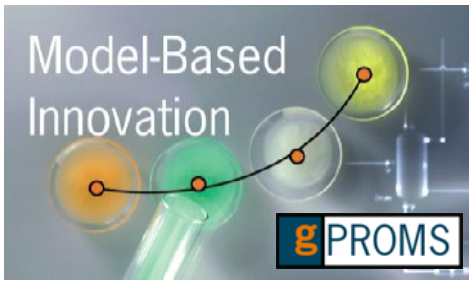


Model-Based Innovation

Concepts & technologies

MBI can be applied to virtually any process context …

- *MBI techniques have been applied extensively in **crystallisation** processes, where scale-up is difficult.*
- *MBI is widely used in emerging technologies such as **fuel cell** development, where time-to-market is critical.*
- *MBI is an ideal approach to designing or selecting **new catalysts**.*
- *Virtually all **reactor** or **reaction system** design can benefit from MBI.*

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.

What does Model-Based Innovation involve?

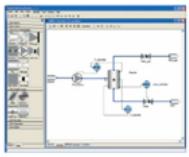
At the core of MBI is Advanced Process Modelling (APM) technology such as PSE's gPROMS, which allows the easy construction and solution of detailed mathematical models of any process, from a simple laboratory stirred-tank reactor to a full-scale industrial plant.

APM techniques such as model validation and experiment design are then applied within well-defined methodologies for model-based experimentation, scale-up, process synthesis and design optimisation, to provide *optimal process, product and equipment designs*.

This document describes how model-based experimentation (shown in the diagram below) is a key technology for integrating R&D with design and operational activities.

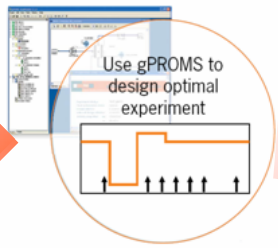
Model-Based Experimentation

Used to generate maximum information from minimum experimentation



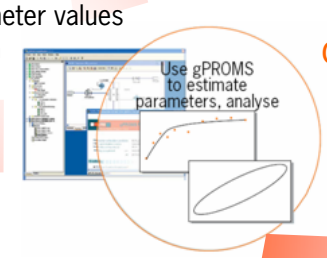
Model-based experiment design

Optimisation techniques are applied to models of experiment to design *optimal* experiments



Model-based data analysis

Model of experiment used to analyse data, and determine parameter values and confidence information



The experiment design cycle

Model-targeted experimentation

Objective is to obtain high-accuracy design parameters with quantified confidence intervals for design models

Actual experiments

Performed according to instructions generated by model-based experiment design

The model company

Model-Based Experimentation explained

Model-Based Experimentation is an experimentation methodology centred on the use of a detailed (mathematical) model of the experimental equipment and physics and chemistry. The model provides the means to *analyse data* from the experiment, to *capture the information* acquired in usable form, then to use that information to *optimise the experimental process* itself.

Model-targeted experimentation

Most experimentation work performed in an MBI context is *model-targeted experimentation*, where the purpose of the experiments is not to optimise any aspect of the equipment or process, but to derive the most accurate possible model. The model is then used for optimisation of many aspects of the design.

A well-designed model-targeted experiment will involve well-defined conditions, such as perfect mixing and isothermal conditions. This helps to simplify construction of models and means that parameters will be valid for scale-up.

Model-supported micro-experimentation. This is a fundamental activity in, for example, new catalyst design, where reaction on single or small numbers of catalyst particles is studied under well-defined conditions. Model-based analysis is then applied to determine kinetic parameters and their associated confidence intervals. This results in highly accurate model parameters for use in optimisation of industrial-scale design.

Model-based experiment design uses the model of the experiment and optimisation techniques to minimise the number and cost of experiments. By ensuring that each experiment generates the maximum amount of information, the accuracy of parameters being estimated is maximised.

Model-based analysis of experimental data. The detailed model of the experimental rig can be used for parameter estimation, to generate both accurate parameters and confidence information from the experimental data. The confidence data can be used in formal risk analysis using state-of-the-art techniques.

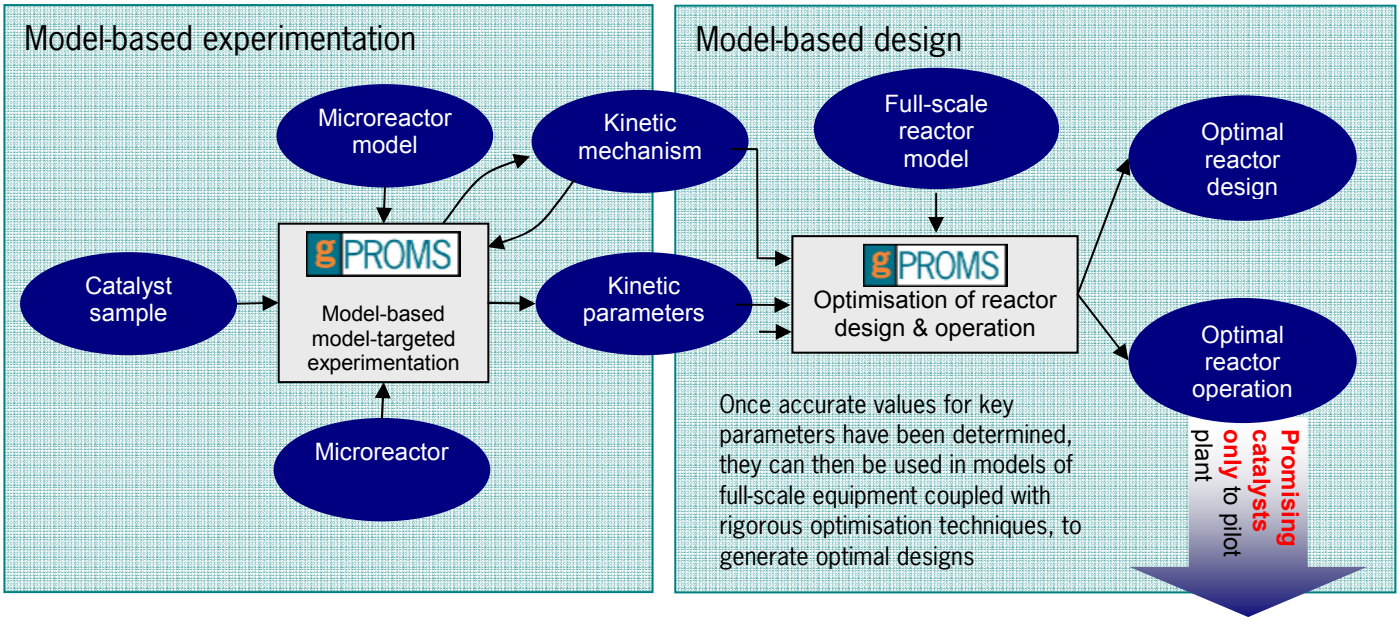
Advanced Process Modelling (APM)

APM tools and methodologies are at the heart of MBI.

These now allow modelling of many types of complex process, products or equipment to a degree of predictive accuracy which is capable of supporting *real innovation* in design and operation.

A typical APM includes material and energy balance, reaction, detailed heat and mass transfer, and physical property and equipment geometry relationships. Hybrid "APM–CFD" methodologies now make it possible to address detailed fluid dynamics effects within complex vessel geometries, improving scale up accuracy even further.

The role of model-based experimentation in Model-Based Innovation – for example, the design of a new catalyst



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