Mixing in Chemical Reactors

CIJs - Confined Impinging Jets

KEYWORDS: Opposed Jets mixers, Design Equation, Active Mixing, Dissimilar fluids

The guidelines for the implementation of opposed jets mixers in the industry were explored in this research. Two geometries were considered: cylindrical chamber - Confined Impinging Jets (CIJs) - and prismatic chamber - T-Jets. Mixing mechanisms for asymmetric flow conditions and fluids with different viscosities and densities were assessed. The range of working conditions to achieve chaotic flow regimes under asymmetric conditions was fully studied in these devices. This knowledge is particularly relevant for reactive polymerizations, where monomers often have different physical properties. Further advances were made in the opposed jets technology. The modulation of inlet flow streams fully controlled the mixing scales and the turbulent energy spectrum, opening several prospects for the application of this technology, for example at lower Reynolds numbers with more viscous fluids.

Introduction

Opposed Jet Mixers are highly efficient mixing devices that consist of a semi-confined mixing chamber having two directly opposed injectors. Research on opposed jets was introduced at LSRE-LCM 30 years ago to solve the mixing issue in Reaction Injection Moulding (RIM). Over the last years, the research at LSRE-LCM has focused on two opposed jets geometries: Confined Impinging Jets (CIJs) and T-Jets. CIJs consist of a cylindrical confined mixing chamber, while T-Jets are prismatic opposed-jets.

Mixing in CIJs has been studied from experimental work and Computational Fluid Dynamics (CFD) simulations. The first studies focused on mixing similar fluids, i.e., fluids with the same viscosities and densities, at symmetric flow conditions (same flow rate in both jets). For these conditions, it was established that the main condition for mixing was the operation above critical Reynolds number Re>120. This critical Re marks the transition between the segregated flow regime, where the fluids flow from the inlet to the outlet, to the chaotic flow regime, where there is the formation of a vortex street that engulfs the two fluids injected to the mixing chamber.

The mixing mechanisms in T-Jets reactors are similar to CIJs, where the main mechanism is a vortex street that sheds from the jets impinging point towards the outlet. The chaotic flow regime in T-jets was identified for the first time at LSRE-LCM using knowledge from 2D CFD simulations made for CIJs. This flow regime is of practical interest due to its capability to promote very fast mixing, although descriptions in the literature are still scarce and restricted to research made at LSRE-LCM and by the group of Prof. Li Wei-Feng from East China University of Science and Technology. In this period, the dynamic flow field in T-jet mixers under a chaotic flow regime was thoroughly characterised by fully resolved 3D CFD simulations.

CIJs and T-Jets mixers are commonly applied in plants involving mixing two dissimilar fluids, i.e., fluids with different densities and viscosities. Experimental and numerical studies on mixing dissimilar fluids and asymmetric flow conditions were performed from 2018 to 2023 at LSRE-LCM. The guidelines for the design and operation of these reactors for dissimilar flow rates and fluids were also established in this period.

The fully resolved CFD simulations in opposed jets mixers are still out of reach for engineering practice. The order of magnitude for the required number of computational cells for

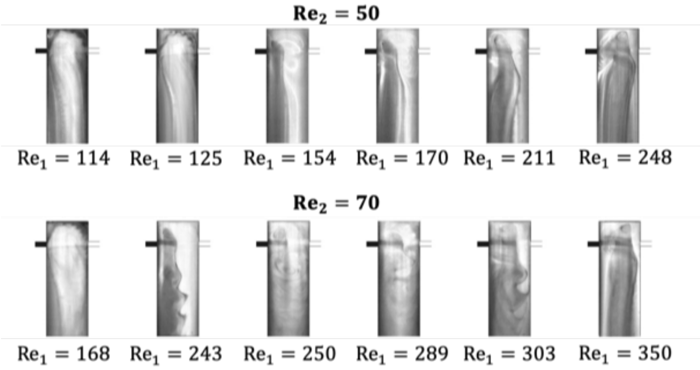

Fig 1. PLIF images of CIJs for a viscosity ratio 5 using symmetric mixing chamber.

the micromixing simulation of a reactor with ~1cm is around 10^{11}. Another aspect explored in this period was a lamellar model that describes the micromixing in CIJs, which enables fully resolved micromixing simulations using hydrodynamic data. This model considers the striation thinning and diffusion at the interface of the mixing fluids, enabling the resolution of all mixing scales.

