CLARIANT

Optimization of product properties via a **HYBRID MODELING APPROACH OF A SEGREGATED REACTOR**

APPLIED CHEMICAL REACTION ENGINEERING

WHY IS CHEMICAL REACTION ENGINEERING KNOWLEDGE OF FUNDAMENTAL IMPORTANCE?

- To ensure scale-up and mixing of complex and multi-phase systems
- To improve process understanding as a basis for design and optimization
- To reduce costs through
  - Shortening of time-to-market
  - Maximizing of yield and selectivity, and realizing a safe process

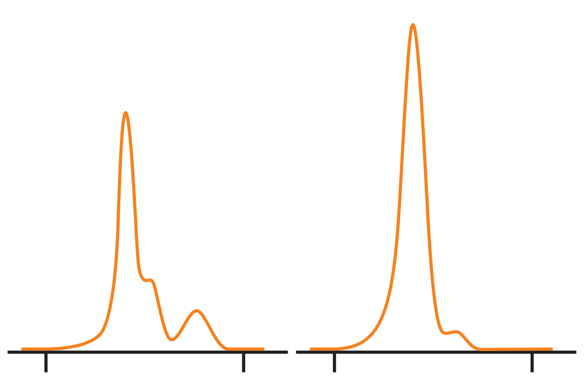
WHAT ARE COMPLEX REACTION SYSTEMS?

- Parallel and consecutive reaction systems
  - A + B → C
A + 2B → D micro mixing
  - A + B → C
B + C → D micro mixing and back-mixing
- Multi-phase systems such as dispersions, suspensions, and emulsions
- Highly exothermic reactions
- Reactions with a considerable viscosity change

HIGHLY VISCOUS POLYMERS

FACTORS INFLUENCING PRODUCT QUALITY

- Polymerization kinetics
- Mixing at viscosities as high as 6 Pas
- Heat removal
- Temperature distribution
- Monomer type and co-monomer
- Starter (initiator)
- Catalyst



LAB TRIALS

- Stirrer optimization and very high power inputs were realized

PRODUCTION

- Scale-up from lab-size is non-trivial so that a hybrid modeling approach was employed for the estimation of
  - Velocity und temperature distribution in the reactor
  - Effects of mixing on the polymer chain length distribution
  - Product quality depending on the polymer chain length distribution

HYBRID MODELING: MIXING AND REACTION ENGINEERING

THE POLYMERIZATION KINETICS IS WELL-KNOWN

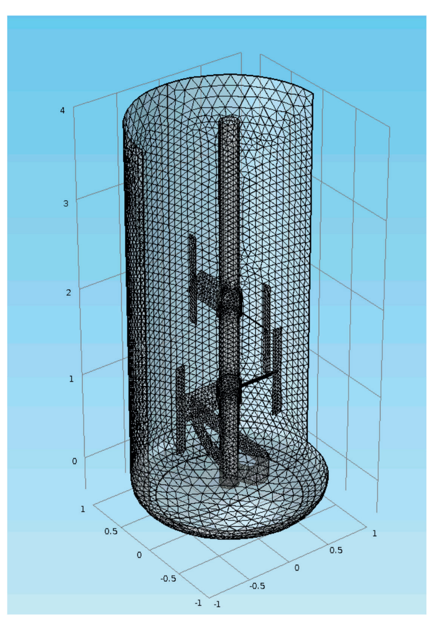
- The polymer chain length distribution can be calculated well for ideally mixed systems
- Segregated conditions exist in the real life though

