gPROMS

Application areas

# Advanced Process Modelling of Polymerisation processes

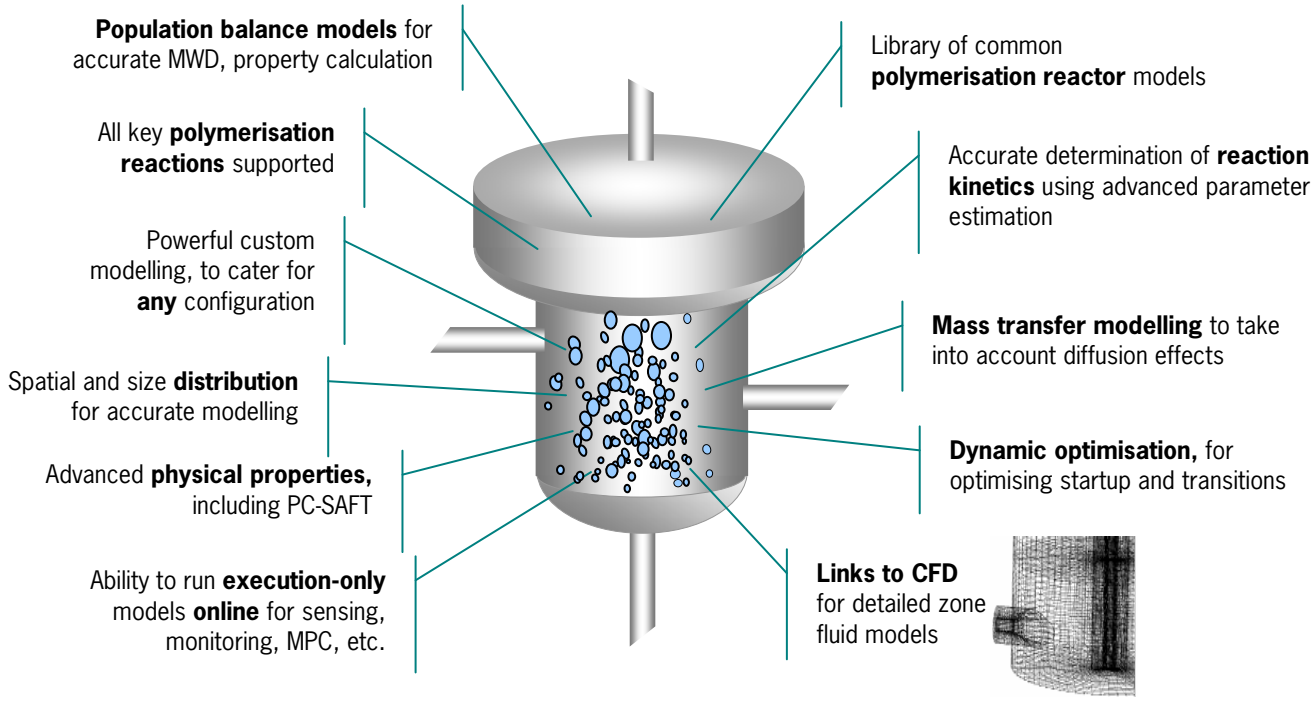
*"Process modelling using gPROMS identified a 30% saving in batch time."*

**Senior Polymer Technology Manager**
BASF Polymers

Polymer manufacture is a complex operation involving many different process variables. As new capacity comes on line in the Middle East and China, the commercial drivers for efficient design and operation are increasing daily.

In general, the more complex the process, the more benefit there is from using process modelling to understand the physics and chemistry, create better designs and optimise operation. Application of Model-Based Innovation techniques can result in millions of dollars of per year in enhanced revenue with little or no capital expenditure.

PSE's state-of-the-art gPROMS process modelling package is increasingly the environment of choice for polymer manufacturers who wish to extract more value from their plants. PSE also provides sophisticated reactor models, and polymer modelling experts who work collaboratively with your personnel to guide experimental and implementation programmes, and ensure fit-for-purpose applications.




## Benefits

*Quality, yield, throughput, and reduction in design and operating risk – **all without major capital investment**.*

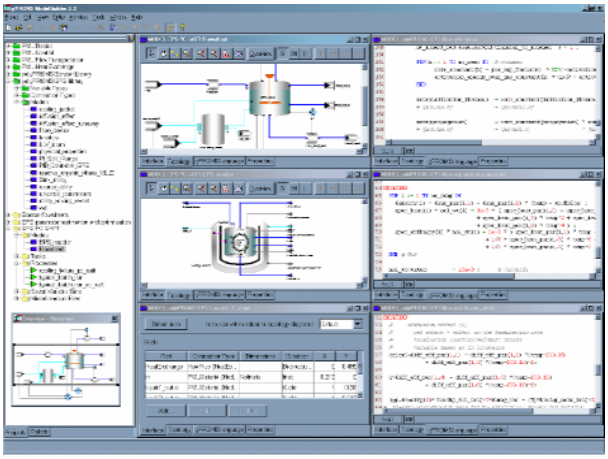
The benefits of modelling can be significant. For a start, you can improve yield, throughput and product quality simply by using optimisation to determine the optimal trajectories of key operating variables, particularly in batch processes. Models can then be deployed to optimise online operation, providing benefits every day.

