

# Advanced Process Modelling

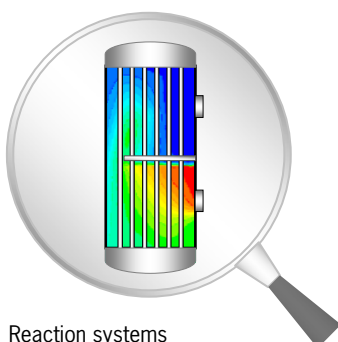
## High-quality information for decision support

### Where is APM applied?

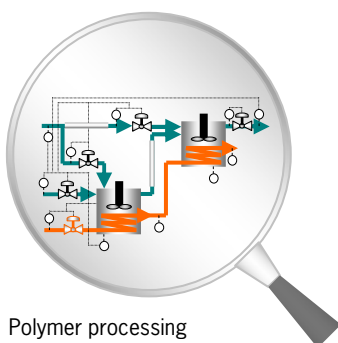
Though called 'process' modelling, APM is not restricted to refinery or large-scale chemical plant.

Typical examples can be found in many different areas of application and at many different scales:

- Design of a new high-conversion multitubular reactor for producing acrylic acid
- Scale up of a crystalliser from laboratory to production scale
- Optimisation of the operation of an atmospheric crude unit
- Design of optimal start-up procedures for an Air Separation Unit
- Design of a new catalyst to produce clean diesel from natural gas
- Optimisation of pill design to ensure optimal delivery of the active ingredient



Reaction systems



Polymer processing

Advanced Process Modelling (APM) is a technology that uses high-accuracy mathematical models of process equipment and phenomena to provide *high-quality information for decision support* in process innovation, design and operation.

The predictive power of an Advanced Process Model results from the combination of first-principles chemical engineering, physics and chemistry with observed ("real-life") data such as laboratory, pilot plant or operational measurements.

APM gives companies significant competitive advantage by providing a tool to capture and deploy corporate knowledge effectively, and thus innovate rapidly.

APM can be applied across the process lifecycle, from laboratory conceptual work, through process and detailed design to online operation. Typical application areas are those that involve complex physical and chemical phenomena, such as reaction engineering, crystallisation, complex separation processes and fuel cell component and system design.

PSE is the leading supplier of APM technology and services: PSE's gPROMS is a sophisticated, modern software environment for construction, validation and execution of high-accuracy models, and the company is a pioneer in the growing application of Model-Based Innovation.

### What are the benefits of Advanced Process Modelling?

A key benefit of Advanced Process Modelling is the high-quality information it provides to underpin decision support in process and product innovation, and process design and operation. Typical benefits are:

- **Faster innovation**, with **reduced innovation risk**, cost and time-to-market. Model-Based Innovation techniques allow rapid screening and verification of designs, with reduced reliance on physical testing
- **better process designs**, with lower design margins, leading to reduced capital expenditure, higher reliability and lower operating cost
- **better operations**, with greater flexibility of operation through better understanding of operating limits and the ability to operate closer to constraints with confidence, plus the many advantages of Model-Based Automation.
- **better product designs**, through the ability to test product designs and tailor manufacturing processes to deliver required product attributes
- better compliance with **health, safety** and **environmental** requirements
- **effective risk management**, by using the reliable *quantitative data* on which to base R&D and design decisions, allowing you to manage risk with confidence.

## How does APM relate to other modelling and simulation technologies?

A gPROMS APM is typically a first-principles model that embodies fundamental chemical engineering, physics and chemistry relationships, validated against observed data. This gives it a higher level of predictive accuracy and wider range of application than any other type of model currently in widespread use.

APM differs from the traditional technologies available to the process industries, such as process simulation and Computational Fluid Dynamics (CFD), in:

- its degree of predictive accuracy for complex chemical phenomena
- the range of application (from micro- to macro-scale) of models
- the extent to which it can be applied across the process lifecycle, from laboratory analysis through process engineering to online operation.

APM is, however, **entirely complementary to existing technologies**, and can augment their application significantly. For example, a high-accuracy reactor or distillation model can be deployed within a traditional process flowsheet simulator, in order to investigate process design alternatives (see below) once the detailed unit model has been designed.

### Example: reactor Advanced Process Model

The diagram below shows the “lifecycle” of a high-accuracy Advanced Process Model of a multitubular reactor.

#### gPROMS Advanced Process Models are documents, not software ...

A gPROMS model contains just the description of the physical and chemical relationships governing the process. Solution of the resulting equations is taken care of automatically.

This means that a well-written Advanced Process Model is effectively a **document**. It can be easily read and understood by someone with the right level of process knowledge, making it easy to maintain and extend.

For this reason, models are ideal vehicles for **capturing and building vital corporate knowledge**, as well as **transferring that knowledge** between different stakeholders across the corporation.

