gPROMS Concepts

Model-Based Innovation

Effective risk management through modelling

MBI answers …

Application of Model-Based Innovation can help answer questions such as these:

- *"Should I spend my $250K budget on transport property research or a pilot plant to determine reaction rates"*
- *"How can we cut the experimentation phase from six months to three months?"*
- *"How does the uncertainty in our reaction data affect the flare stack design margins?"*
- *"Can we avoid constructing a costly pilot facility?"*
- *"How do we guarantee that the scaled-up process will work?"*

One of the key applications for PSE's gPROMS Advanced Process Modelling (APM) environment is Model-based Innovation (MBI), a relatively new technology enabled by significant advances in modelling technology over the last decade.

Model-Based Innovation involves combining high-accuracy models of process or products with modern innovation methodologies to provide high-quality information for innovation decision support. This helps companies to manage risk in innovation, design and operational enhancement based on accurate quantitative information.

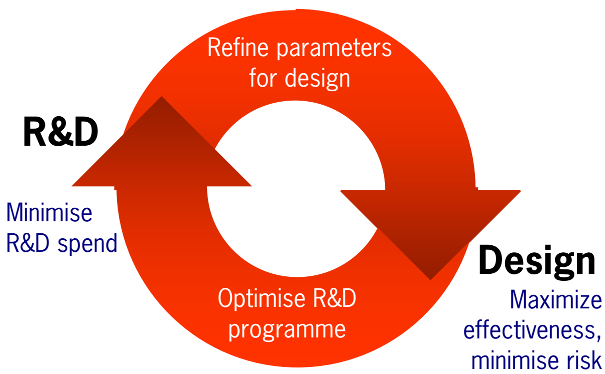
The result is faster innovation, improved designs of processes and products, enhancement of existing operations and more effective R&D programmes.

PSE's ModelCare® Model-Based Innovation service covers all process industry sectors, and can be applied from laboratory R&D, through process and detailed design, to online operation. *In fact, MBI is a key mechanism for integrating R&D, design and operational activities, to achieve mutually beneficial objectives.*

The benefits of Model-Based Innovation

The application of MBI can result in significant competitive advantage through modelling, as outlined above. Some specific benefits are:

- **effective risk management**. Modelling provides *quantitative data* on which to base R&D and design decisions, allowing you to manage risk with confidence.
- **fast screening of alternatives**. Modelling quickly shows you which alternatives to discard and which to pursue.
- **streamlining of experimental programmes.** Model-based experiment design can reduce time and cost of experimentation *significantly*.
- **direction of Research & Development spending**. The information generated by MBI techniques can be used to rank R&D investment alternatives by value.
- understanding the relationship between **experimental uncertainty and design margin** (see overleaf)
- availability of **accurate validated models for design**, leading to effective and accurate process or product design right from the research stage.



"MBI is a key mechanism for integrating R&D, design and operational activities, to achieve mutually beneficial objectives"

PSE's ModelCare

PSE's ModelCare service is designed to help companies innovate rapidly with relatively low investment and fast payback. A key aim of ModelCare is to transfer MBI know-how to customers to help them build their own capability.

Model-Based Innovation methodology: three messages

New technology and approaches are the reason that Model-Based Innovation is emerging as a key technology:

1. Modelling technology has come of age

Advanced Process Modelling tools and methodologies now enable modelling of many types of complex process, products or equipment – from detailed reactor systems to pills delivering drugs in the human body – to sufficient accuracy to support real innovation in design and operation; hybrid “APM – CFD” methodologies now allow investigation of detailed effects of equipment geometry on the behaviour of complex processes, enabling accurate scale up; models can now be used directly for rigorous optimisation of design and operating conditions, without the need for trial-and-error simulations.

