Study of the styrene emulsions formation in a micro reactor using Fluent CFD Tool

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Resumo: The use of microfluidics can improve the control of polymerization reactions and a numerical study of the process variables, validated by a set of experimental data, is necessary for the better understand the phenomenon. In the present work, a Syrris 250μL micro-reactor with T-mixer was used. The simulations were performed in the T-mixer, as it is where the formation of emulsions occurs. The turbulence model used was the k-ε and for interaction of the phases, VOF model was selected. The results obtained in the modeling were compared with the results obtained experimentally and it was concluded that the obtained particle diameters are consistent with reality.

Key-Words*:* Microfluidic, T-mixer, styrene, emulsions, CFD, Fluent

Introduction: Microfluidic devices are used to analyze chemical and biochemical reactions, since they require only a small amount of sample and are capable of accelerating the process [1]. In fact, the great relation between surface and volume, the expansion of thermal and mass transport, makes it possible for the study and control of fast and exothermic reactions [2][3]. Anionic and cationic polymerizations have also been studied [4][5], since these polymerization techniques are characterized by high initiation and propagation rates, but the mixture of the reactants can be a problem. The use of the micro-blend prior to polymerization reduces the dispersion of the molecular weight distribution of the synthesized polymers. When a T-junction is used in place of a micro-mixer, the polyester dispersion of copolymers was greater than or equal to 1.73 [6]. In 2005 was reported that free-radical polymerizations in 500μm diameter micro-tubes did not present different results from traditional laboratory scale reactors for low exothermic reactions [7]. However, for high exothermic reactions, the molecular mass distribution was narrower than for the traditional system. It was concluded that this is due to the surface / volume ratio of the reactor micro-tube, which allows better removal of the heat released during the polymerization. All of these studies suggest that the use of micro-tubes and micro-mixers can significantly improve the control of polymerization reactions. Because of this a numerical study of the process variables, together with the experimental validation, becomes necessary, which results in a better understanding of the phenomenon

Experimental and Simulation: The Syrris micro reactor used in this work has a 250μL microchip with two inputs and one output; The mixing of the phases takes place in the static T-mixer. The formulation used was removed from articles that performed the polymerization in micro reactors. A study of the styrene emulsion polymerization reaction in continuous tubular micro reactors, with the aim of verifying the percentage of solids content and the relationship with clogging, being recommended not to exceed it by 30% [8]. In order to avoid clogging, this formulation was taken as the starting point. The simulations are stationary and use the k-ε model for turbulence and the multiphase VOF model. All the simulations were conducted in the static T-mixer, in order to visualize the formation of emulsions and obtain the droplet size according to the ratio of the flows. Were studied two flow rates, 1:1 and 1:10, where continuous phase (Qc) and dispersed phase (Q_D) are respectively water and styrene. The geometry follows the dimensions provided by the manufacturer, with the channel having a rectangle shaped cross-section with semicircles on the sides, with a height of 250μm and a width of 300μm. The mesh contains 6,731,334 elements; The large number of elements is due to the refinement near the pipe wall and the required size of the elements to observe the interface between the emulsion and the continuous fluid. The flow of the currents, as well as their properties, is present in table 1.

Table 1 – Boundary Conditions

	Q_C	Q_D
1:1	16,4 μL/min	16,4 μL/min
1:10	164 μL/min	16,4 μL/min
DENSITY	0.99705 g/cm³	0.9016 g/cm³
VISCOSITY	0.008903 g/cm.s	0.00695 g/cm.s

Results and discussion: By creating a plane along the Z-axis in the center of the pipe, it is possible to observe that for a flow ratio of 1: 1 there was no mixing of the phases or appearance of emulsions (Figure 1a). By observing the vectors (Figure 1c) it is also possible to verify that both fluids have equal velocity until they meet, where there is a speed increase of the styrene, due to its narrowing in the tubing. When the water flow is increased by 10x, there is a break in the continuous flow, forming micro emulsions (1b). It is possible to measure its diameter with the aid of CAD software (DraftSight) for experimental comparison. According to Asua (2003), the polymers generated by the emulsion polymerization reach the diameter of the emulsions. By observing the velocity vectors, the velocity increase is significant around the emulsions (Figure 1d). By comparing the simulation with the experimental data, it is possible to notice the similarity between the obtained diameters. The experimental data presented show values of polymer particles of 255.8 and 244.0 µm (Figure 2), while the simulation show a value of 243 µm for flow rates of Qc = 164 µL / min and Q_D = 16.4 µL / min. For flow rates of Qc and QD = 16.4µL / min, no emulsions were obtained either in the simulation or in the experiments, because the water flow was not enough to overcome the styrene interfacial tension.

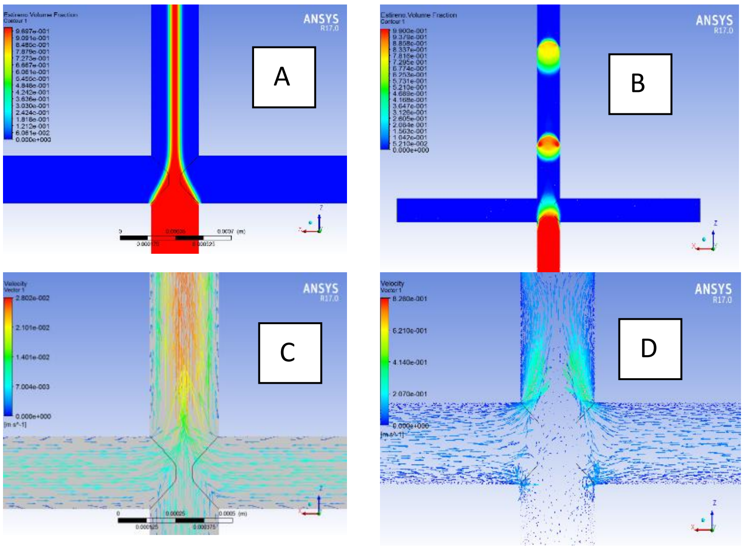

Figure 1 - a) Density profile for flow ratio 1: 1; b) Density profile for flow ratio 1:10; c) Velocity vectors for 1: 1 flow ratio; d) Velocity vectors for flow ratio 1:10.

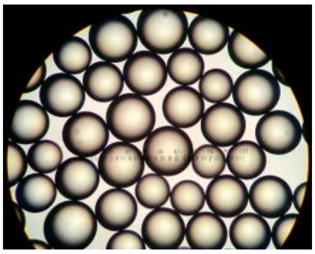

Figure 2 - Polymer particles obtained experimentally.

Conclusion: The CFD simulations satisfactorily represented the diameters of emulsion polymer particles experimentally obtained for flow rates with a ratio of 1:10; Emulsions with 1: 1 flow rates were not obtained in simulations and in experiments, which indicates the simulations represent well the operational conditions of the process.

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