

## **SIMULATION BASED PRODUCT DEVELOPMENT IN HIGH-PRESSURE POLYMERIZATION TECHNOLOGY**

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### **ABSTRACT**

Product development in high-pressure polymerization technology is a specifically demanding task. First, operation procedures from large-scale technical practice cannot be scaled down to typical lab application one to one. Second, competitive high-pressure polymerization plants operate on a scale of significant more than 100 kt/a production capacity. Both, the significant scale up as well as limitations in miniaturizing laboratory equipment are still a remarkable challenge in designing strategies for product development in high-pressure polymerization technology. The contribution will look on how simulation technologies can help to overcome these challenges and where actual the limitations occur.

The first target is the prediction of microstructural polymer properties being determined by process conditions and strategy. During the recent years, there has been remarkable progress. Specifically, the combination of deterministic modeling with Monte-Carlo techniques, so-called hybrid technology, brought significant improvement with respect to detail of predicted molecular structure and limitation of computational efforts. By this, the detail is sufficient for feeding rheological models. However, demands on computational equipment together with the speed of computation is high enough to establish such technologies in standard research. Using examples of such investigations the portability of such technologies will be discussed. The second target is to use this information to build a bridge in order to transform structural information to rheological models. By this, based on process design application properties become accessible by simulation.

With increasing insight into the polymer structure, aspects of reactor operation come into focus again that have been accepted for a long time as non-ideal behavior to be adapted as the impact of the correlation of process conditions in polymer microstructure had been the dominant problem. Now, the focus of modeling is redirected again to the non-uniform distribution of species along the radial reactor axis together with the resulting consequences. The consequences of radial species distribution in high-pressure polymerization reactors will be inspected together with their origin and impact on varying heat transfer in reactor tubes.

Systematic discrepancies in reactor modeling being observed applying unified reactor models over a wide variety of processes and manufacturing sites indicate that it is worthwhile to search for their origin. This makes us revisiting fundamentals. Both, elementary reaction kinetics and thermo-physical properties come into focus again. The access to thermo-physical properties of reaction species under process conditions such as 3000 bar and 300 °C is rare. Even inexistent is the information about their mixtures. First attempts of a direct access of such quantities will be shown.

For years the modeling of such complex systems was strictly oriented forward pushing the limits in detail in describing the polymeric microstructure. Consistent model design and multifold application in technical practice helped to learn about the potential of development and weak points. It is remarkable to note how fundamental investigations for such purposes of modeling redirect the interest back to root of fundamental mechanisms. By this, classical disciplines experience a renaissance.