CHALLENGES DUE TO NON-IDEAL MIXING IN THE PRODUCTION REACTOR

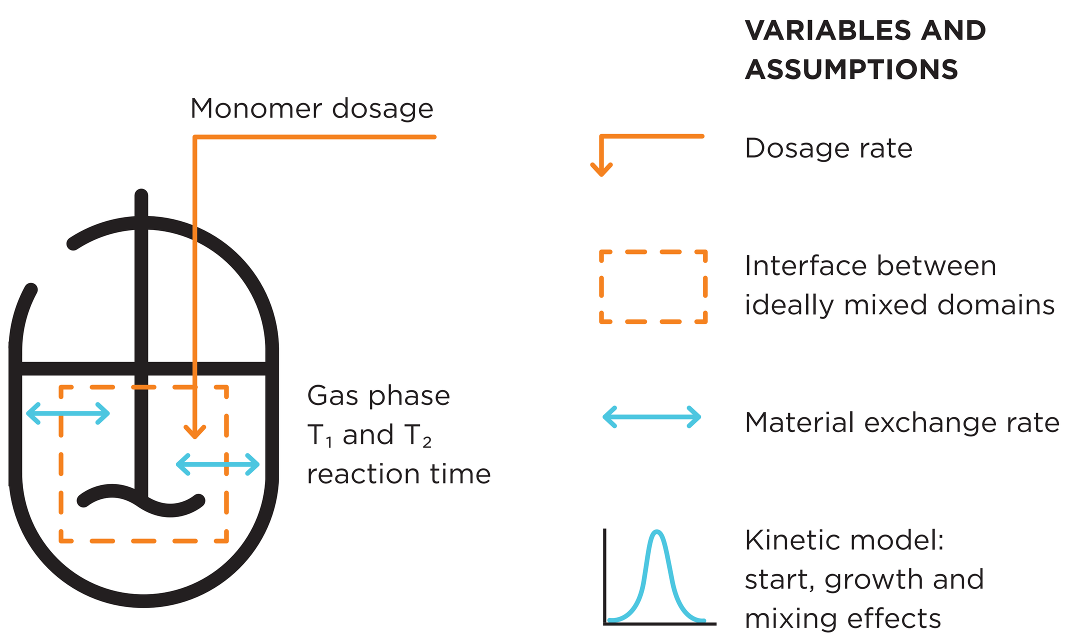
- Viscosity effects on the reaction system
- Coupling heat removal with reactions kinetics
- Low mixing intensity based on increasing viscosity as the reaction proceeds
- Coupling polymerization kinetics with CFD

