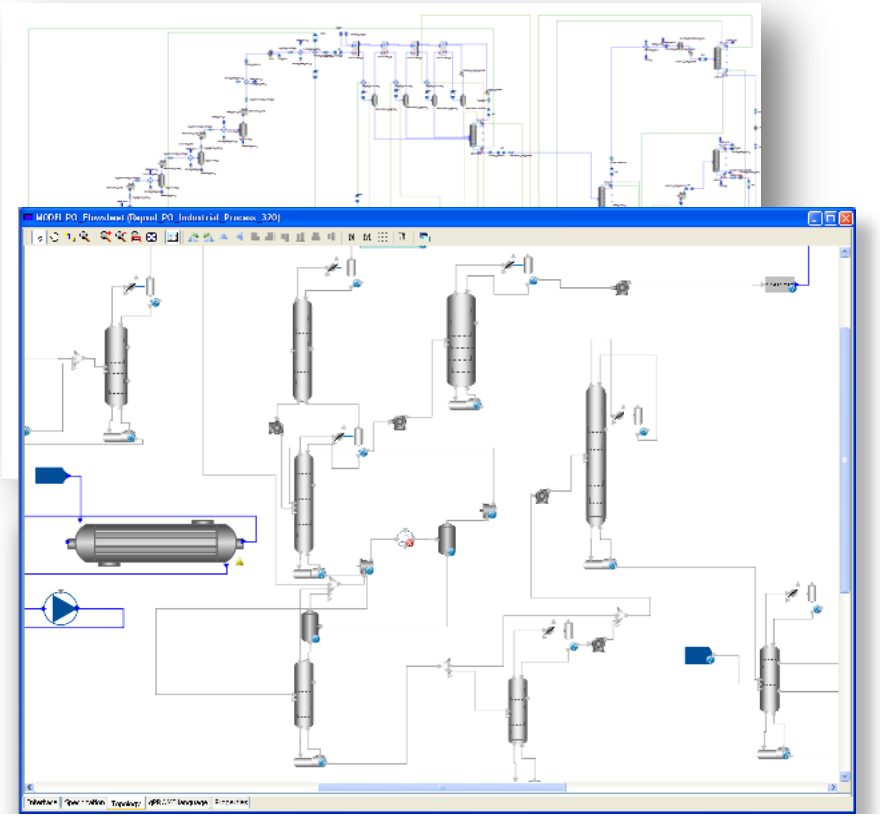
ADVANCED PROCESS MODELLING FORUM **2014**

# gPROMS ProcessBuilder

## Conclusions & Perspectives

Costas Pantelides – Managing Director

# gPROMS ProcessBuilder
## Environment



**HPPO process – plant-wide optimisation**

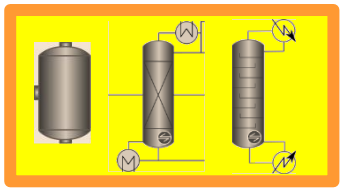
**49 continuous & discrete decision variables**

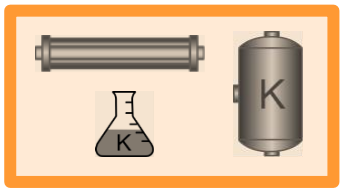
**v1.0 based on**
**gPROMS Platform v4.1**

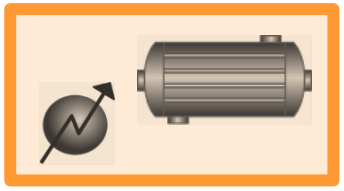
- True **equation-oriented power**
  - Steady state & dynamics
  - Speed of solution
    - sensitivity analysis
  - Convergence of tightly integrated flowsheets
    - multiple recycles, thermal couplings etc.
  - Non-standard specifications
  - Optimisation
    - continuous & discrete decisions
  - Deployment of proprietary libraries & models
  - Custom modelling
  - Export model to web/runtime deployment
- …with **usability**
  - Drag-and-drop flowsheeting
  - Robust solution

