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Use of CFD in modeling MMA solution polymerization in a CSTR

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HIGHLIGHTS

- CFD was employed to study MMA solution polymerization in a CSTR.
- CFD model was successfully validated using experimental data from literature.
- The model incorporates thermal and chemical initiations, CTA and gel effect.
- Effects of operating conditions on conversion and homogeneity were investigated.
- CFD model enables us to optimize the process and forecast the product quality.

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ABSTRACT

A computational fluid dynamics (CFD) model was developed to study methyl methacrylate (MMA) solution polymerization in a lab-scale stationary continuous stirred tank reactor (CSTR) equipped with a six bladed 45° pitched impeller. Azobisisobutyronitrile (AIBN) and ethyl acetate were taken as the initiator and solvent, respectively. The CFD modeling approach incorporated an integration of the continuity, momentum, and species transport equations along with a polymerization source term. The latter was a function of thermal and chemical initiations, transfer to monomer and solvent as well as the gel effect. Multiple reference frame (MRF) technique, laminar regime, and isothermal condition were considered in the modeling. To validate the CFD model, the simulation results of conversion in a stationary CSTR of MMA polymerization were compared with the data reported in the literature. The CFD model was then employed to investigate the impacts of the impeller speed, reaction temperature, residence time and inlet monomer (or solvent) concentration on the conversion and homogeneity of reaction mixture inside the reactor. Contours of monomer mass fraction conceptually facilitated to visualize the reaction progress in the reactor.

1. Introduction

Continuous stirred-tank reactors (CSTRs) are ubiquitously used for mixing and reaction systems. In particular, polymerization in CSTR reactors has been a challenge [1]. Furthermore, in a polymerization system, the polymer reactor behavior becomes quite complex due to inherent non-linearity arising from polymerization kinetics and a rapid increase of viscosity. Mixing, reactor temperature, inlet monomer, solvent and initiator concentrations are among factors that can have profound effects on polymerization rate in a CSTR [2–4]. Thus, mixing in a polymer reactor vessel is obviously not ideal. In a CSTR, the control of heat is alleviated due to more efficient removal of reaction heat with the effluent and these reactors are economically attractive for industrial production with relatively infrequent changes in product properties [4]. Besides, a polymerization system in a CSTR is less influenced by the formation of thick polymer layers at the walls. However, only detailed simulations of the flow pattern and the kinetics for a given reactor with a specific geometry allows identifying the optimal reactor type. To develop an appropriate model for this type of reactor, a computational fluid dynamics (CFD) model must be developed for the flow field generated by the impeller in combination with the kinetics of the reaction [1]. Mixing can also affect the polymer properties. Rapid increase in viscosity with monomer conversion causes drastic variations of heat and mass transfer in reaction mass. Good mixing can be achieved by mechanical agitation, which breaks up the fluid elements into small parts, and molecular diffusion, which homogenizes the level of species concentration gradients inside the small parts [5]. Real flow in continuous polymerization reactors usually presents intermediate flow pattern between the completely micro-mixed and completely segregated conditions. The degree of micro-mixing may have little effect on the conversion of monomer throughout the reactor, but it can strongly affect the molar mass and branching distribution [4].

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