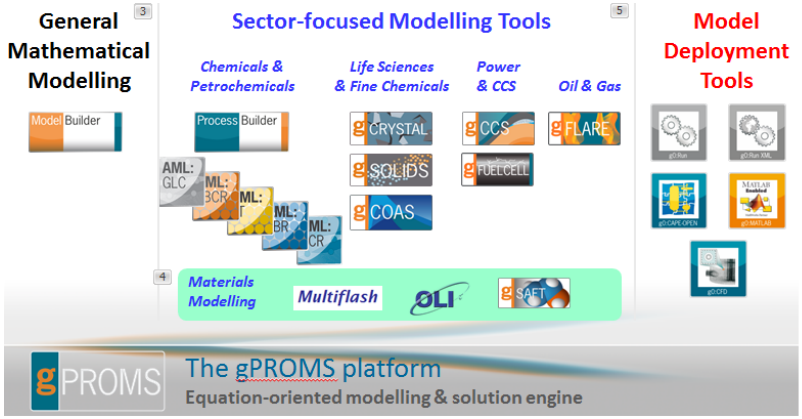
Development Priorities 2013-2014
gPROMS Platform

1. Usability

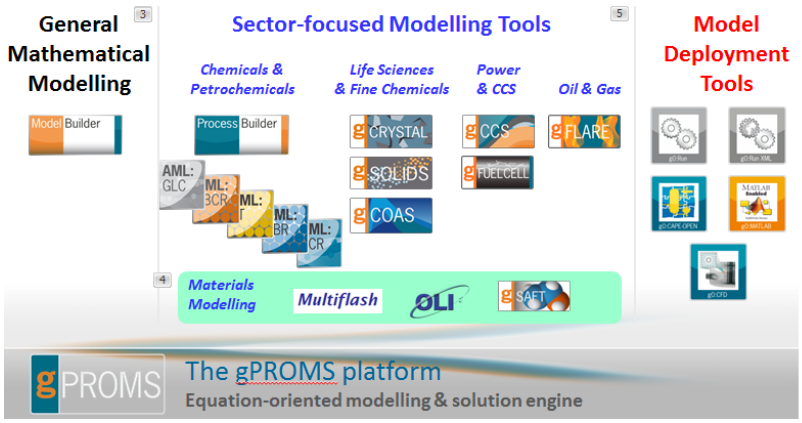
- Make "flowsheet" the central paradigm of user interaction
  - Model construction
  - Problem specification for all types of activity
    - simulation, optimisation, parameter estimation, experiment design
  - Results analysis
  - Diagnostics
- Integrate material/physical property specification within environment
- Provide comprehensive support for units of measurement



2. Robustness

- Eliminate causes of failure at source
  - e.g. bad problem specifications
- Enhance Model Initialisation Procedures
- Improve robustness in solution methods
  - convergence criteria
  - variable scaling
- *[Improved diagnostics]*

gPROMS Platform



3. Solution performance

- Introduce fu[illegible]her automatic model pre-proces[illegible]
  - e.g. m[illegible]
- Exploit de[illegible]are/ software infras[illegible]
  - 64-bit Windows
  - distributed computation

4. gPRODUCT workflows & user experience

- Increase customisability of gPROMS Platform
- Support enhanced modes for user interaction
  - e.g. in model dialogs

Future Proofing

- [illegible]rove efficiency of development & [illegible]roduction of major new [illegible]from 2014 onwards via…
  - [illegible]ng
  - [illegible]interfaces
  - re-arch[illegible]ng key numerical s[illegible]
  - . . . . . .