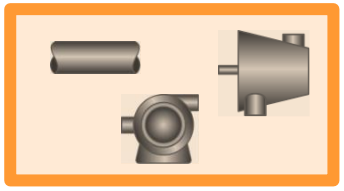
# gPROMS ProcessBuilder v1.0

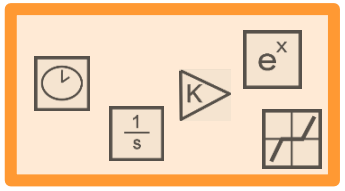
## Content









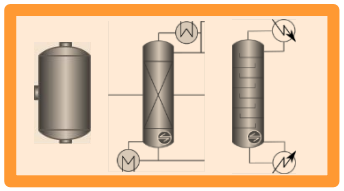

| Separations – Fluid-Fluid | Steady-state | Dynamic |
|---|---|---|
| Component splitter | ☑ | |
| Flash drum | ☑ | ☑ |
| Decanter | ☑ | ☑ |
| 3-phase separator | ☑ | ☑ |
| Distillation column (tray, equilibrium) | ☑ | ☑ |
| Distillation column (packed-bed, HETP) | ☑ | ☑ |
| Distillation column (packed-bed, 1D rate-based) | ☑ | ☑ |
| Distillation column (packed-bed, 2D rate-based) | ☑ | ☑ |
| Distillation column (reactive) | ☑ | ☑ |

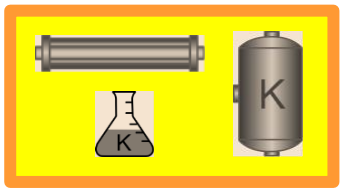
| Separations – Adsorption | Steady-state | Dynamic |
|---|---|---|
| Adsorption bed | | ☑ |
| Schedule for periodic processes (PSA, TSA) | | ☑ |

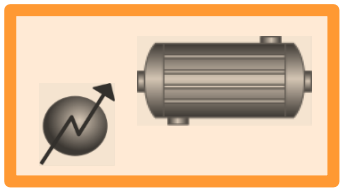
| Separations – Membranes | Steady-state | Dynamic |
|---|---|---|
| Membrane module | ☑ | ☑ |

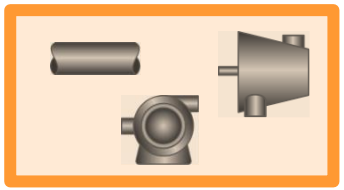
# gPROMS ProcessBuilder v1.0

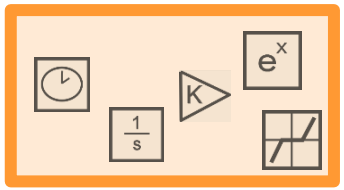
## Content









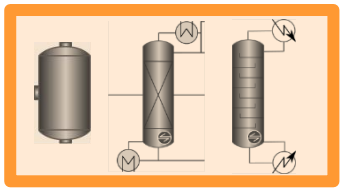

| Separations – Fluid-Fluid | Steady-state | Dynamic |
|---|---|---|
| Compon | | |
| Flash dr | | |
| Decante | | |
| 3-phase | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Separat | | |
| Adsorpt | | |
| Schedul | | |

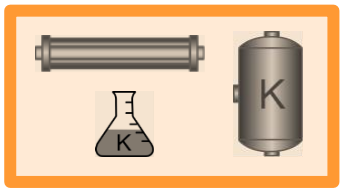
| Reaction | Steady-state | Dynamic |
|---|---|---|
| Conversion reactor | ☑ | |
| Gibbs reactor | ☑ | ☑ |
| CSTR (kinetic & equilibrium reactions) | ☑ | ☑ |
| PFR (kinetic & equilibrium reactions) | ☑ | ☑ |
| Fixed-bed catalytic reactor (1D) | ☑ | ☑ |
| Fixed-bed catalytic reactor (2D) | ☑ | ☑ |
| Fixed-bed catalytic reactor (2D + intra-particle) | ☑ | ☑ |
| | | |
| Reaction mechanisms:<br>▪ Arrhenius<br>▪ Langmuir-Hinshelwood<br>▪ Michaelis-Menten<br>▪ User specified | ☑ | ☑ |

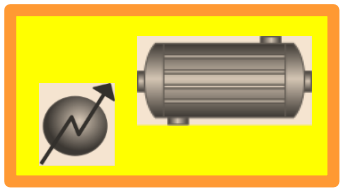
| Separations – Membranes | Steady-state | Dynamic |
|---|---|---|
| Membrane module | ☑ | ☑ |

