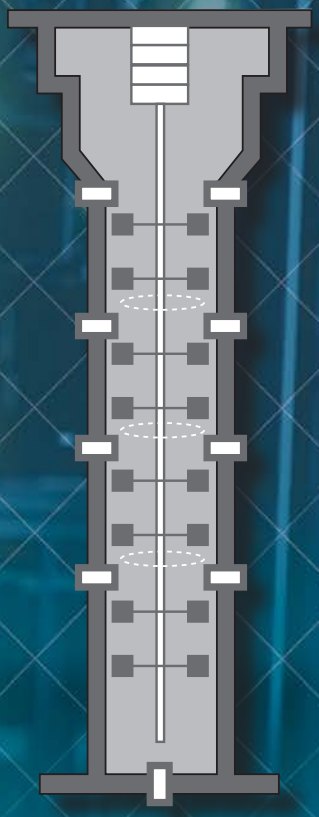
gPROMS

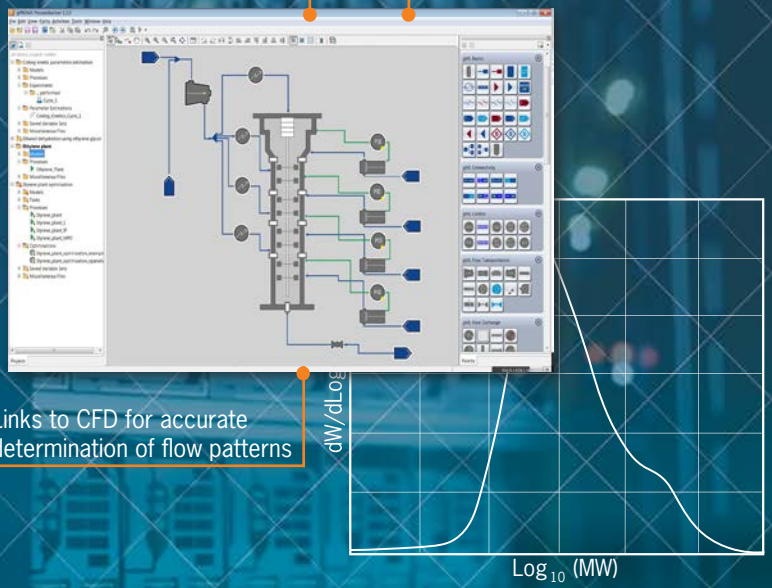
DIGITAL OPTIMISATION OF LDPE AUTOCLAVE REACTORS



- Perform continuous process debottlenecking
- Maximise production rate while maintaining polymer properties
- Find operating conditions required for production of polymer with desired product properties
- Evaluate impact of modifications to reactor internals

Rigorous thermodynamic models for phase behaviour predictions

Full population balance models for accurate MWD calculation



Links to CFD for accurate determination of flow patterns

Developing new polymer grades typically presents a number of challenges. For example, how do you determine the operating conditions for producing desired polymer molecular weight distributions (MWD) in reactor systems with imperfect mixing and complex kinetics?

Advanced process modelling provides the means to capture the effect of changes in operating conditions on the shape of MWDs.

This helps reduce development time for new polymer grades, evaluate new reactor designs, and determine the operating conditions that maximise the production of each grade while preserving polymer properties.

PSE

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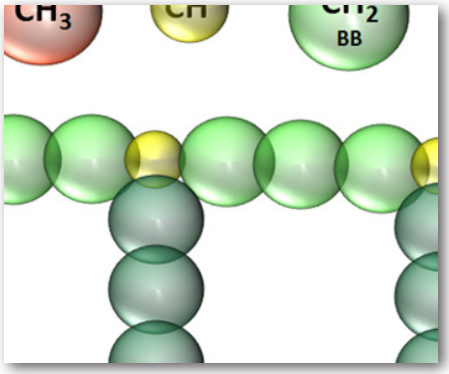
How does it work?

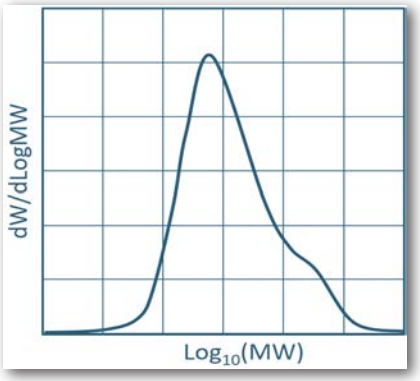
PSE's approach for low-density polyethylene (LDPE) autoclave reactors integrates several advanced modelling and solution concepts:

Advanced polymer thermodynamics



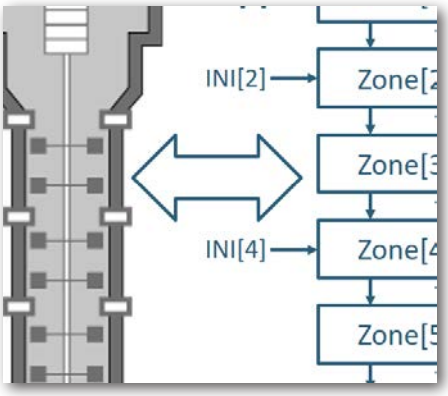
The Statistical Association Fluid Theory (SAFT) y-Mie Equation of State represents molecules as chains of distinct functional groups. Branching is accurately modelled, to provide accurate polymer properties across the MWD. This approach is ideally suitable for the modelling of polymers.

Full MWD modelling



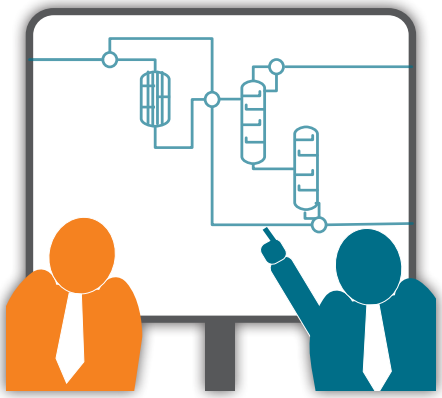
Detailed kinetic modelling considers elementary polymerisation reaction steps in chemically-initiated free radical polymerisation. The model solves for the evolution of the full molecular weight distribution (MWD) using the fixed pivot technique.

A multizonal approach linked to CFD



The hybrid multizonal approach couples a "cold-flow" Computational Fluid Dynamics (CFD) simulation of the reactor with the full chemistry model to represent both the polymerisation process and the complex flow pattern in industrial-size autoclave reactors.

PSE expert services



We provide expert consulting services to ensure rapid and quality assured project delivery, as well as to transfer know-how to internal teams.

> "Using the model … we were able to increase production by more than 10% while preserving end-use polymer properties."
>
> – US polymer producer

Supply

PSE can build custom LDPE reactor models that incorporate your kinetic information, for you to apply in optimising design and operation.

To find out more about digital optimisation of LDPE autoclave reactors in gPROMS ProcessBuilder, visit

psenterprise.com