Quality Assurance

Model deployment within the organisation

Model deployment within the organisation

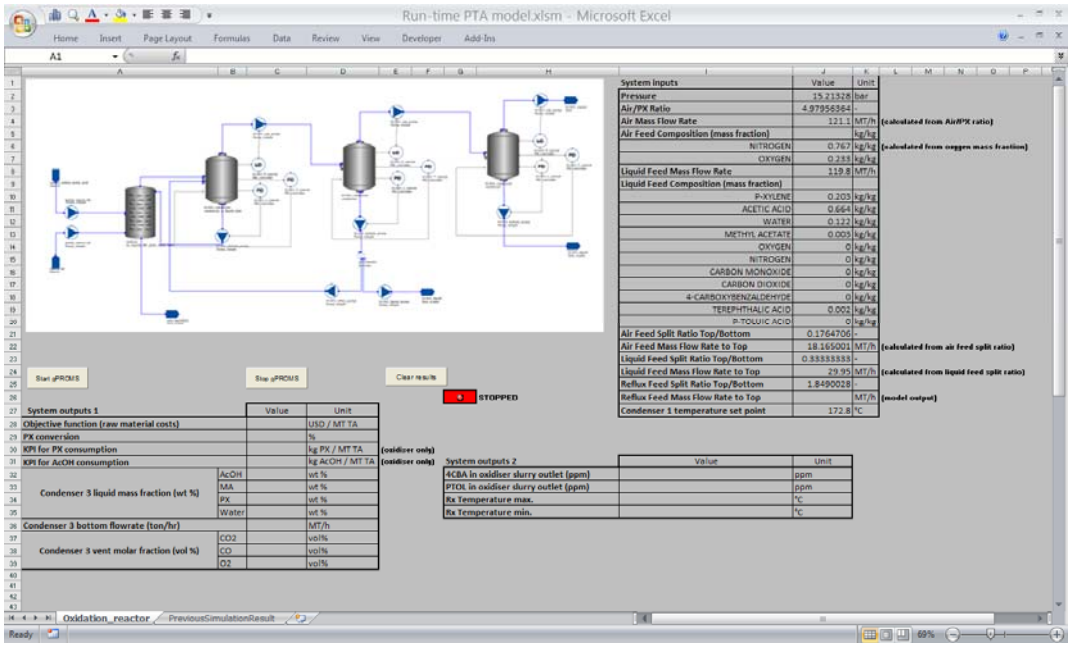
Tier I	Tier II	Tier III
First-principles modellers ("custom modelling")	Drag-and-drop flowsheeting using model libraries	"Non-modellers" requiring access to model-based calculations
Primarily R&D	R&D Engineering	Engineering Operations Commercial

gPRODUCTs

gPROMS Objects

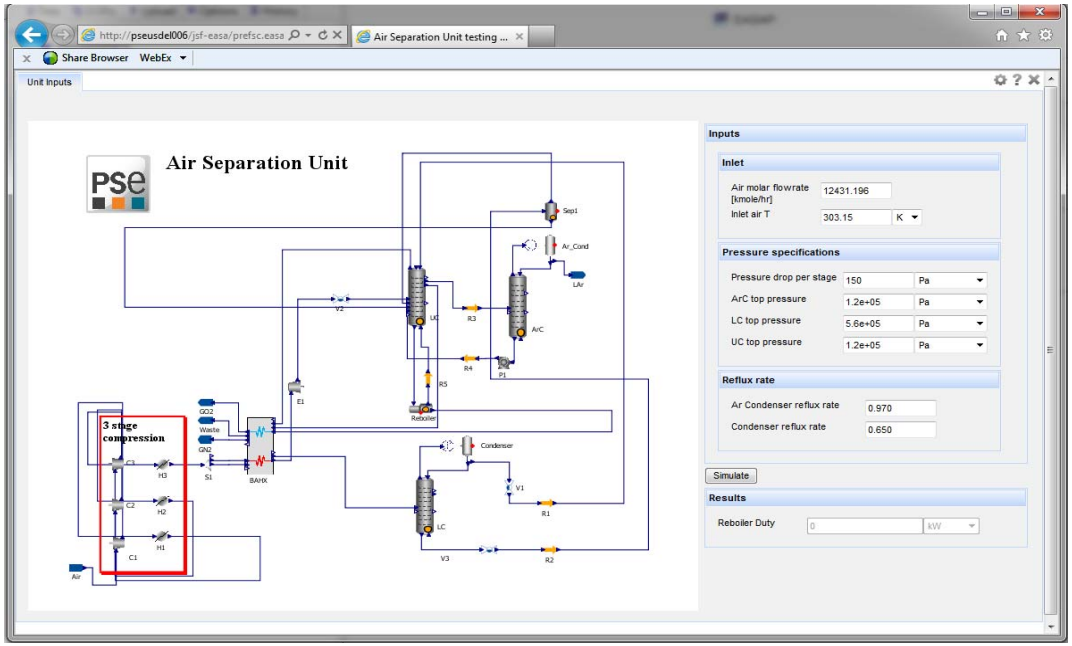
Tier-III deployment mechanisms

gO:RUN: Local model deployment



Optimisation of Purified Terephthalic Acid plants (Microsoft Excel®)

gO:RUN_xml: Web-based model deployment



Simulation of Air Separation Units (web browser + EASA®)

