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Characterization of micromixing in T-jet mixers

K. Krupa [a], Maria I. Nunes [b,*], Ricardo J. Santos [a], John R. Bourne [c]

[a] LSRE – Laboratory of Separation and Reaction Engineering, Associated Laboratory LSRE/LCM, Faculdade de Engenharia da Universidade do Porto, Rua Dr. Roberto Frias, 4200-465 Porto, Portugal
[b] Centre for Environmental and Marine Studies (CESAM), Departamento de Ambiente e Ordenamento, Universidade de Aveiro, Campus Universitário de Santiago, 3800-193 Aveiro, Portugal
[c] 1 King Stephen's Mount, GB – Worcester WR2 5PL, UK

HIGHLIGHTS

- Determination of micromixing characteristics and mixing times of novel T-jet mixers having rectangular cross-sections.
- Chamber width-to-depth ratios of 1–1.5 reduce mixing times and raise throughput relative to shallow chambers.
- Mixing is favored by jet expansion ratios of 4–6.
- At constant jet Reynolds number a small injector promotes faster micromixing and plug flow.
- All results are related to flow regimes determined by PLIF.

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ABSTRACT

To assess micromixing in T-jet mixers, having various geometries and flow rates, a set of test reactions was employed. This consisted of the reactions between 1-naphthol/2-naphthol and diazotized sulfanilic acid in aqueous solution. The results showed that the Reynolds number has a large effect on the rate of mixing. Furthermore, the geometrical parameters also influenced the product distribution of the test reactions. Increasing the ratio between the mixing chamber width and the inlet jet width improved mixing. Shallow chambers can show poorer mixing while increasing the depth enhances both mixing and reactor capacity. A characteristic mixing time was defined and determined as a function of Reynolds number in the range 300–3000 for the various reactor geometries. The effects of chamber width and depth as well as of jet width on product distributions and mixing times were related to the flow regimes found earlier by Planar Laser Induced Fluorescence.

1. Introduction

Mixing is one of the most important processes in the chemical industry, especially in nanoparticle precipitation and reactive polymerization. Typically, the process of mixing uses a tank equipped with one or more agitators, having the main disadvantage of promoting intense contact of fluid with very different ages, which can lead to product contamination or formation of secondary products (Santos et al., 2002). Static mixers were developed to circumvent those disadvantages and Confined Impinging-T-jet mixers (CIJ) and T-jet mixers are the most common types of opposed jet mixers.

A CIJ mixer consists of two opposed jets that collide and flow through a mixing chamber towards an outlet tube (Gillian and Kirwan, 2008; Santos et al., 2002). From previous works it is known that the mixing in opposed jets depends mainly on operational conditions, namely on the Reynolds number, and the geometry of the mixing device (Malguarnera and Suh, 1977; Sultan et al., 2012).

Several authors observed the influence of geometrical and operational parameters, particularly the Reynolds number, on the flow regimes and the mixing. From these works five flow regimes are distinguished:

- Segregated flow regime, where two parallel streams of fluid are formed and flow from injectors to the outlet without mixing (Engler et al., 2004; Soleymani et al., 2008; Sultan et al., 2010);
- Vortex flow regime – the segregation plane between the streams coincides with the mixing chamber axis and is characterized by two streams of fluid that have helicoidal

* Corresponding author. Tel.: +351 234 370 349; fax: +351 234 370 309.
E-mail address: isanunes@ua.pt (M.I. Nunes).

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vortices with a rotation axis aligned with the mixing chamber axis (Engler et al., 2004; Nunes et al., 2012; Soleymani et al., 2008; Sultan et al., 2010, 2012);

- Engulfment flow regime where the fluid streams issuing from each jet rotate over the chamber axis and promote transport of fluid from one half of the chamber to the other half (Engler et al., 2004; Soleymani et al., 2008; Sultan et al., 2010);
- Self-sustainable chaotic flow regime, reported by Sultan et al. (2012), is characterized by the formation of a vortex street evolving throughout the mixing chamber, which promotes fast mixing of the fluid streams issuing from the opposed jets;
- Turbulent flow regime is the dynamic flow regime where the jets are engulfed by action of the vortices that have a wide range of diameters (Santos and Sultan, 2013; Schwarzer et al., 2006).

Experimental and modeling studies have been carried out to explain the mixing process, but a clear picture has not yet emerged. Some experimental studies were focused on direct visualization of the flow (Tucker III and Suh, 1980a, 1980b), whereas others used laser-induced fluorescence (Santos et al., 2002, 2008, 2009; Sultan et al., 2010) or examined the polymer products (Kolodziej et al., 1982; Nguyen and Suh, 1985) to quantify the mixing.