Last, active mixing strategies in opposed jets mixers using the modulation of inlet flow streams were also studied, imposing a frequency and an amplitude.

Current Development

Experimental and numerical studies on the mixing mechanisms in CIJs showed that the necessary conditions for effective mixing are the balance of the opposed jets and the Reynolds number of the most viscous liquid stream. For CIJ, the critical Reynolds number of the more viscous liquid stream is above 150 for a viscosity ratio from 2 to 9. Fig.1 shows the Planar Laser-Induced Fluorescence (PLIF) images for a viscosity ratio 5. These PLIF images required the matching of refractive indices. Thus, it was needed to develop a Refractive Index Matching methodology using calcium chloride and introduce a set of equations to design the physical properties of the model fluids (density, viscosity and refractive index).

It was also made clear proof that the conditions for effective mixing in T-Jets mixers are mainly affected by the geometrical parameters. The jets in T-jets are bent before the contacting

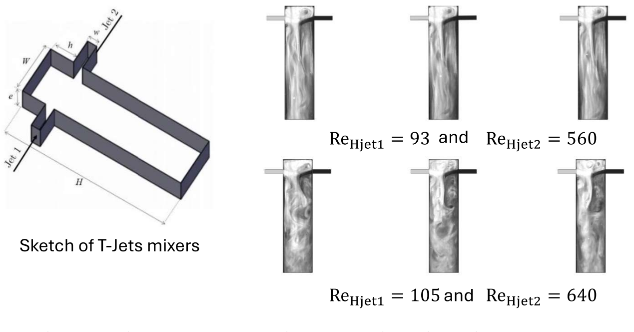

Fig 2. PLIF images of T-Jets mixers for a viscosity ratio 3.

point, and thus, the mechanisms for mixing dissimilar fluids are different.

From the evidence gathered in this work, the ratio of the physical properties of dissimilar fluids also affects the operation parameters for the onset of chaotic flow regimes. 3D CFD simulations of T-Jets mixers were performed and validated by comparison with experimental PLIF data. Fig.2 shows the experimental studies of mixing dissimilar fluids with a viscosity ratio 3 in T-Jets mixers. These results show that the chaotic flow regime is onset when two fluids are impinged at the centre of the chamber, and the conditions of the most viscous liquid stream must be above the critical Reynolds number.

The mixing scales were also assessed based on the flow dynamics and micromixing data. Furthermore, the effect of geometric parameters on the flow regime was further assessed, namely, the ratio between the mixing chamber width and jet width and the ratio of the chamber width to the chamber depth. It is now clear that the shear rate from the walls is an important factor for the onset of dynamic flow regimes; the vorticity generation for chaotic regimes feeds on the wall shearing. On the other hand, too much viscous dissipation hinders the chaotic flow dynamics. This study also proves that the mixing scales for this flow regime are set from the reactor design, of which the most important parameter is the ratio between the jet and chamber widths.

In this period, an analysis of the lamellar microstructure generated by CIJs was made using a Lamelar Micromxing (LM) model. This model was solved using striation thickness data from the models proposed by Lee and his collaborators (1980) and Baldyga and Bourne (1983) and compared with the experimental data reported by Nunes and his collaborators (2012). The LM model incorporates the description of chaotic mixing mechanisms in a 1D model and uses the transport equation with diffusion coupled to a space that warps the concentration gradients by the effect of the shear field, which causes the striation thinning of two reactant strias.

Results from the LM model show that the striation thickness function proposed by Lee gives the best estimation of the striation thickness evolution for a range of Reynolds number $200 < Re < 600$. The description of the micromixing from the LM model and the respective validation clearly show that this model could be used as a simulation tool in chemical reactors.