- Controlled model deployment
  - well-defined/restricted sets of model inputs & outputs
  - secure model IP
- Ease of use
  - no knowledge of modelling required

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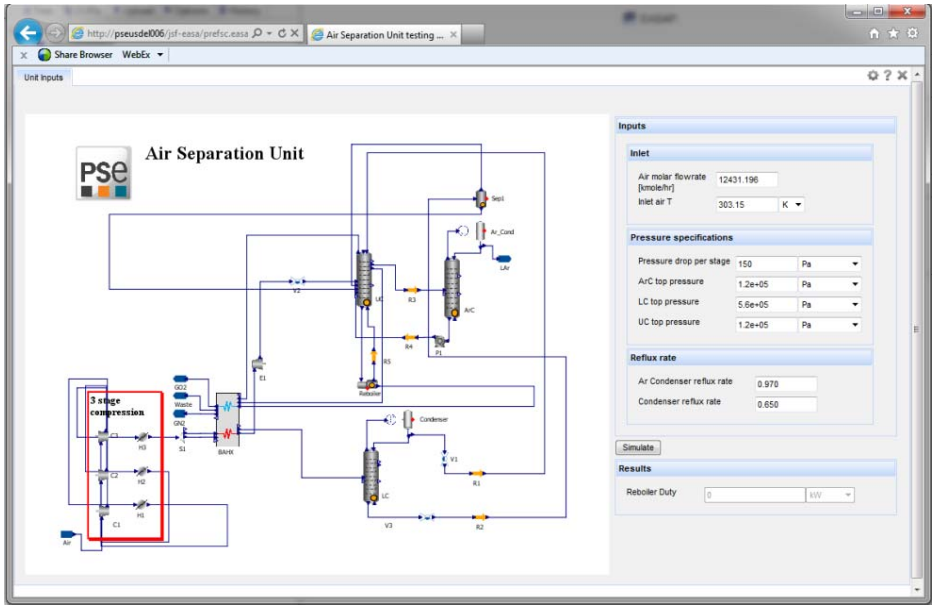
Web-based model deployment



web browser

EASA®

gO:RUN_xml

- Users can access models via web browser from anywhere
  - no software installation required
- Centralised model installation, execution, maintenance
  - same model version used across entire organisation
  - efficient use of powerful compute servers
- Full access control & logging
  - on a per-user per-model basis
  - IP protection, significantly lower risk of reverse engineering

Model deployment within the organisation

Tier I	Tier II	Tier III	Tier IV
First-principles modellers ("custom modelling")	Drag-and-drop flowsheeting using model libraries	"Non-modellers" requiring access to model-based calculations	Models embedded in online/real-time systems
Primarily R&D	R&D Engineering	Engineering Operations Commercial	Operations
gPRODUCTs		gPROMS Objects	Online Model-Based Applications

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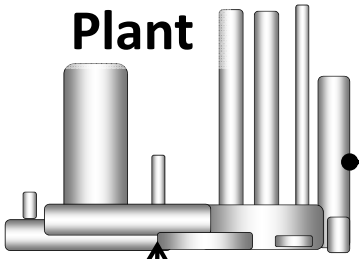
Online Model-Based Applications



Raw plant data

❶ State estimation/ Online model calibration

Up-to-date calibrated model

Current plant state

Regulatory Control System

Regulatory Controller set-points

❻ Set-point/ trajectory optimisation

❺ Model reduction/ linearisation

❹ Nonlinear optimal control

❸ Decision support via future scenario(s) simulation

❷ Monitoring & diagnosis

Optimal set-points/ trajectories

Reduced/ linear model(s)

