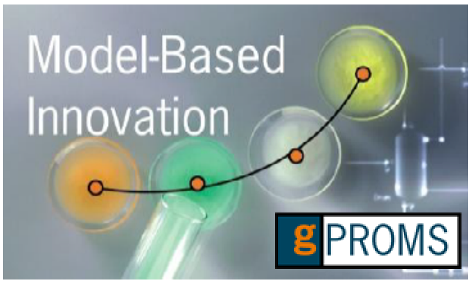



# Typical applications in brief

## Chemical Process Industries

**Model-Based Innovation is systematically used for:**

- *Design of new reactors*
- *Design of new catalysts*
- *Scale-up of complex operations such as crystallisation*
- *Development of new technologies such as fuel cells*
- *Reducing pilot plant testing*
- *Reducing R&D costs and time*

Model-Based Innovation combines high-fidelity models of processes or products with modern R&D methodologies to provide *high-quality information* for *innovation decision support*, thus allowing companies to manage risk based on accurate quantitative information.

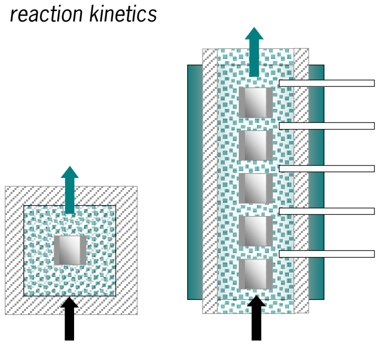
The result is faster innovation, improved designs of processes and products, enhancement of existing operations and more effective R&D programmes.

### Why Model-Based Innovation rather than just "modelling"?

Some applications of MBI – such as the HiDiC example below – involve simply using modelling to reduce innovation risk. However, full Model-Based Innovation uses special techniques such as *model-based experiment experimentation* to ensure that process design and R&D activity are formally related through a modelling framework. This brings benefits in both directions, and results in accelerated innovation and more cost-effective – and time-effective – R&D[1].

### Example #1 – Design of a novel acrylic acid reactor

*Single and multi-pellet model-targeted experiments to determine accurate reaction kinetics*



PSE worked closely with LG Chem, Ltd, Korea's largest chemical manufacturer, using Model-Based Innovation techniques to design a novel reactor/catalyst configuration for an Acrylic Acid process.

First, PSE provided a high-fidelity reactor model constructed using the gPROMS Advanced Model Library for Fixed-Bed Catalytic Reactors (AML:FBCR). This was linked to LG Chem's existing Fluent CFD model of the shell side geometry.

Then PSE Consultants directed the "model-targeted" experimental program within LG Chem's labs to determine high-accuracy values for reaction kinetics and key process parameters such as bed conductivity. This resulted in a model with an extremely high degree of predictive accuracy.


The model was then used to develop catalyst profiles that would give uniform temperatures and concentrations across the reactor, resulting in significantly improved performance and overall stability.

As a consequence LG Chem were able to finalise the detailed design themselves at a considerable cost saving. Equally important, the company has now entered the market as one of the world's four companies with their own Acrylic Acid technology.

The new investment is particularly noteworthy, as LG Chem will be using its own developed production technology. LG Chem's new process is an enhanced technology that improves the production efficiency and stability through a new reaction system and innovative purification technique.

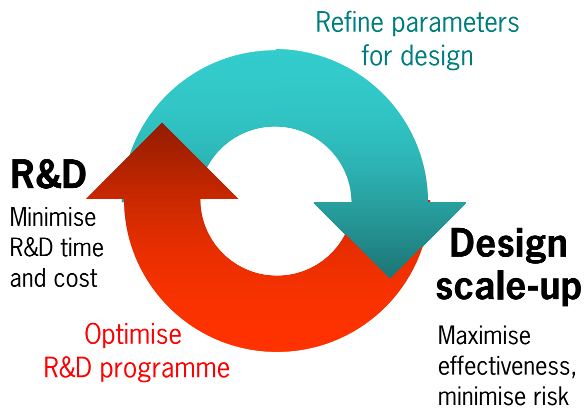
Other than LG Chem, only three major chemical companies such as Nippon Shokubai Co. Ltd., BASF and Mitsubishi Chemical Corp. have their own technology to produce acrylic acid.

*With acknowledgment to LG Chem, Ltd.*

[1] See the brochure "Model-Based Innovation – concepts" for more information.

## Example #2 – Reliable, confident scale-up of crystallisation processes

Crystallisation processes are notoriously difficult to scale up. For instance, an approach that produces coarse crystals on a small scale in the lab may produce fine crystals in industrial-scale equipment, leading to poor filterability and hence a reduced production capacity. How do you design a new crystalliser that can be guaranteed to work?



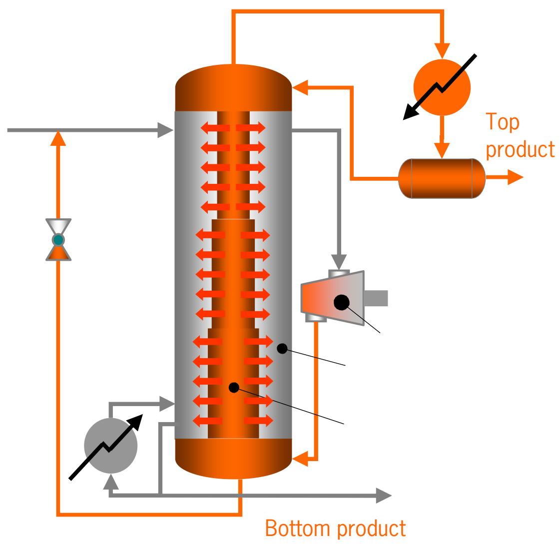

The answer – as with design of any equipment – is to take into account all relevant phenomena in the design. In the case of crystallisation this involves many experimentally-determined parameters (e.g. nucleation and growth rates) coupled with solution of population balance relationships.

Crystallisation is one of the areas that benefits most from Model-Based Innovation techniques. For example, models of lab-scale equipment can be used with *Model-Based Experiment Design* techniques to design of the optimal set of experiments.This maximises the information content of experimental results while while minimising time and cost of experimentation, leading to optimal product performance and process behaviour.

*By coupling the R&D and design processes, R&D time can be minimised and design made much more effective*

PSE regularly works with companies to accelerate their innovation in crystallisation process design and operation, from industrial scale processes for compounds such as terepththalic acid, bis-phenol A or sucrose to much smaller-scale pharmaceutical operations. These techniques have been successfully applied in companies such as Mitsubishi Chemical, BP Chemicals, PURAC, Danisco and SQM Nitratos.

## Example #3 – UP TO 60% energy saving with novel distillation techniques




*HIDIC concentric tube column*

Heat-Integrated Distillation Columns (HIDiCs) can save up to 60% of the energy used for distillation, itself some 40% of the total energy used in the process industries.

However HIDiCs are yet not widely implemented. Why not? The reason is that, because of the difficulty in verifying that a design will start up and operate correctly, there is a high perceived degree of risk associated with their implementation.

Modelling provides an ideal way to minimise the risk of implementation. It enables companies to verify designs and establish safe and viable operating envelopes, to optimise safe and effective start-up procedures, to design control schemes that maximise operational flexibility, and many more.

It also helps to accelerate implementation, and, once the column is operational, provides a means to troubleshoot any operational problems.

*HIDiCs are not yet widely implemented in the process industries. Why not?*

PSE's work with a leading Japanese government research organisation has demonstrated the power of the model-based approach to HIDiC implementation.