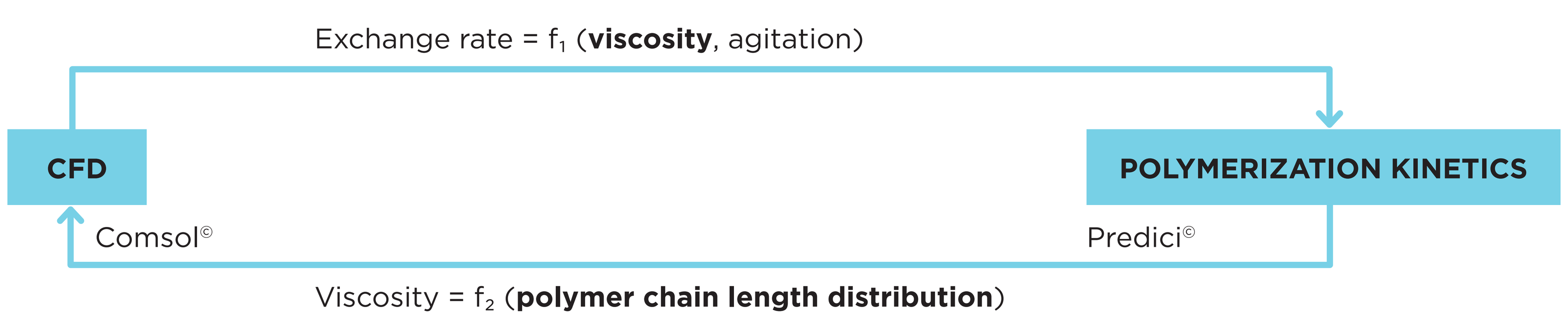
COUPLING CFD AND POLYMERIZATION KINETICS

REACTOR

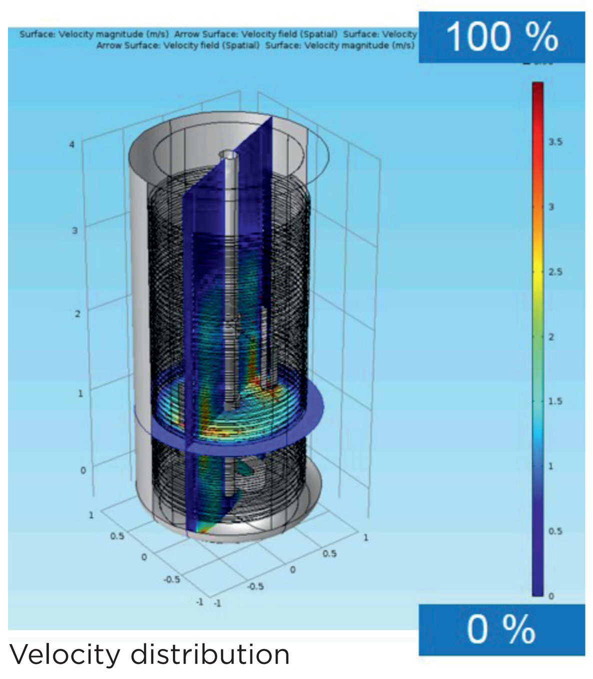


Reactor geometry with the corresponding mesh

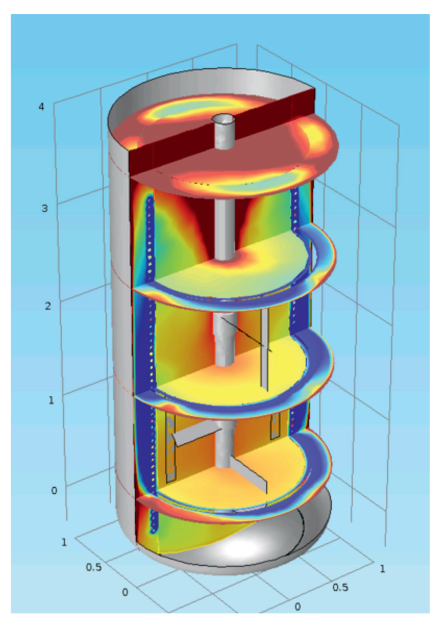




RESULTS

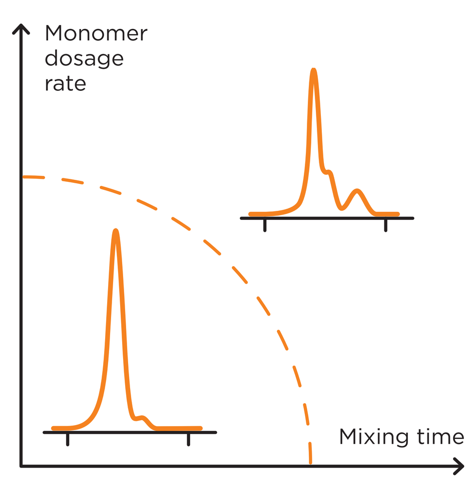


Velocity distribution (viscosity >6 Pas)

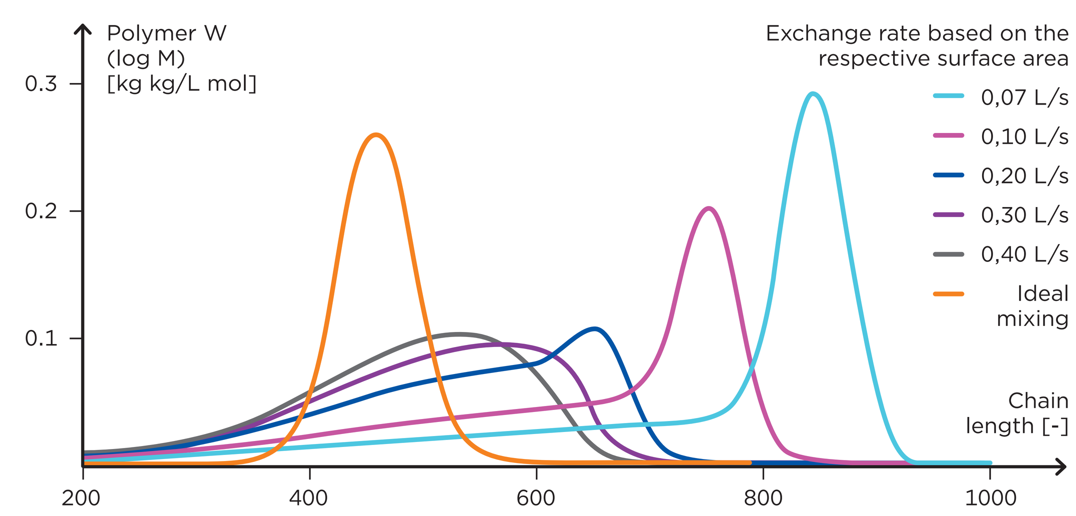


Temperature distribution

- Successful process scale-up for a new product
- Improved product properties through
  - reduced dosage rate
  - finer temperature control
- The gained knowledge was transferred and applied to further reactors



Production optimization



Simulated chain length distribution depending on the material exchange rate

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what is precious to you?

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