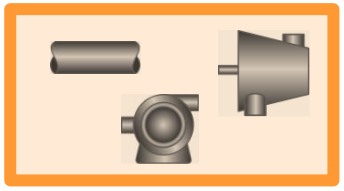
# gPROMS ProcessBuilder v1.0

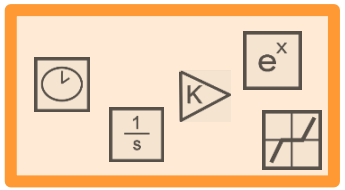
## Content











| Separations – Fluid-Fluid | Steady-state | Dynamic |
|---|---|---|
| Compon | | |
| Flash dr | | |
| Decante | | |
| 3-phase | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Separat | | |
| Adsorpt | | |
| Schedul | | |

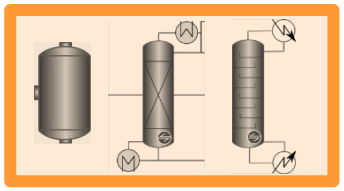
| Reaction | Steady-state | Dynamic |
|---|---|---|
| Conversion reactor | ☑ | |
| Gibbs reactor | | |
| CSTR (kinetic | | |
| PFR (kinetic & | | |
| Fixed-bed cata | | |
| Fixed-bed cata | | |
| Fixed-bed catalytic reactor (2D + intra-particle) | ☑ | ☑ |
| | | |
| Reaction mechanisms:<br>▪ Arrhenius<br>▪ Langmuir-Hinshelwood<br>▪ Michaelis-Menten<br>▪ User specified | ☑ | ☑ |

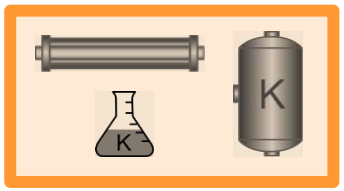
| Heat exchange | Steady-state | Dynamic |
|---|---|---|
| Heater | ☑ | ☑ |
| Cooler | ☑ | ☑ |
| Two-stream heat exchanger | ☑ | ☑ |
| Multi-stream heat exchanger | ☑ | ☑ |

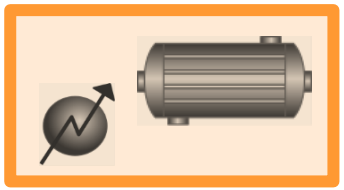
| Separations – Membranes | Steady-state | Dynamic |
|---|---|---|
| Membrane module | ☑ | ☑ |

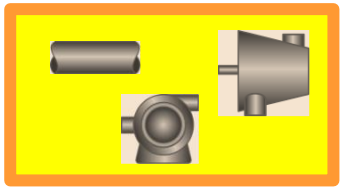
# gPROMS ProcessBuilder v1.0

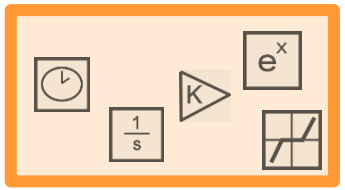
## Content











| Separations – Fluid-Fluid | Steady-state | Dynamic |
|---|---|---|
| Compon | | |
| Flash dr | | |
| Decante | | |
| 3-phase | | |
| Distillati | | |
| Distillati | | |
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| Distillati | | |
| Distillati | | |

| Reaction | Steady-state | Dynamic |
|---|---|---|
| Conversion reactor | ☑ | |
| Gibbs reactor | | |
| CSTR (kinetic | | |
| PFR (kinetic & | | |
| Fixed-bed cata | | |
| Fixed-bed cata | | |
| Fixed-bed catalytic react | | |
| Reaction mechanisms:<br>▪ Arrhenius<br>▪ Langmuir-Hinshelw<br>▪ Michaelis-Menten<br>▪ User specified | ☑ | ☑ |

| Heat exchange | Steady-state | Dynamic |
|---|---|---|
| Heater | ☑ | ☑ |
| Cooler | | |
| Two-stre | | |
| Multi-str | | |

| Flow transportation | Steady-state | Dynamic |
|---|---|---|
| Pipe | ☑ | ☑ |
| Pump | ☑ | ☑ |
| Valve | ☑ | ☑ |