Many studies on T-jet mixers focus on the influence of Reynolds number on the flow regimes, but the geometric and other operational parameters also play an important role in micromixing. The flow regime in T-jet mixers has a strong effect on mixing and depends on many parameters, such as the momentum ratio of the jets, the jet's Reynolds number, and the chamber-to-injector width or chamber width-to-depth ratios (Schwarzer et al., 2006). Bothe et al. (2010) used a test chemical reaction in the engulfment flow regime. From this work it was concluded that the smaller reactor yielded better conversion. Kusch et al. (1989) used Bourne's test system for the quantification of micromixing in opposed jet mixers over a range of Reynolds number from 50 to 600, which is the typical range of operation of industrial Reaction Injection Molding (RIM) machines. In the previous work (Kusch et al., 1989) the used fluid was water. Nunes et al. (2012) studied the same reactor with another reaction scheme and using a fluid with higher viscosity, thus the hydrodynamics in these experiments was closer to the actual conditions used in RIM. From both works (Kusch et al., 1989; Nunes et al., 2012) it was clear that the formation of desired products rapidly decreased as the Reynolds number decreased. Other authors covered a wider range of Reynolds numbers in opposed jet reactors and assessed the effect of turbulence scales on micromixing (Gillian and Kirwan, 2008; Mahajan and Kirwan, 1996) or validated turbulence models from chemical reaction data (Liu and Fox, 2006).

In this work mixing quality at the molecular scale will be assessed by using test reactions, namely the competitive–consecutive system introduced in 1992 (Bourne et al., 1992). The final product distribution depends on the mixing quality, so the system can be considered as a molecular probe to quantify the quality of a mixing process (Nunes et al., 2012). The details of the reaction system are shown in the next section.

The effect of the operational parameters, the Reynolds number and the geometry of T-jets on mixing will be assessed at the T-jet mixer outlet and related to flow regimes found by Planar Laser Induced Fluorescence (PLIF).

1.1. Test reaction scheme

Bourne and co-workers have developed a number of competitive reaction schemes to study micromixing (Baldyga and Bourne, 1997, 1999; Bourne et al., 1981; Fournier et al., 1996).

The test system adopted in this work was the reactions between 1- and 2-naphthols with diazotized sulfanilic acid, whose simplified scheme is:

$$A_1+B\overset{k_1}{\rightarrow}R$$
$$R+B\overset{k_2}{\rightarrow}S$$
$$A_2+B\overset{k_3}{\rightarrow}Q \tag{1}$$

where A_1 and A_2 are 1- and 2-naphthol respectively, B is diazotized sulfanilic acid, R represents two monoazo isomers, S is a bisazo dye and Q is known as Orange II. All reaction products are aqueous soluble dyes.

The kinetic rate constants in aqueous solution at 20 °C and ionic strength of 444.4 mol m^{-3} are: $k_1=15.3\times10^3$ m^3 mol^{-1} s^{-1}, $k_2=3.04$ m^3 mol^{-1} s^{-1} and $k_3=88.8$ m^3 mol^{-1} s^{-1} (Nunes, 2007).

The reaction between A_2 and $B$is faster than that between R and B but slower than the reaction between A_1 and B.

The product distribution of this test system can be defined by two variables: the fractions of the limiting reagent B which are converted to S and to Q, denoted by X_S and X_Q, respectively (see Eqs. (2) and (3)).

$$X_S=\frac{2C_S}{C_R+2C_S+C_Q} \tag{2}$$

$$X_Q=\frac{C_Q}{C_R+2C_S+C_Q} \tag{3}$$

where C is the concentration.

As mixing intensity increases, the selectivity, X_Q, decreases and X_S tends to zero. This means that in a well-mixed system the product S is not formed. The minimum value of X_Q occurs when the reactants are fully mixed and so the mixture is homogeneous at the molecular scale (Demyanovich and Bourne, 1989; Kusch et al., 1989). This minimum yield will be given later.

One advantage of this test system is the fact that the reactants and solvents used are not expensive and the products of reaction R, S and Q , absorb at different wave-lengths and their concentrations are relatively easy to determine spectrophotometrically (Bourne et al., 1981; Nunes, 2007).

2. Experimental setup

A drawing of the T-jet geometry used in the experimental work is shown in Fig. 1. It consists of two opposed feeding channels, which issue into a mixing chamber at an angle of 180° to each other. The flows enter the mixer symmetrically and leave through the open side of the main mixing chamber. The T-jets used in this work have some specificities that resulted from previous studies on the effect of the geometry on mixing in these mixers (Sultan et al., 2012, 2013). Some of the specificities that are worthwhile to pinpoint are the headspace above the inlet channels, the rectangular injectors extending throughout the mixing chamber depth, and the large ratio of jets expansion in the chamber, the chamber width in some cases is sixfold the injector's width. The headspace was observed in an early study of Santos et al. (2002) to have a strong impact on flow dynamics. The rectangular injectors extending throughout all the chamber depth were used by other authors for micro reactors (e.g. Bothe et al. (2008) and Gobby et al. (2001)), but the main reason for this configuration was the goal of introducing a geometry that could be easily scaled-up from a non-critical dimension, in this case the depth (Sultan et al., 2013). The jets expansion ratio (chamber width to inlet channel width ratio) of sixfold was based on the observation that this ratio is a critical parameter for the dynamics of mixing in the work