Unmeasured control objectives

❼ Model Predictive Control

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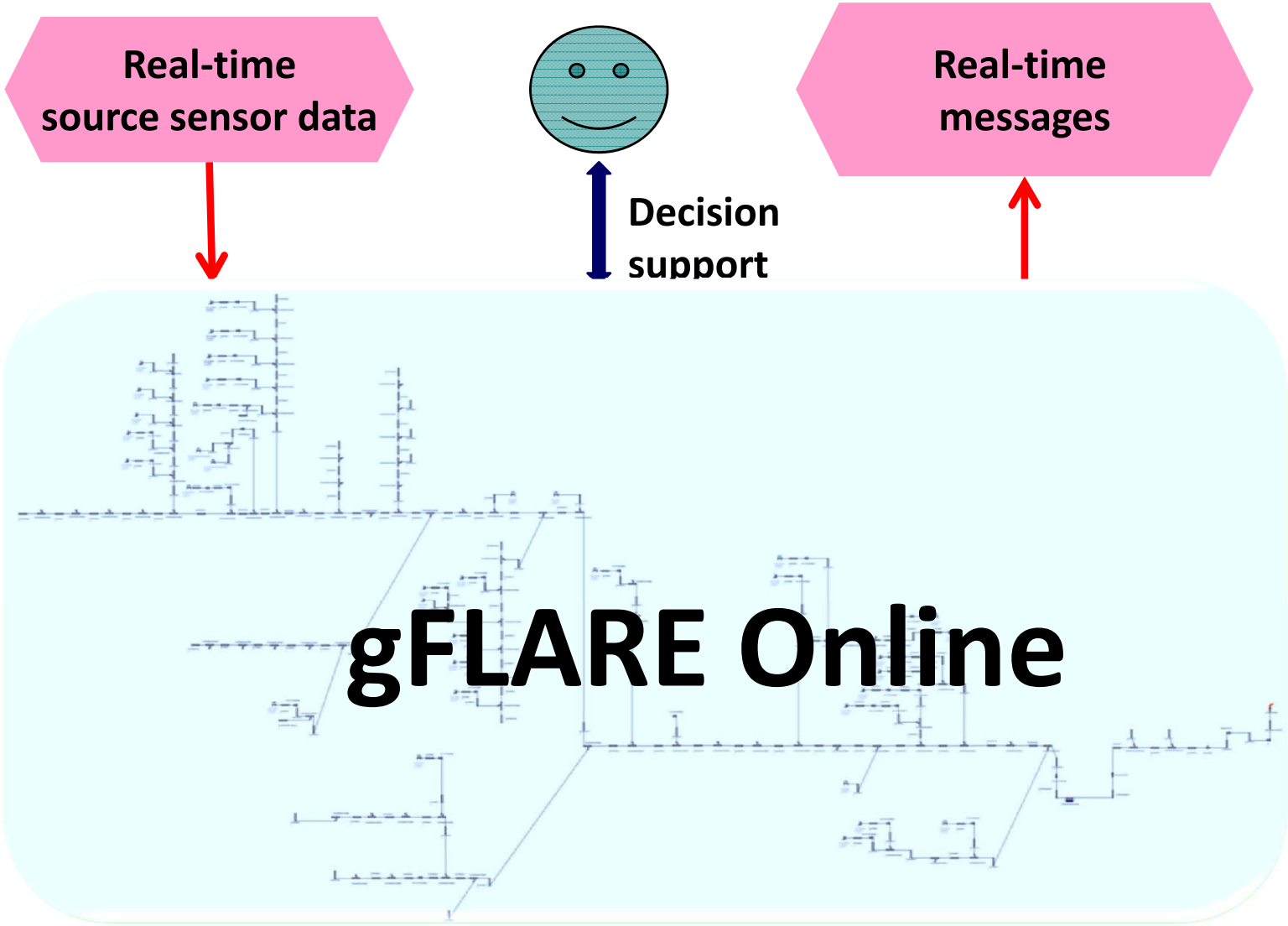
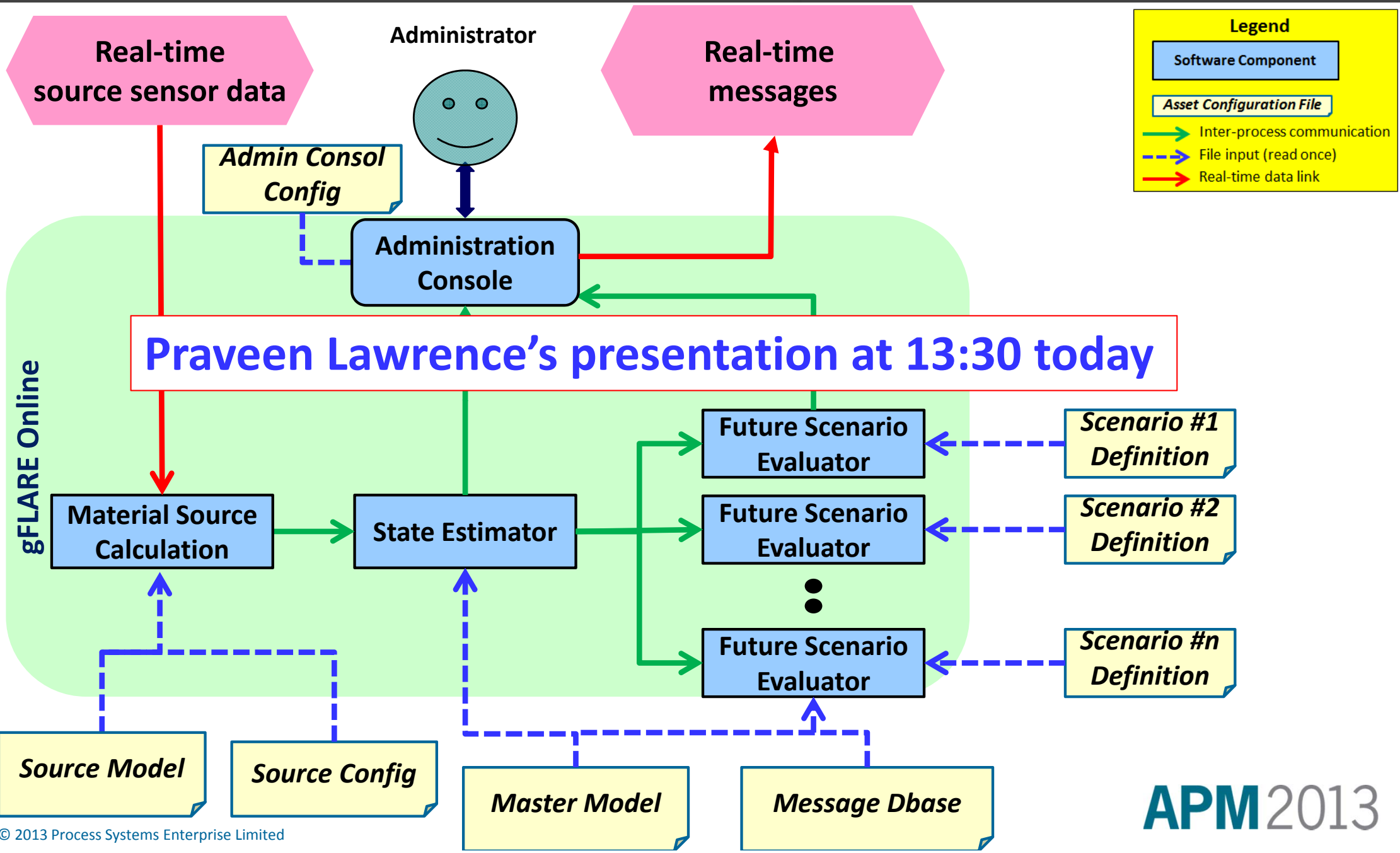
Online Model-based Monitoring & Decision Support