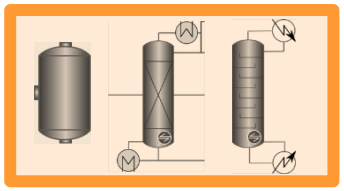
| Separat | |
|---|---|
| Adsorpt | |
| Schedul | |

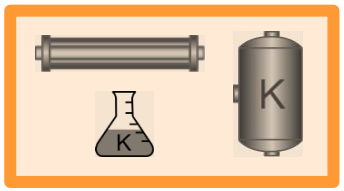
| Compression | Steady-state | Dynamic |
|---|---|---|
| Compressor | ☑ | ☑ |
| Expander | ☑ | ☑ |

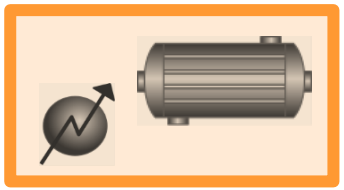
| Separations – Membranes | state | |
|---|---|---|
| Membrane module | ☑ | ☑ |

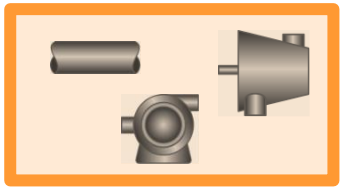
# gPROMS ProcessBuilder v1.0

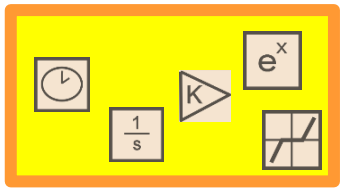
## Content










| Separations – Fluid-Fluid | Steady-state | Dynamic |
|---|---|---|
| Compon | | |
| Flash dr | | |
| Decante | | |
| 3-phase | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |
| Distillati | | |

| Reaction | Steady-state | Dynamic |
|---|---|---|
| Conversion reactor | ☑ | |
| Gibbs reactor | | |
| CSTR (kinetic | | |
| PFR (kinetic & | | |
| Fixed-bed cata | | |
| Fixed-bed cata | | |
| Fixed-bed catalytic react | | |

| Heat exchange | Steady-state | Dynamic |
|---|---|---|
| Heater | ☑ | ☑ |
| Cooler | | |
| Two-stre | | |
| Multi-str | | |

| Flow transportation | Steady-state | Dynamic |
|---|---|---|
| Pipe | ☑ | ☑ |
| Pump | | |
| Valve | | |

| Instrumentation and control | Steady-state | Dynar |
|---|---|---|
| **Controllers**<br>▪ Gain, PID, delays | ☑ | ☑ |
| **Logic**<br>▪ Switches | ☑ | |
| **Linear systems**<br>▪ Transfer function, state-space model | | ☑ |
| **Discrete**<br>▪ Dead zone, hysteresis, saturation | ☑ | ☑ |
| **Mathematics**<br>▪ Functions, basic operations | ☑ | |
| **Signal Sources**<br>▪ Constant, ramp, step signal, function | ☑ | ☑ |

| Separat |
|---|
| Adsorpt |
| Schedul |

Reaction mechanisms:
- Arrhenius
- Langmuir-Hinshelw
- Michaelis-Menten
- User specified

| Compres |
|---|
| Compres |
| Expande |

| Separations – Membranes |
|---|
| Membrane module |

# UNIT OPERATION MODELS

| | Steady-state | Dynamic |
|---|---|---|
| **Separations – Fluid-Fluid** | | |
| **Separations – Adsorption** | | |
| **Separations – Membranes** | | |
| **Reaction** | | |
| **Heat exchange** | | |
| **Flow transportation** | | |
| **Compression** | | |
| **Instrumentation and control** | | |
| **Controllers**<br>▪ Gain, PID, delays | ☑ | ☑ |
| **Logic**<br>▪ Switches | ☑ | |
| **Linear systems** | | ☑ |

- "Basic" models
- "Advanced" models
  - 1d/2d rate-based distillation
  - 2d/3d fixed-bed reactors
  - adsorption
- Focus on
  - engineering content
  - model robustness
    - Model Initialisation Procedures
    - minimal mathematical formulation based on user specifications

