



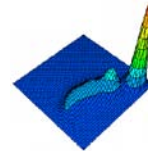
# Mathematical modelling power for Engineers and Scientists

PSE's gPROMS was developed originally at Imperial College London for solving large and complex process systems using *first-principles models of system physics and chemistry*.

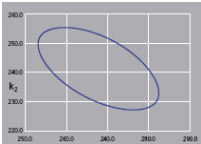
However gPROMS has evolved to be much more than just a process modelling tool. It can be used to solve large sets of differential and algebraic equations in many different contexts.

## Do you need to:

... solve large-scale equation systems?



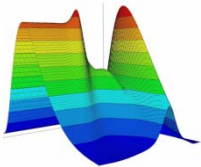
... estimate parameters from experimental data?



... work with ODE and partial differential systems?

$$\frac{\partial C_1}{\partial t} = -v \frac{\partial C_1}{\partial z} + D_z \frac{\partial^2 C_1}{\partial z^2} + D$$

... concentrate on physics, avoid programming?



## The gPROMS advantage

gPROMS has a number of key advantages as a modelling environment for scientific research. Here are just some:

*“Multiple applications:  
simulation, optimisation,  
parameter estimation”*

*“gPROMS physics and  
chemistry models link to  
CFD in six different ways”*



- gPROMS is an **equation-oriented, simultaneous solution** environment. No **programming is required**: users enter first-principles relationships as equations. gPROMS takes care of the solution automatically.
- The powerful modelling language caters for **lumped and distributed systems** (size, spatial, residence time). gPROMS can solve systems involving 1m+ equations.
- The same model can be used for **multiple applications**: simulation, optimisation parameter estimation, in steady-state or dynamic (transient) mode.
- Powerful **model-based data analysis tools** allow model parameters to be estimated from experimental data, and provide information for quantitative risk management.
- **Model-based experiment design** techniques can be used to minimise experiment time and cost while maximising information from each experiment.
- Comprehensive **QA facilities** ensue that the all-critical numbers used in design and optimisation are auditable at any time.
- gPROMS physics and chemistry models **can link to CFD** hydrodynamic models in six different ways.

**Project environment**

Easy creation of custom models and own connection types

Easily-maintainable corporate model libraries

Equipment palettes for quick access to library models

**Multiple activities using same model: simulation, parameter estimation, optimisation and experiment design**

Easy incorporation of laboratory and pilot data into first-principles models

Drag-and-drop flowsheeting

Auto-complete and syntax checking

**Comprehensive results management facilities**

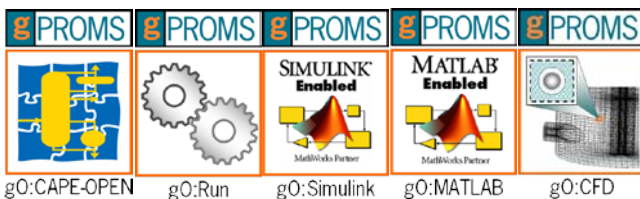
Comprehensive Quality Assurance tools for reliable, auditable data

Open architecture – easy links to external software

Interchangeable graphic and gPROMS language views maintained fully consistent at all times

**Export models**

Execution in external software environments on behind Excel or VB interface



**Powerful modelling language**

- Lumped and distributed systems
- Flexible case and conditional structures
- Full array handling with parameter propagation
- Easy calls to external software (e.g. physprops)
- Integro-Partial Differential Algebraic Equation (IPDAE) formulation for complete modelling power
- Modelling of large-scale systems (1m+ equations)
- Easily maintainable and auditable

**Links to CFD**

Six different ways to link CFD and gPROMS models

**Advanced model libraries**

For fixed-bed catalytic reaction, solution crystallisation, gas-liquid contacting and fuel cells

