Study of mixing and chemical reaction in RIM

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Abstract

A 2D hydrodynamic model of the mixing chamber of a reaction injection molding (RIM) machine, previously established for the flow field simulation with computational fluid dynamics is now extended for the study of mixing and chemical reaction. Mass transfer is studied from simulations of tracer's dynamics, which are used for direct imaging of the mixing mechanisms and for micromixing efficiency quantification. The effect on the mass transfer simulations of the most important numeric and operational parameters, such as the grid density, the Schmidt number and the Reynolds number, is assessed. Tracer simulations are also used to quantify the macromixing with the computation of the residence time distribution. Dynamic simulation of chemical reaction in RIM is also presented, and the impact of micromixing mechanisms is studied.

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Keywords: Chemical reactors; Laminar flow; Mixing; Mass transfer; CFD; RIM

1. Introduction

Reaction injection molding (RIM) is an industrial process for plastic parts production, mainly polyurethanes, where two or more reacting monomers are rapidly mixed in a small cylindrical chamber, the *mixing chamber*, characterized by extremely short liquid passage times, in the range of 10–100 ms. The resulting reacting mixture is then discharged into a *mould*, where most polymerization takes place. The monomers are introduced into the mixing chamber by two opposing jets, with injection velocities usually ranging from 10 to 100 m/s. Due to the high viscosity of the injected monomers, up to 1 Pa s, and in spite of the extreme dynamics expected for the jets' impingement when they are decelerated over the short space of one diameter of the mixing chamber, 5–10 mm, the flow field is still basically laminar.

The Reynolds number for the RIM process was defined by Malguarnera and Suh (1977) at the injectors as

$$Re = \frac{\rho v_{\text{inj}} d}{\mu}, \tag{1}$$

where v_{inj} is the average velocity at the injectors with diameter d, and ρ and μ are the fluid density and viscosity, respectively. In operations of industrial relevance, this number can fall in the range of $100 \leqslant Re \leqslant 500$. In this range, mixing only takes place above a *critical Reynolds number* of 120, as experimentally demonstrated by Santos (2003), where the flow regime switches from a laminar steady state without mixing, to a laminar chaotic regime with strong and dynamic mixing.

Since at these low Reynolds numbers chaotic flows can nowadays be simulated accurately by *direct numeric simulation* (DNS) using *computational fluid dynamics* (CFD) software, in Muzzio and Liu's (1996) own words, this is "a promising route for the investigation of reactive mixing process". However, in the late 1970s and early 1980s, before

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DNS was yet an option to be considered, RIM technology was being introduced and immediately reaching a fast expansion in industrial applications. Since DNS was not possible at that time, and mixing knowledge is critical to the final RIM products (Kolodziej et al., 1986) the pioneering mixing simulation studies on RIM were based on heuristic physical modeling approaches.

The first attempts to model mixing were made with the lamellar model (Ranz, 1979; Ottino et al., 1979;Kusch et al., 1989) which was used to calculate the final striation thickness, and in the case of Kusch et al. (1989) to predict a test reaction product distribution. Other early attempts include the work of Lee et al. (1980), which developed a model for the striation thickness of fluid lamellae based on a derived stretching function of Tucker and Suh (1980), which, based on the assumption that the final striation thickness is determined by the size of the smallest eddies, proposed that it should vary with the Reynolds number as, $Re^{-3/4}$. Based on the statistical theory of turbulent diffusion, Baldyga and Bourne (1983) developed a model to predict the striation thickness distribution for T-mixers. The resulting size distribution was in good agreement with the experimental data of Kolodziej et al. (1982), although the fraction of striation thicknesses below the limit of $10\,\mu m$, necessary for polymerization to become chemically controlled, was found to be too low. Bourne and Garcia-Rosas (1985) postulated that the additional striation should have occurred in the runner and calculated it.

This type of models have the major disadvantage of not accounting for the actual flow field, and some of the assumptions used, such as fully developed local turbulence, are not particularly suitable to the laminar hydrodynamics in the mixing chamber of a RIM machine.

Nowadays modeling and simulation of the flow field for this problem is feasible using CFD codes. From CFD simulation considerable insight into the reactor hydrodynamics can be gained, since all the hydrodynamic variables are known at every instant and every point of the physical domain (Kosály, 1987). Albeit the longstanding importance of RIM process economics', and the actual feasibility for CFD simulations, only very few research works on the subject can be found in the literature. Of these, and in particular from the ones most closely related to the RIM problem, the following should be singled out due to their importance:

- Steady-state simulation of a 3D mixing chamber used in precipitators, which are opposed jets mixers with ten times the typical dimensions of RIM machines mixing chambers, was done by Zhao and Brodkey (1998) and Unger et al. (1998). Nakamura and Brodkey (2000) extended these studies to the dynamic simulation of the flow field with tracer injection.
- Wood et al. (1991) made CFD simulations of the 3D transient flow field of a RIM machine's mixing chamber. The simulation results were compared with LDA and

with visualization experiments. The results from the dynamic simulations presented roughly the same dynamic characteristics, based on Strouhal's number determinations, as the LDA data. Johnson and Wood (2000) further extended the study of typical frequencies with CFD simulation of a mixing chamber with a rectangular cross section.

- CFD simulations were used to study the effect of jets momentum imbalance in the flow field of opposed jets reactors by Johnson (2000a). The averaged flow field from the 3D dynamic simulations showed that the impingement point is off-centered if the jets' momentum ratio is different from unity. The off-center of the impingement point could lead to hydrodynamic nozzle plugging near the lower momentum jet. Johnson (2000a,b) studied different alternatives to get the impingement point near the center of the chamber and tested them solely by direct simulation.

The scarcity of published literature on confined impinging jets hydrodynamics generates enormous difficulties in the interpretation of the even scarcer experimental mixing studies with chemical reaction, such as those of Kusch et al. (1989), Mahajan and Kirwan (1996) and Johnson and Prud'homme (2003).

Nevertheless, since CFD simulations are nowadays capable of coupling hydrodynamics with chemical reaction and resolve dynamically the smallest scales of momentum and mass transfer, i.e., actually simulating the *micromixing* process, in Weinstein and Adler (1967) terminology, then DNS can be an alternative for accessing the impact of micromixing on fast reactions promoted with confined impinging jets, and with some success as it will be shown later. Furthermore, for such mixers, with a chaotic laminar regime, several operating and design aspects can be analyzed directly from flow field simulations. A good example is the momentum ratio between the jets, which was proven experimentally by Malguarnera and Suh (1977) to be a critical parameter that should be very close to the unity. In order to comply with this stipulation for chemical systems demanding the separate injection of streams with flow rate ratios different from unity imposed by stoichiometric requirements, simple mixing chamber design alternatives were successfully tested with CFD by Santos et al. (2002).

To test the design and operational parameters in a mixing study, a specific strategy for the quantification of the quality of mixing must be chosen. Several approaches based on DNS can be used: computation of *particle paths* (Howes et al., 1991;Mickaily-Huber et al., 1996; Byrde and Sawley, 1999; Aubin et al., 2003); *stretching rates* computation (Roberts and Mackley, 1995; Lamberto et al., 2001; Aubin et al., 2003); and simultaneous simulation of the convective and diffusion transport of chemical species (Muzzio and Liu, 1996; Zalc and Muzzio, 1999; Adrover et al., 2002). This last strategy, the *continous approach*, can be very attractive, since macro- and micromixing can be fully characterized