# gPROMS ProcessBuilder v1.0

## Content

## UNIT OPERATION MODELS

| | | |
|---|---|---|
| **Separations – Fluid-Fluid** | **Steady-state** | **Dynamic** |
| **Separations – Adsorption** | **Steady-state** | **Dynamic** |
| **Separations – Membranes** | **Steady-state** | **Dynamic** |
| **Reaction** | **Steady-state** | **Dynamic** |
| **Heat exchange** | **Steady-state** | **Dynamic** |
| **Flow transportation** | **Steady-state** | **Dynamic** |
| **Compression** | **Steady-state** | **Dynamic** |
| **Instrumentation and control** | **Steady-state** | **Dynamic** |
| **Controllers**<br>▪ Gain, PID, delays | ☑ | ☑ |
| **Logic**<br>▪ Switches | ☑ | |
| **Linear systems** | | ☑ |

## MATERIAL MODELS

Multiflash

*+ DIPPR databank*

gSAFT

*+ SAFT-VR SW / SAFT-$\gamma$ Mie databanks*

# gPROMS ProcessBuilder v1.0

## Product configuration options

Process Builder

PSE

## UNIT OPE

## RIAL MODELS

| | | | |
|---|---|---|---|
| **Separations – Fluid-Fluid** | gPROMS environment (inc. Case file viewer) | ✓ | |
| | Flowsheet construction & specification | ✓ | |
| | Custom modelling | | ✓ |
| | Simulation (steady-state & dynamic) | ✓ | |
| | Optimisation (steady-state & dynamic) | ✓ | |
| | Parameter estimation | | ✓ |
| | Experiment design | | ✓ |
| | Export to gPROMS Objects | | ✓ |
| | Custom model library management licence | | ✓ |
| | Hybrid Multizonal CFD Inteface | | ✓ |
| **Separations – Adsorption** | **Libraries: ProcessBuilder** | | |
| | gML:Basics, Connectivity, Signal, Flow Transportation, Heat Exchange | ✓ | |
| | gML:Compression | | ✓ |
| | gML:Reaction | | ✓ |
| | gML:Separations - Fluid-Fluid | | ✓ |
| **Separations – Membranes** | gML:Multipack (Compression, Reaction, Separations - Fluid-Fluid) | | ✓ |
| | gML:Separations - Adsorption | | ✓ |
| | gML:Separations - Membranes | | ✓ |
| | AML:Gas-Liquid Contactors | | ✓ |
| | AML:Fixed-Bed Catalytic Reactors | | ✓ |
| | AML:FBCR - FLUENT interface | | ✓ |
| | AML:FBCR - STAR-CD interface | | ✓ |
| **Reaction** | **Physical properties** | | |
| | gSAFT | | ✓ |
| | gPROMS Properties (MS Windows only) | ✓ | |
| | gPROMS Properties - DIPPR | ✓ | |
| **Heat exchange** | | | |
| **Flow transportation** | | | |
| **Compression** | | | |
| **Instrumentation and control** | | | |
| **Controllers**<br>▪ Gain, PID, delays | | | |
| **Logic**<br>▪ Switches | | | |
| **Linear systems** | | | ☑ |

