Physical properties

Virtually any physprops package

gPROMS® family products are used across virtually all process industry sectors, from cement manufacture to pharmaceuticals to food.

There is no universal physical properties package that can supply all requirements. For this reason PSE's approach is to provide a wide range of optional rigorous physical property packages that cater for different needs.

gPROMS Multiflash properties

Infochem Multiflash, supplied by KBC Advanced Technologies, is the standard gPROMS physical properties package.

Multiflash is a highly rigorous properties package that supports all commonly-used thermodynamic and transport properties, including a wide range of equation of state and activity coefficient thermodynamic models.

Multiflash is specifically designed for equation-orientated modelling, providing tight convergence of internal iterations and analytical partial derivatives with respect to temperature, pressure and composition.

PSE can supply Multiflash with the DIPPR database supplied by the AIChE, providing component data for thousands of components.

OLI electrolyte properties

PSE provides OLI Systems' OLI® electrolyte properties package for aqueous electrolytic systems.

Electrolyte chemistry is particularly complex and challenging to understand and predict, especially for real industrial systems containing many components and operating over broad ranges of temperature, pressure and concentration.

PSE's efficient implementation of the OLI Engine makes it easy to access these properties from gPROMS ModelBuilder® and other gPROMS family products.

CAPE-OPEN physical properties

PSE has strongly supported the CAPE-OPEN initiative and its successor CO-LaN since inception.

gPROMS provides a CAPE-OPEN physical properties socket into which any CAPE-OPEN compliant physical properties package can be plugged – for example Aspentech's Aspen Properties®, PROSIM's SIMULIS® Thermodynamics, Aspentech's COMThermo® and many others.

gSAFT: the future of advanced thermodynamics

Statistical Associating Fluid Theory, or SAFT, is an advanced molecular thermodynamic method that can predict a wide variety of thermodynamic properties of mixtures accurately based on physically-realistic models of molecules and their interactions with other molecules.

PSE has implemented the SAFT-VR and the SAFT-γ Mie group contribution methods developed at Imperial College London in the gSAFT® product. gSAFT is currently being supplied to lead customers by special arrangement.

Proprietary physical property packages

gPROMS provides a general open interface for interfacing of external property and thermodynamic tools.

Virtually any physical properties package can be interfaced to gPROMS with a few days' effort.

More Information

Physical properties

- gSAFT
- Physical properties

gPROMS overview

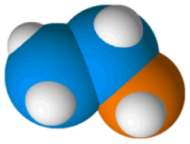
- gPROMS home
- gPROMS Objects

INFOCHEM Multiflash

- comprehensive
- high-accuracy
- industry-standard
- designed for advanced modelling environments

CO-LaN Associate Member

gSAFT: Find out more ...



Did you know?

gPROMS models can call Aspen Properties® via the CAPE-OPEN interface

gPROMS activities: Global system analysis

Rapid and effective exploration of the process decision space

The main use of process simulation and modelling tools is to analyse "what-if" scenarios in order to improve process design and operation. Currently this is done manually as a point activity, using repeated simulation runs.

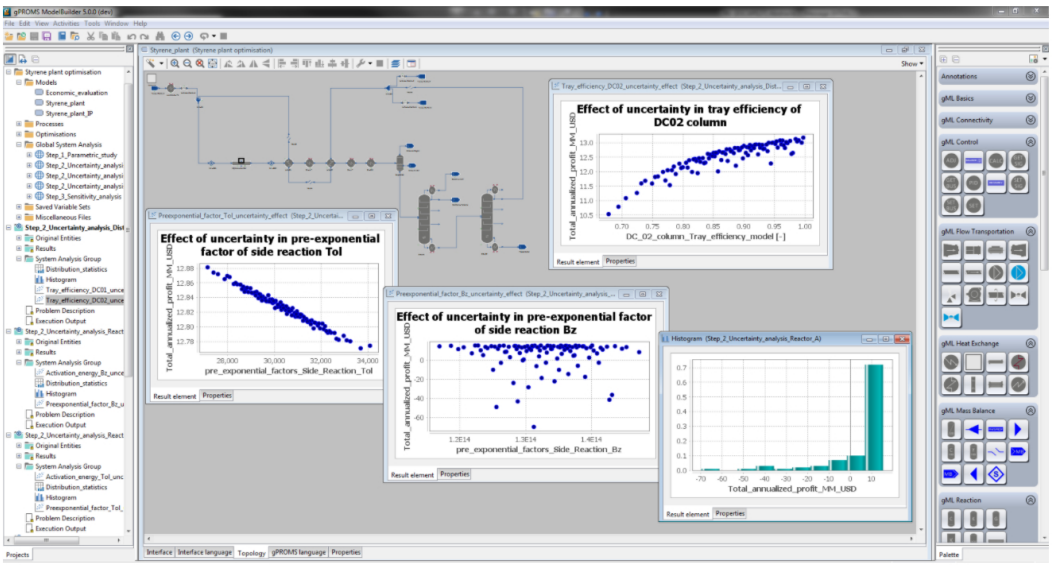
Global systems analysis (GSA) allows the comprehensive exploration of the behaviour of a system over domains of any user-selected subset of its input variables ('factors'), and output variables ('responses').

This provides a quick, easy and systematic way to explore the complex process design and operational decision space using high-fidelity models.

How does it work?

GSA can be applied very easily to any gPROMS model. The gPROMS ProcessBuilder screenshot below shows some results of GSA applied to the design of a styrene monomer plant.

In this example, the effect of uncertainty in the reaction kinetics and the tray efficiencies on the total annual profit of the plant was quantified.



To start, the user chooses:

- any subset of the model input variables ('factors'). These may include external disturbances, control actions and model parameters such as reaction kinetic constants. The factors may vary over domains specified in terms of lower and upper bounds. They may be deterministic or probabilistic, in the latter case their variation being described in terms of univariate or multivariate probability distributions.
- the output variables of interest ('responses'). These are typically key performance indicators (KPIs) that are of critical interest for plant design or operation.

Having selected factors and output variables of interest the model is then executed hundreds or even thousands of times, depending on the analysis. The results are then presented in a variety of ways, allowing easy understanding on the influence of factors on the responses.

What are the benefits?

Key benefits of GSA are the ability to perform sensitivity analysis and uncertainty quantification on complex process systems in a systematic and highly efficient manner.

This allows rapid and effective exploration of the process design and operational decision space, with rapid screening and ranking of alternatives.

More about GSA ...

More Information

gPROMS overview

- gPROMS home
- The gPROMS platform
- gPROMS ProcessBuilder
- gPROMS FormulatedProducts
- gPROMS ModelBuilder
- gPROMS Digital Applications Platform
- gPROMS Web Applications Platform

gPROMS platform capabilities

- Platform overview
- Custom modelling
- Parameter estimation
- Optimization
- Global system analysis
- Physical properties
- Hybrid Multizonal CFD

GSA can be applied to any gPROMS model very easily, irrespective of the model size or complexity. The GSA implementation:

- employs efficient techniques for sampling the input space based on low-discrepancy sequences
- is designed for deployment on distributed computing hardware
- has built-in resilience, e.g. in terms of being able to deal with failure of individual samples
- computes important aspects of responses such as measures of their probability distributions and their global sensitivity indices with respect to the input factors.
- incorporates extensive facilities for visualising and analysing the results

Availability

GSA is available as an option in gPROMS FormulatedProducts and gPROMS ProcessBuilder.