

Advanced Process Modelling examples

Better, faster, safer decisions in all areas of the process industries

gPROMS®'s high-fidelity predictive modelling capabilities are applied to a wide range of design and operational challenges in many different industry sectors.

Typical examples of Advanced Process Modelling used for model-based innovation and model-based engineering – some performed by the customer, some by PSE Consulting – are listed below.

In virtually all cases, they have resulted directly in *significant savings* or *enhanced revenue*, or *accelerated innovation and development*. In many cases they have resulted in *new understanding of the fundamental phenomena*, allowing for informed decision making that results in *better design* and *better operation*.

Process design

- **Whole-plant optimization of a new propylene oxide process**
Simultaneous optimization of reactor and separation sections to achieve tens of millions of Euros' improvement in process economics. See Hydrocarbon Processing article €€€ savings. [Repso]
- **Design of falling-film sulphonation reactor**
Determined optimal reactor design, operating conditions and start-up procedure to minimise off-colour product and reduce cleaning frequency. \$\$ savings. [US consumer goods manufacturer]
- **Design of new multitubular reactor for petrochemical process**
New design for reactor shell and optimal utilisation of catalyst. First design to achieve uniform yield from all tubes in multitubular arrangement; performed own detailed design and saved significant costs on reactor. [LG Chem, Ltd]
- **Design of optimal multitubular reactor for terephthaldehyde production**
See Hydrocarbon Processing article. [LG Chem, Ltd]
- **Design of new membrane separations**
Developed an easy-to-use tool for the client's engineers to be able to rapidly assess new gas separation designs, with the resulting gPROMS model incorporated in Hysys. [US industrial gases process licensor]
- **Design of new continuous and batch processes for production of norbornene and tetracyclododecene**. Designed plant that can reliably process wide range of feedstocks, varying in proportion of the two main products (from 1:5 to 5:1); \$\$ revenue enhancement. [Japanese petrochemicals producer]
- **Optimal design of licensed large-scale industrial crystallization process**
Developed high-accuracy models to enable process licensor to optimize the design of a licensed large-scale industrial crystallization process, for enhanced process economics. [BP Chemicals]
- **Distillation of ethanol/water mixtures with the use of entrainers**
Optimized process and selected best entrainer for required task. [US petrochemicals producer]
- **Design of Heat Integrated Distillation Columns (HIDiC)**
Designed new distillation column which can run without reboiler, demonstrating 60% overall energy savings. [Japanese petrochemicals producer]
- **Design and operation of new pharmaceutical reactor**
Guided experimental programme for the identification of complex chemistry, then used resulting data for design of new reactor with improved mixing and mass transfer. Derived new batch operating procedure to minimise side reactions and impurities. [UK/Italian pharmaceutical manufacturer]
- **Design of novel multitubular reactor for Fischer-Tropsch production of designer diesel**. Detailed AML:FBCR kinetic model linked to a CFD model of the shell side fluid dynamics proved the design without the need to build a pilot plant, saving \$250K. [US technology company]

Equipment design

- **Design of novel multitubular reactor for maleic anhydride**
New reactor design with improved yield and selectivity currently under patent application. [US petrochemicals producer]
- **Desulphurisation of flue gases**
Designed new desulphurisation equipment an optimized operating conditions to ensure maximum removal of sulphur in order to comply with anti-pollution laws. [Chilean plant equipment manufacturer]
- **Design of liquefied natural gas (LNG) storage tanks**
Provided detailed loading/unloading dynamic models of LNG storage tanks to achieve \$\$ savings on compression equipment and energy use. [UK oil & gas supplier]
- **Design of new depressurisation vessel for African offshore oilfield**
Demonstrated that the use of expensive alloy was necessary for only small part of the vessel, saving \$1.5m in construction costs. [BP]
- **Crystallization in in-line mixing equipment**
Studied particle size distribution formed in complex, non-standard crystallization device, aimed at achieving enhanced product quality

More Information

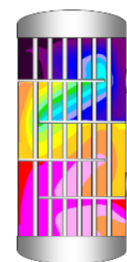
In this section

- [APM overview](#)
- [How does it work?](#)
- [Digitalization](#)
- [Digital process design](#)
- [Digital process operations](#)
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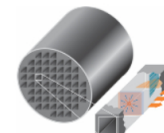
See also

- [Model-based engineering](#)
- [Model-based innovation](#)
- [Model-targeted experimentation](#)

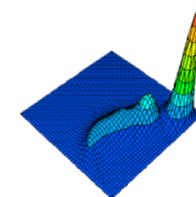
“ The hybrid gPROMS-Fluent model we built with PSE of our multitubular reactor gave us perfect insight into the internal working of the process
DR SANG PHIL HAN LG CHEM, LTD ”



From model to metal: model-based engineering design of a multitubular reactor



Monolith reactor for fuel processing (fuel cells)



Concentration profiles in a pulsed reactor

and consistency. [US consumer goods manufacturer]

- **Development of optimal fibre production**, involving detailed design of bushing equipment. [US glass fibre manufacturer]

Process development

- **Development of new process for methyl ethyl ketone (MEK)**

Analysed data from lab scale equipment to identify true reaction kinetics, which were then used in the design of full-scale process including novel gas/solid contacting device. Company now has own process [Japanese petrochemicals producer]