*ltiflash*

*PPR databank*

SAFT

*AFT-VR SW /*

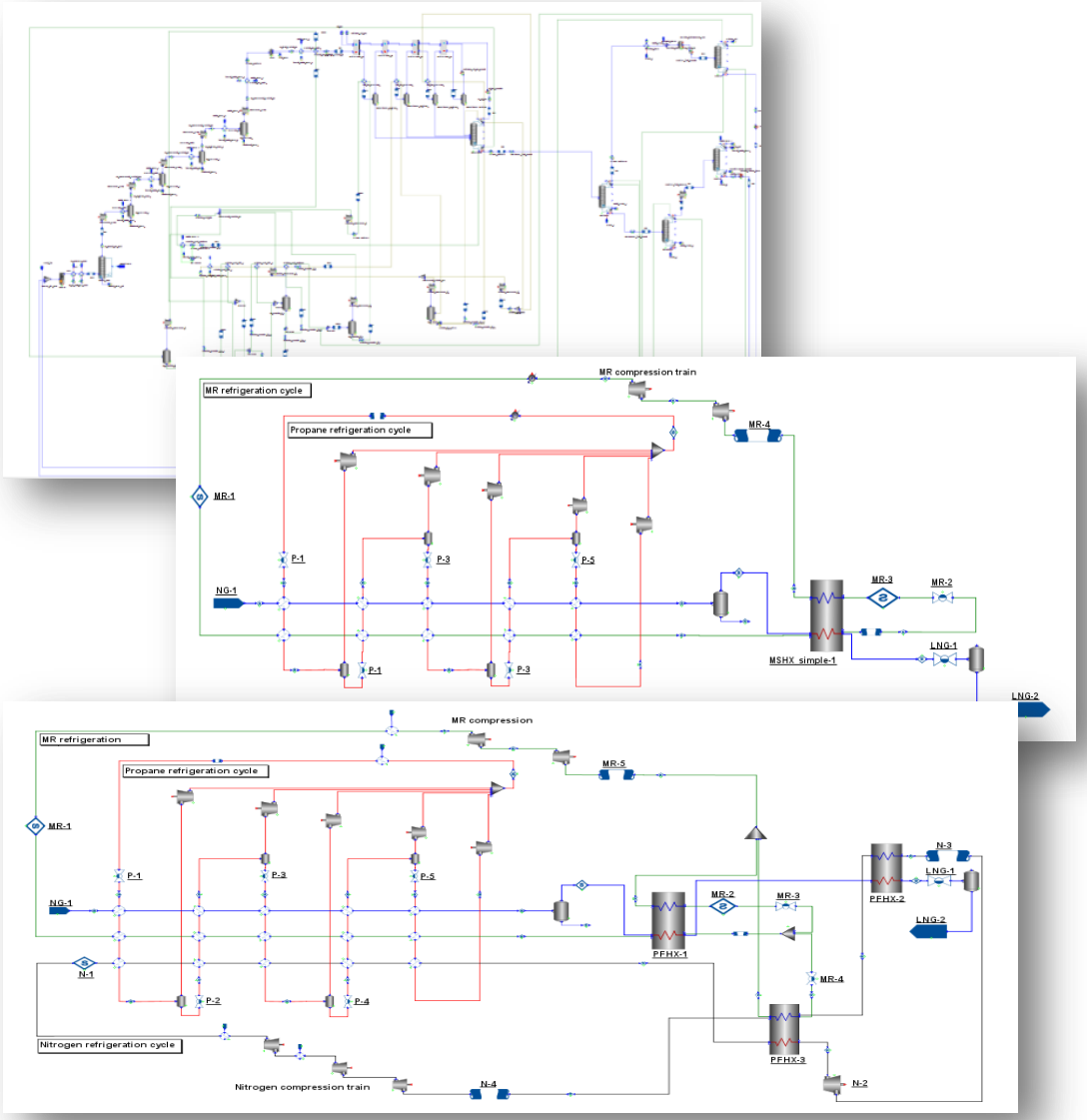
*AFT-γ Mie*

*latabanks*

# gPROMS ModelBuilder v1.0

## Current status

- Unit operation models
  - steady-state elements mostly completed
  - addition of dynamic elements under way
- Application/testing on key processes
  - Olefins
  - Gas processing (NG/LNG)
  - Industrial gases
  - Syngas / hydrogen
  - Batch/reactive distillation
- Ongoing evaluations by selected users
  - migration paths from gPROMS ModelBuilder