In CIJs, the turbulent energy for mixing is injected from the smaller scales of the inlet streams width and grows into larger vortices extending to the chamber width. The energy distribution associated with the flow scales mainly concentrates in the inertial sub-range, ranging from the injectors width to the mixing chamber width. This research introduces the control of the 2D turbulent energy spectrum from an external stimulus, the modulation of the jets' flow rate, which induces several dynamic behaviours. A new flow regime is induced from active mixing, where a state of resonance with a single flow frequency throughout the CIJs is associated with the formation of large vortices occupying the entire width of the mixing chamber. Fig.2 shows the externally induced resonance in the flow that sheds a street of vortices with the frequency of the inlet flow modulation.

This research will contribute to further implementing opposed jets in the industry, broadening the range of applications since different conditions can be set. This work was made in collaboration with Dr Cláudio Fonte, from the University of Manchester, who has vast experience in mixing in opposed jets mixers.

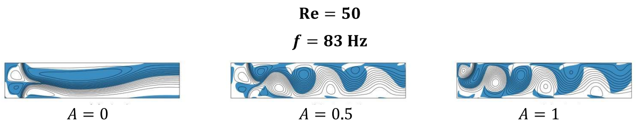

Fig 3. Streamlines and vorticity sign at Re=50 for different amplitudes and frequency 83 Hz.

Future Perspectives

Studies on the full range of flow conditions for the mixing of dissimilar fluids open prospects for implementing CIJs and T-Jets in industrial processes that involve the mixing of dissimilar fluids. For example, emulsification processes or gas-liquid systems. These results will enable to establish future collaboration with the food, cosmetics and chemical industries.

Research on the control of mixing scales and the turbulent energy spectrum from the modulation of inlet flow streams will open several prospects for the modulation of active mixing in static mixers. In the case of CIJs, chaotic flow can be onset from excitation frequency for lower inlet flow rates. This study will be extended to other heart technologies at LSRE-LCM, such as NETmix and T-Jets mixers. Sofia Brandão, PhD student, will perform these studies, supported by FCT scholarship 2023.00452.BD.

Based on these results, fundamental principles for active mixing will be developed from dynamic system analysis. Although very precise, full Computational Fluid Dynamics (CFD) simulations of active mixing in these modulated reactors require time-resolved intensive computational resources. Therefore, reduced order methods based on artificial intelligence will be implemented in the future.

Related Sustainable Development Goals

Outputs

PhD Theses

[1] Margarida Brito, *Mixing Mechanisms in 2D Reactors,* PDEQB, FEUP, 2021

Selected Publications

[1] Brito MSCA et al., Chemical Engineering Research and Design, 195, (2023);
[2] Brito MSCA et al., Chemical Engineering Journal, 465, 142892, (2023);
[3] Brito MSCA et al., Chemical Engineering Science, 258, 117756 (2022);
[4] Brito MSCA et al., Chemical Engineering and Technology, 45, 355-364, (2022);
[5] Brito M.S.C.A., Processes, 10, 1260 (2022).
[6] Brito, MSCA et al., Chemical Engineering Science, 211, 115299 (2020);
[7] Sultan, M.A. et al. Chemical Engineering & Technology, 42, 119-128, (2019);
[8] Brito, MSCA, Chemical Engineering Research and Design, 134, 392-404, (2018).

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Funding

HXmeso, POCI-01-0145-FEDER-030445, 2018-2022
2Dmix, POCI-01-0145-FEDER-016851, 2016-2019
LSRE-LCM Base Funding, UIDB/50020/2020, 2020-2023
LSRE-LCM Programmatic Funding, UIDP/50020/2020, 2020-2023
LA LSRE-LCM Funding, UID/EQU/50020/2019, 2019
LA LSRE-LCM Funding, POCI-01-0145-FEDER-006984,2013-2018
HyGreen&LowEmissions, NORTE-01-0145-FEDER-000077, 2021-2023
FCT Scholarships: PD/BD/135060/2017 (M. Brito)