Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Influence of Mixing Characteristics on Polymerization Reactors

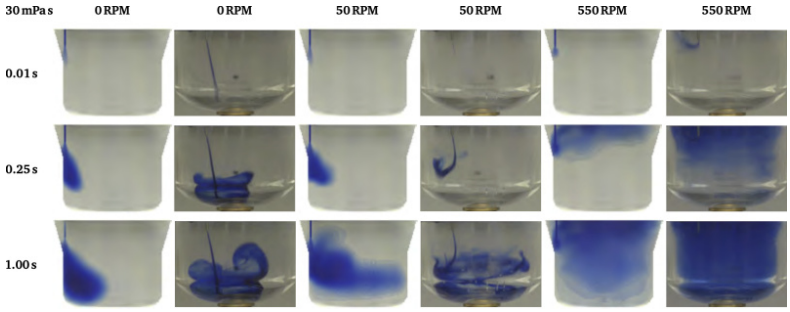


Figure 1: Images of the reactor at different times and stirrer velocity. Left: picturecreated from a 2D projection of the CFD simulation. Right: pictures taken inthe lab for comparison.

Introduction

The industrial production of high-density polyethylene (HDPE) through the catalytic polymerization of ethene is an important process, as HDPE is essential for a wide range of applications, from packaging materials to automotive components. Polymerization can be carried out in the solution, suspension or gas phase, with solution polymerization typically being carried out in stirred reactors. Polymerization is highly dependent on the mixing effects within the reactor, which affect product properties, conversion and reactor composition. Variations in stirring speed, residence time, composition and reactor geometry can affect the final polymer properties. Detailed computational fluid dynamics (CFD) simulations are used to investigate these parameters. These simulations couple the flow behavior in the reactor with the polymerization kinetics and provide insight into the process. Due to the complexity and scale of these simulations, high performance computing (HPC) is required. In this project, a lab-scale polymerization reactor of the working group is investigated.

Methods

To study the catalytic polymerization of ethene, computational fluid dynamics (CFD) simulations were carried out using the following methodology: A computer-aided design (CAD) model was constructed based on the laboratory-scale reactor. This CAD model was used to create the mesh on which the CFD calculations were based. The CFD software used for these simulations was ANSYS Fluent, which provides a robust platform for analyzing fluid dynamics and reaction kinetics. The kinetics of the polymerization process was implemented using a C/C++ programmable interface to Fluent's user-defined functions (UDFs). This approach allowed custom reaction kinetics to be incorporated directly into the simulation, ensuring accurate modeling of the polymerization process. The kinetic model used the method of moments to determine the average polymer

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Clusters
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Software
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Institute
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University
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properties of the HDPE produced, providing a detailed understanding of the polymer properties.

Results

During the project, several methods were tested to simulate the residence time behavior in the reactor. These methods included Lagrangian particle tracking, transient simulations using a species transport model, and an approach using a user-defined scalar. In particular, the Lagrangian particle tracking method was used to test how well the flow behavior could be represented by the particle trajectories. Different trajectory generation settings were tested to optimize the representation of the flow dynamics. In addition various turbulence models were tested to evaluate their influence on the residence time behavior. These models helped to understand how turbulence affects mixing. The stirrer speed and the viscosity of the mixture were varied to study their effect on the mixing effects. A projected 2D view was generated from the 3D CFD data. The aim of this projection was to reproduce the images of the reactor taken in the laboratory to allow a direct comparison. Figure 1 shows the comparison of injection experiments for three different stirrer rotation speeds. The time shown is the time after injection of the tracer substance.

Discussion

The research has shown which methods are more effective in simulating the residence time behavior in the reactor and which methods are less optimal. A projected 2D view could be generated from the CFD simulations which represent the trends from the experimental reactor images. For the injection without stirrer rotation the short-circuit flow can be seen in the experiment as well as the simulation. For the highest stirrer speed the mixing starts from the top in contrast to the mixing from the bottom for the slower stirring speed. The focus of future work will expand to include free radical polymerization of ethene, aiming to simulate the production of low-density polyethylene (LDPE). It is planned to couple the CFD results with Monte-Carlo simulation to obtain a full molecular-weight distribution of the produced polymer.

Publications

Schwarz, E.; Busch, M. Modeling Mixing Characteristics in a Mini-Plant Polymerization Reactor (Poster), 11th PhD-Student Workshop by the Working Party of Polymer Reaction Engineering, Potsdam, Germany, September 8-10, (2023)

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