# In conclusion…

# Advanced Process Modelling

Getting the most out of past investment

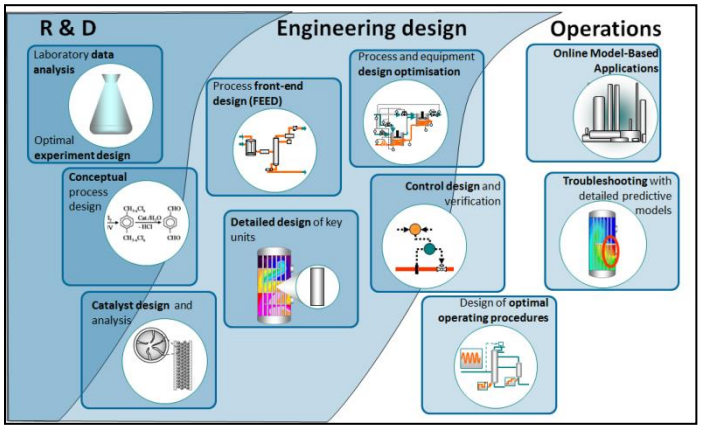
Targeting future investment

Managing innovation

**Managing risk in an uncertain world**

Process Builder

**Major step towards organisation-wide deployment of APM**



ADVANCED PROCESS
MODELLING FORUM **2014**

# Thank you

# gPROMS ModelBuilder v4.0

## Product configuration options

| | | |
|---|---|---|
| **Platform** | | |
| gPROMS environment (inc. Case file viewer) | ✓ | |
| Flowsheet construction & specification | ✓ | |
| Custom modelling | ✓ | |
| Simulation (steady-state & dynamic) | ✓ | |
| Optimisation (steady-state & dynamic) | ✓ | |
| Parameter estimation | ✓ | |
| Experiment design | | ✓ |
| Export to gPROMS Objects | ✓ | |
| Custom model library management licence | | ✓ |
| Hybrid Multizonal CFD Inteface | | ✓ |
| **Physical properties** | | |
| gSAFT | | ✓ |
| gPROMS Properties (MS Windows only) | | ✓ |
| gPROMS Properties - DIPPR | | ✓ |

"gE:Web" - Google Search | PSE: gE:Web — the PSE En

www.psenterprise.com/gproms/enterprise/geweb.html

Company Concepts Sectors Products Services Contact

PSE > gPROMS > enterprise solutions

# gE:Web – Enterprise Web Publishing Solution

## Publish and deploy gPROMS models via the web or intranet

The gPROMS Enterprise Web Publishing Solution makes the power of gPROMS models developed in the gPROMS ModelBuilder and the other members of the gPROMS product family accessible across the enterprise.

It supports all types of gPROMS-based calculations, including steady-state and dynamic simulation and optimisation, and parameter estimation.

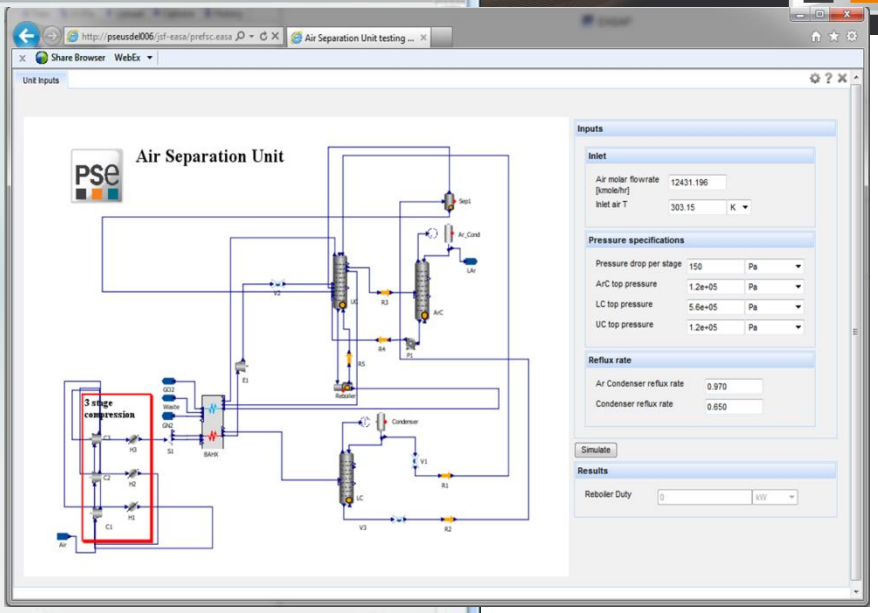
## Why use gE:Web?

The gE:Web solution provides a powerful and convenient way to, for example, allow central R&D or engineering personnel to develop and 'publish' model-based tools for use in supporting day-to-day decisions by operations or purchasing personnel.

Typical use is in applications such as:

- day-to-day plant optimisation of plant operations
- processing of plant data – for example, for data reconciliation and yield accounting
- look-ahead dynamic simulation or optimisation for operating decision support
- support of feedstock purchasing decisions
- catalyst activity monitoring.

## Benefits of gE:Web




## Adding value via gE:Web

- easy re-use of valuable modelling investment
- easy transfer of powerful models between modelling experts and other users
- brings gPROMS model-based decision support to operations or purchasing teams
- deployment of models across the enterprise

## Typical applications

gPROMS product family – 2014

# The gPROMS ProcessBuilder v1.0

## General mathematical modelling

Model Builder

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