Example: gFLARE Online



Online Model-based Monitoring & Decision Support

gFLARE Online software architecture



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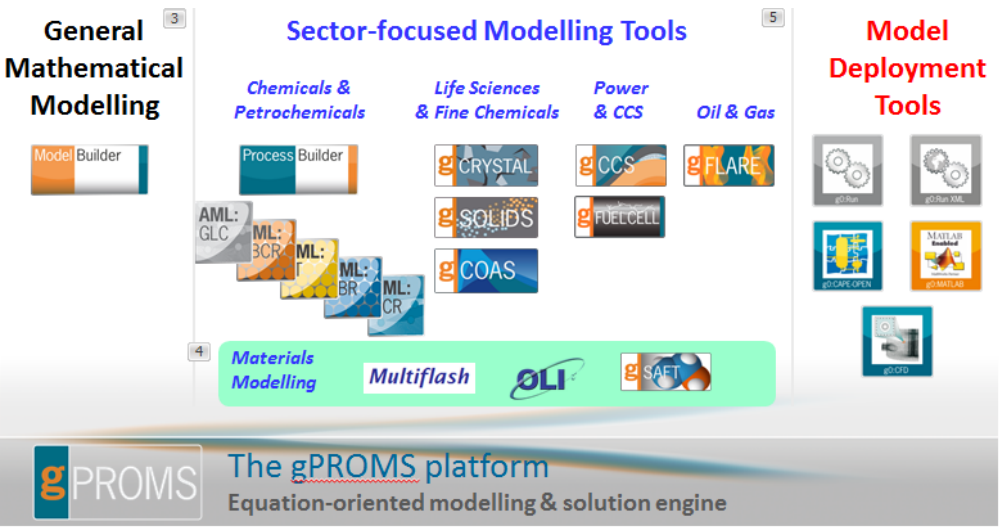
In conclusion…

gPROMS product family



- Advanced Process Modelling tools
  - power + usability
  - deep process knowledge & understanding
- Effective & consistent deployment of corporate IP across the organisation
- Future proofed by PSE's investment & innovation

