Hessisches Kompetenzzentrum
für Hochleistungsrechnen

Influence of Mixing Characteristics on Polymerization Reactors I

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Clusters
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Software
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Introduction

Low-density polyethylene is produced under extreme conditions at temperatures of up to 300 °C and pressures of up to 3000 bar. The final properties of the polymer depend on how the reactants are mixed within the reactor. Inadequate mixing can lead to the formation of hot-spots, which increases the risk of decomposition. The mixing also affects the initiator decomposition and therefore the chain propagation. This effect cascaded to the temperature profile in the whole reactor influencing the microstructure of the polymer chains. To study these effects, a laboratory-scale reactor with three separate zones was devel- oped. Each zone can be operated independently, enabling the polymerization process to be initiated in a controlled manner. The aim was to simulate the behavior of this reactor using Computational Fluid Dynamics (CFD) modeling. CFD simulations com- bine modeling of fluid flow, heat transfer, and chemical reactions. The results can be used to predict the molecular weight distribution of the polymer, which determines its mechanical and processing behavior. Modeling such a system using CFD simulations is computationally demanding, given that the reactor geometry consists of several million computational cells and the chem- ical reactions are coupled. Without access to high-performance computing, the time required for a single simulation would be infeasible. Therefore, the Lichtenberg cluster was essential for completing the work within a reasonable time-frame.

Methods

For the CFD model setup, a three-dimensional computer-aided

design (CAD) represen- tation of the lab-scale reactor was used as the foundation for discretization into the computational mesh. The mesh was constructed to accurately capture the reactor geometry, including the stirrer blades and the separating disks among the three reaction zones. The flow field of all species was simulated in ANSYS Fluent, which solves the conservation equations for mass, momentum, and energy. Polymerization reactions were incorporated via a C/C++ interface to Fluent's user-defined functions (UDF), enabling direct integration of the reaction kinetics, including the complete kinetic mechanism of ethylene polymerization. The model accounts for the influence of temperature, pressure, and species concentrations on reaction rates and thermophysical properties. The continuous polymerization experiments are represented using a steady-state simula- tion. CFD outputs, such as temperature and polymer conversion, are directly obtained. Molecular weight distributions require a post-processing step: the converged CFD data are exported and processed with a compartmentalization algorithm, which subdivides the computational domain into smaller, spatially continuous zones exhibiting similar mixing behavior. This procedure clusters mesh cells with comparable values of a char- acteristic variable into well-mixed regions. The number of compartments is constrained by a minimum volume threshold to maintain meaningful results. This post-processing step is done with Python. The mean values of temperature, pressure, species concentrations, and polymer moments within each compartment are extracted and input into a stochastic Monte-Carlo sim- ulation. This simulation models the growth of individual polymer chains by randomly sampling reaction events according to their frequencies. It tracks branch formation and chain lengths, allowing prediction of the molecular weight distribution.

Results

Simulations were performed for various experimental conditions with initiator addition in either a single zone or multiple zones. The simulated zone temperatures closely matched experimental measurements, and polymer conversion was accurately predicted. Using the converged CFD results, the compartmentalization algorithm subdivided the reactor into multiple compartments. The spatial arrangement of these compartments reflected the underlying flow patterns and mixing behavior, with consistent results across all simulation cases. Monte Carlo simulations were then carried out for each case. For single-zone initiation, the predicted molecular weight distribution agreed well with experimental data, accurately capturing both low- and high-molecular-weight regions. In two-zone initiation experiments, the simulation reproduced the low-molecular-weight fraction effectively, but significant deviations appeared in the high-molecular-weight re- gion. The simulated distribution lacked the second peak observed experimentally, indi- cating that the model underestimates the formation of long polymer chains.

Discussion

Using the Lichtenberg cluster, multiple experimental cases were simulated with CFD and compared to experimental data. Comparison of modeled molecular weight distribu- tions demonstrates both the strengths and limitations of the current model, highlighting areas for refinement in future work. Nevertheless it has to be emphasized that all simulations were conducted without mod- eling factors typically applied to account for systematic non-idealities. Future efforts will focus on improving the reaction network and compartmentalization algorithm to better capture these effects.

Publications

Schwarz E., Weigel C., Busch M.: Modeling Low-Density Polyethylene Polymerization in a Multi-Zone Autoclave using coupled CFD and Monte-Carlo Simulation, Proceedings of the ASME 2025
https://doi.org/10.1115/PVP2025-154652

Schwarz E., Weigel C., Busch M.: Modeling Low-Density Polyethylene Polymerization in a Multi-Zone Autoclave using coupled CFD and Monte-Carlo Simulation (Presentation); Pressure Vessels & Piping Conference Montreal (Canada), July 20-25, 2025

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