- **Development of low-cost process alternative for bis-phenol A production**

Developed design based on low-cost multitubular falling-film evaporator to replace large, expensive and difficult-to-operate scraped-surface vessel in a licensed chemical process resulting in \$\$\$ saving and simplified maintenance. [Japanese chemical company]

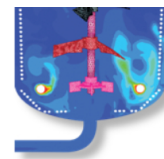
- **Development of reforming microreactor**

Used high-accuracy model of microreactor using microkinetic and diffusion modelling to drive model-targeted experimentation to determine detailed reforming kinetics. Development accelerated significantly. [BP Chemicals]

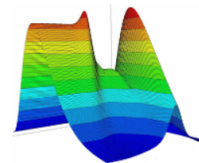
- **Design and development of hydrogenation reactor**

Applied MBI techniques in design of reactor for unsteady state operations with potentially central role in Japanese hydrogen economy. [Japanese chemical company]

- **Development of new types of storage tanks for liquefied natural gas (LNG)**. Guided the experimental programme to assess the viability of these new designs, thereby reducing the number and cost of experiments by an order of magnitude. [UK oil & gas supplier]



35% reduction in batch co-polymerisation time



Start-up size distribution for crystallizer

Process operations

- **Optimization of dioctyl phthalate (DOP) processes**

Optimized recipe for existing plant, resulting in doubling of profit margin. Designed new batch plants (including new operating recipe) for construction in various Asian countries, as well as designs for continuous plant to replace batch plant. [Japanese petrochemicals producer]

- **Optimization of catalyst change-over frequency**

Determined optimal frequency for multiple-reactor styrene monomer production unit, resulting in new set of optimized operating procedures [Shell Chemicals]

- **Optimization of methanol plant catalyst lifetime**

Optimized methanol plant operating conditions for maximum catalyst life, with simultaneous optimization of catalyst formulation. See Hydrocarbon Processing article [Süd-Chemie]

- **Reduced batch time for batch crystallizer**

Optimized recipe for batch crystallization for pharmaceutical-grade lactose, identifying 44% reduction in batch time for same quality product. [Friesland Campina]

- **Optimal operation of crystallizer**

Derived optimal recipe for batch crystallizer, leading to much narrower particle size distribution and hence significant improvements in downstream solids handling leading allowing an increase in production. [UK pharmaceutical manufacturer]

- **Safety analysis of distillation column startup**

Performed highly detailed analysis of events involved in major industrial accident, resulting in identification key factors leading to the accident. [US refinery operator]

- **Start-up of air separation units**

Optimized start-up procedure for 3-column air separation plant, with model subsequently used in operator training system. [Japanese industrial gases supplier]

- **Batch polymerisation 35% improvement in batch time**

Achieved 35% improvement in batch time for complex batch polymerisation process. [UK polymer additives manufacturer]

- **Optimization of expandable polystyrene (EPS) production**

Optimized batch recipe identifying 30% reduction in processing time with no change in product quality. [BASF]

- **Removal of CO2 from hydrocarbon streams using reactive absorption**

Optimized column operation, including utilisation of caustic soda and pumparounds, with accurate prediction of product composition down to ppb levels using advanced rate-based separation models. [Linde Engineering]

- **Multistream heat exchanger modelling**

Developed general model of multistream heat exchanger for use in operator training; development time reduced from envisaged 6 months to 15 days. [Honeywell Process Solutions]

- **Optimization of heap leaching operations**

Provided detailed modelling of leaching operations for use in operational improvements. \$\$ energy savings [Chilean minerals company]

- **Optimization of grade transitions in polyethylene**

Derived optimal policies from switching from one grade of polymer to another, while reducing the off-specification product by more than 60%. Savings in time equivalent to 1 week's extra production per year. [Norwegian petrochemicals producer]

- **Crystallization of bisphenol-A**

Troubleshooting and startup optimization of large-scale multi-unit industrial crystallization process to obtain required crystal size distribution, resulting in benefits of millions of dollars annually in additional on-spec product, enhanced throughput and reduced energy cost. [Japanese petrochemicals producer]

- **Removal of volatiles from polymer particles**

Optimized operating conditions to ensure maximum removal of volatiles in column. [US petrochemical producer]

- **Development of optimal control scheme for azeotropic distillation unit**

Developed scheme that resolved long-term problems in controllability encountered over years of operation. [Shell Chemicals]

- **Development of economically optimal design for azeotropic distillation unit**

Redesigned the same unit, identifying around half a million dollars per annum saving. [Shell Chemicals]

Product design and development

- **Design of cardboard boxes for detergent powders**

Used detailed diffusion models to study permeation of moisture from air into boxes, and recommended changes in box design and thickness. [US consumer goods manufacturer]

■ **Design of SOFC fuel cells**

Detailed design of the fuel cell, the fuel cell stack and the fuel preparation sub-system. *[UK fuel cells developer]*

■ **Design of PEM fuel cells**

Detailed design of the fuel cell and the fuel cell stack. *[Many US & Japanese fuel cells developers]*

■ **Provision of decision support for many aspects of fuel cell component and system design** *[Toyota, Samsung, Mitsubishi Heavy Industries, Ceres Power, others]*

There are many, many more applications in many application areas where PSE or our customers have applied Model-Based Innovation or Model-Based Engineering techniques to great benefit. Please contact us for more details.

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