2: Modelling and experimentation can be closely coupled

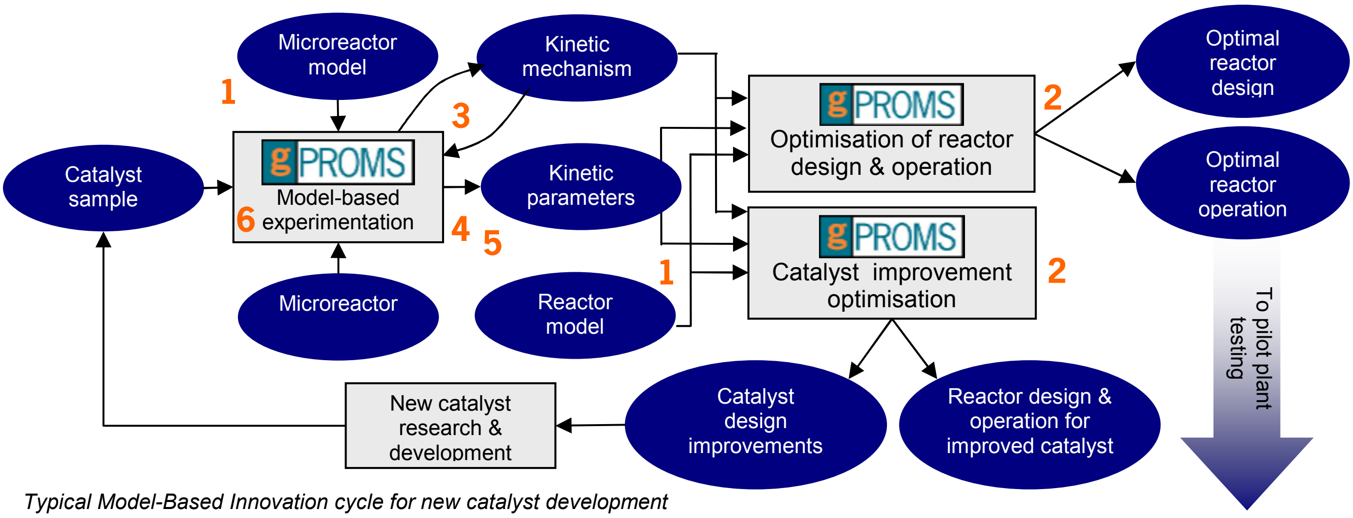
As shown below for the design of a new catalyst, increasingly modelling **[1]**, optimisation **[2]** and experimentation are being combined, using: **model-targeted experimentation,** where the purpose of experiments is to *derive an accurate model* **[3]** *or model parameters***[4]**; model-based **analysis of experimental data[5],** using models coupled with sophisticated parameter estimation capabilities to generate parameter and confidence information; **model-based experimentation [6],** to minimise the number of experiments and maximise the accuracy of the estimated parameters.

What are model parameters and why are they important?

Parameters are the empirical values found in any design calculation, such heat transfer coefficients and reaction kinetic constants. Their values are usually derived from laboratory, pilot plant or operational measurements.

The value of a parameter can have a critical effect on a design. The more accurate the parameters, the more accurate the design, and the lower the risk and capital and operating costs.

Virtually the entire experimentation process is aimed at establishing parameter values. In modelling, this process is called **model validation**.



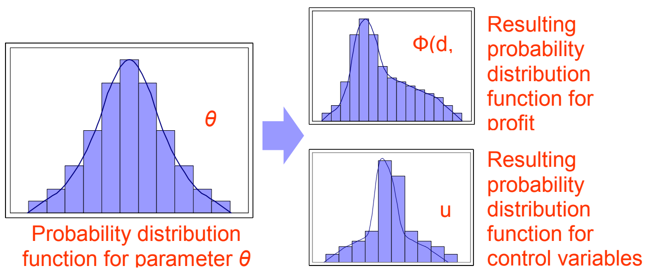
Typical Model-Based Innovation cycle for new catalyst development

3: Modelling can establish a quantitative link between uncertainty and risk

Even formally validated models are still subject to uncertainty in their parameter values. It is important to be able to map this uncertainty to uncertainty in Key Performance Indicators (KPIs) of the process, to allow a trade-off between research and risk.

All parameters are uncertain, but not all of them are critical. Some parameters may have a small effect on KPIs; uncertainty in other parameters may be counteracted by control actions. Models can help establish the **quantitative relationship** between fundamental R&D uncertainty in process development and technological risk during process operation.

By establishing which parameters affect KPIs most, research investment can be directed towards the most critical parameters.



How probability distribution for a parameter translates into profitability and controllability distributions.