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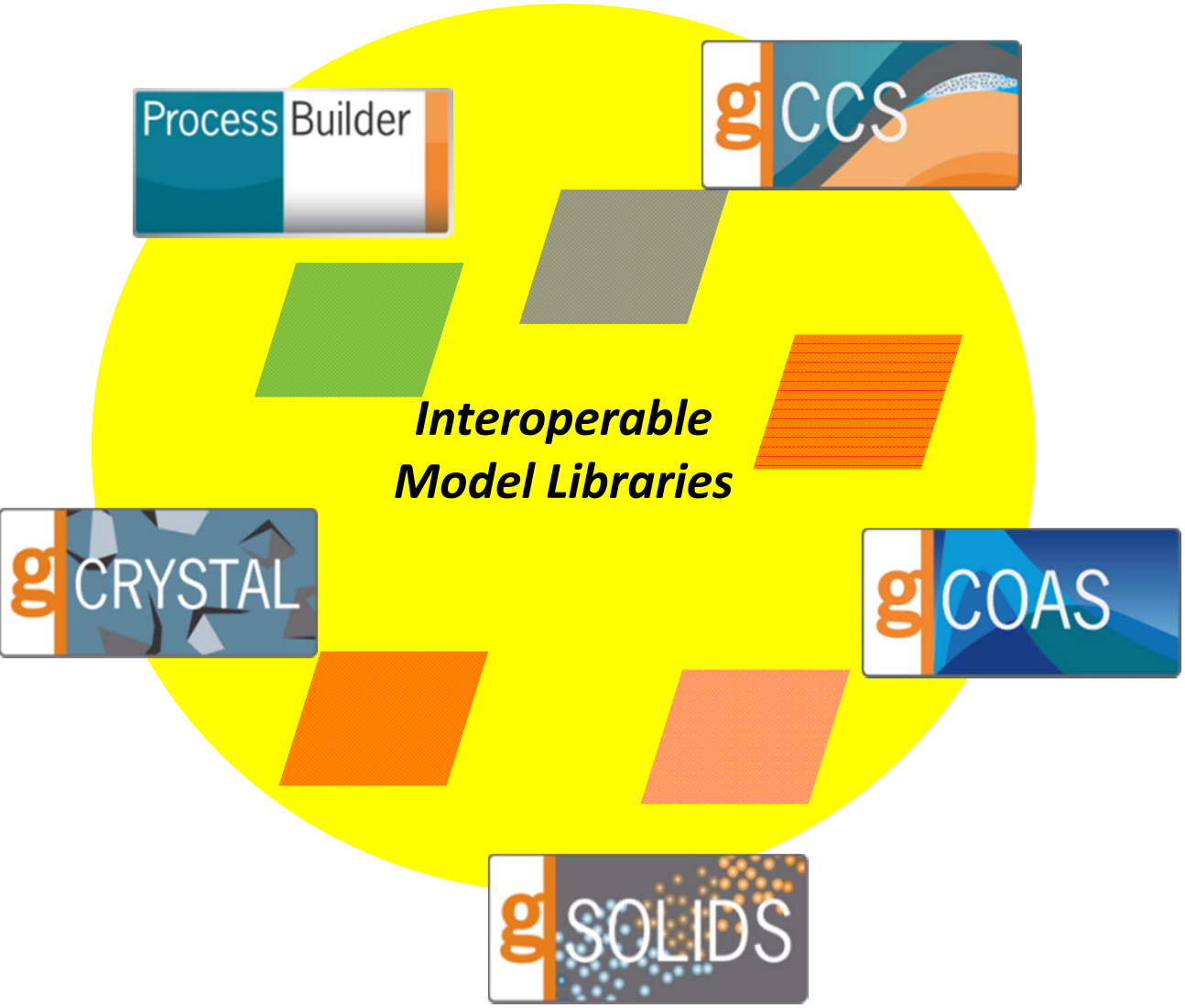
gPROMS product family interoperability



- gPRODUCTs can use each other's model libraries
- Model Libraries comply with "PSE Standard" for
  - metrology
  - variable & connection types
  - look & feel in dialogs & reports
  - variable naming conventions
- Flexible licensing
  - standard vs. optional model libraries

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Thank you!

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