Modelling helps you understand processes better, and make better use of laboratory and operational data. This enables you to troubleshoot poor operation and increase process reliability in existing processes, and introduce new technology – designed to maximise end user product qualities – with confidence and reduced risk.

With kind permission of

BASF The Chemical Company

## Example 1: EPS Batch polymerisation

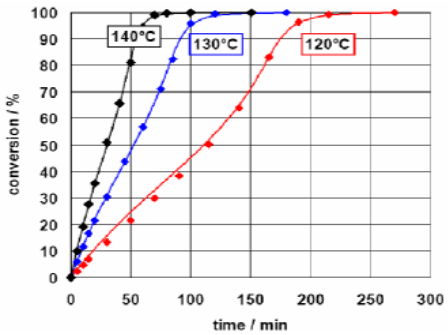


By building a high-fidelity detailed kinetic model of its batch Expanded Polystyrene (EPS) process and applying dynamic optimisation techniques, BASF was able to identify a 30% reduction in batch time.

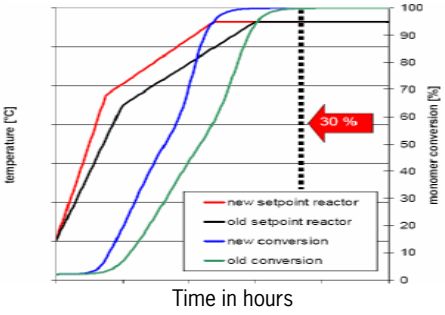
The first-principles gPROMS batch process model (left) included detailed reaction kinetics, with parameters estimated from experimental data. In addition it modelled heat and material balances, geometry details, transport and thermodynamic properties (calculated using the PC-SAFT equation of state) and plant operating procedures.

Dynamic optimisation was used to minimise batch time.

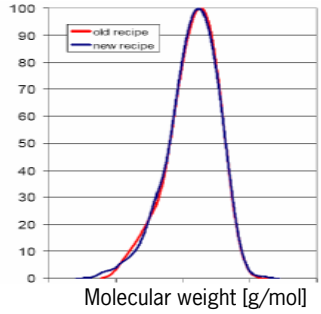
Validation results in good fit between measurements and predictions




Reaction time reduced by 30%

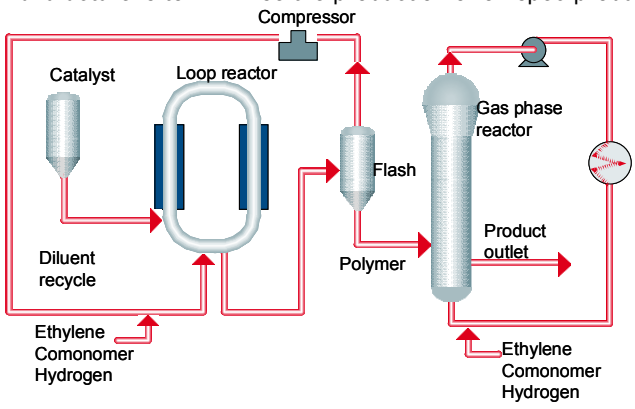



Molecular weight distribution is unchanged



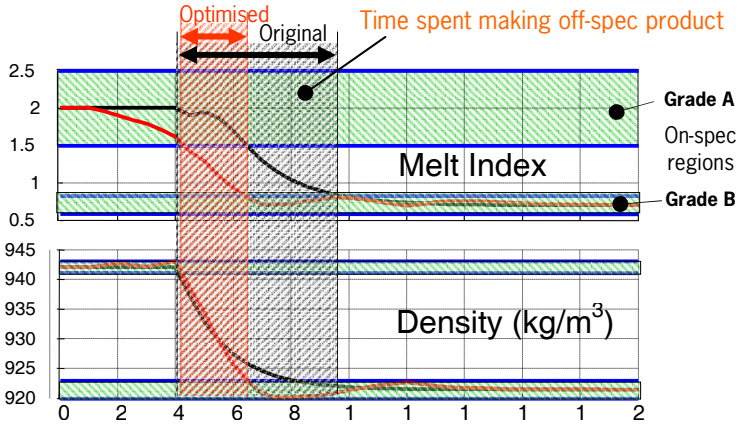

## Example 2: Optimal grade change in a Polyethylene (PE) process

Polyethylene has rigorous quality specifications for different grades. One of the major challenges in polyethylene manufacture is to minimise the production of off-spec product during grade change.




Borealis' BORSTAR™ process (left) uses slurry loop and gas-phase reactors for producing high-grade PE. Borstar PE has a bi-model molecular weight distribution that gives it a wide range of high quality end-user properties.

During grade change, it is necessary to move from one set of melt index and density values to another, through an off-specification region.




By using dynamic optimisation, then implementing the optimal trajectories using an advanced Model-based Predictive Controller, it was possible to demonstrate a time saving of nearly 60 % on a grade change.

Assuming a changeover frequency of one week on average, this represents around **one week's additional production** per year.

With kind permission of

BOREALIS

PSE