Mixing Fundamentals

KEYWORDS: Static mixers; Lamellar Mixing, Stokes Regime,

Mixing in Split-and-recombine (SR) mixers and Confined Impinging Jets (CIJs) mixers was the basis for this fundamental research. Lagrangian Mixing Simulation was done using Lagrangian entities to describe convective mixing without the contribution of diffusion in CIJs as an advanced benchmarking tool. Basic flow structures (modes) of the dynamic flow regimes in these reactors were obtained from Proper Orthogonal Decomposition (POD). This analysis enabled a new vision of POD results and their application to the design of mixers. Regarding the experimental characterisation of mixing mechanisms in static mixers, new methods for Reactive Planar Laser Induced Fluorescence (RPLIF) technique were explored in this work. The analytical description of the flow in SR mixers was used to set a mixing design equation that enables the complete spatial description of mixing scales.

Introduction

Mixing is an important topic at LSRE-LCM, one that underlies many important contributions from this group to society. Driven by the development of technologies based on mixing science, several fundamental studies stemmed naturally aiming to have a better grasp of the mixing phenomena. Fundamental studies on mixing focused in split-and-recombine mixers and confined impinging jets (CIJs) mixers. This research has demonstrated the 2D mixing mechanisms based on the striation thinning of fluid lamellae for Stokes flow regimes in split-and-recombine mixers, and chaotic flow regimes in opposed jets mixers.

The 2D nature of flow and mixing in these reactors stems from the fact that the mixing dynamics are well-represented by 2D time-dependent maps, and the energy transfer mechanisms between flow scales are described from bidimensional turbulence theory.

The full simulation of the chaotic flow regime in 2D reactors requires a great amount of computing resources; thus LSRE-LCM has been focused on implementing methodologies to reduce the computation time and resources. Two methods have been implemented: Lagrangian Mixing Simulation (LMS) and Proper Orthogonal Decomposition (POD). LMS uses the velocity histories extracted from Computational Fluid Dynamics (CFD) simulations to characterise mixing through the measurement of interfacial area generation, interfacial area generation rate and calculation of mixing scales.

POD is a statistical operation that identifies the main characteristics of chaotic flows and separates them into a few modes decoupled from the flow dynamic. POD enables the reconstruction of the dynamic flow from modes related to coherent flow structures. These modes depict flow structures that are the basis of dynamic flow and associate an energy level with each one. Furthermore, the POD flow reconstruction enables a large compression of the flow data set.

Mixing mechanisms have also been studied from experimental work at LSRE-LCM. A reactive-PLIF method was explored in this work. Fluorescein and rhodamine B (RhB) are the two selected reactive tracers in PLIF experiments. Fluorescein is used as a marker in an acid-base reaction because its fluorescence is sensitive to the pH of the reaction medium. Variations in fluorescence will identify the pH changes in the reaction course. A second RPLIF method using RhB was also tested in this work. A Fenton reaction system that promotes the oxidation of RhB tracer and links the evolution of fluorescence emission regions to the contacting of reagents at the molecular scale.

Current Development

The flow in SR mixers was studied from a 3D CFD simulation using ANSYS Fluent. Mixing was simulated by setting the Volume-of-Fluid model. The geometry addressed consists of a network of 4 converging "T"s. The two working fluids have the same physical properties and are injected at Stokes flow regimes. CFD results show that a non-homogeneous striation thickness distribution is formed at the outlet of each mixing element. Fig.1 shows the striation thickness distribution, which is related to the velocity profile in a square section duct. The position of the interface between the two fluids was predicted from the mass balance in each mixing element using the analytical flow profile, resulting in a design equation for mixing in SR mixers:

$$\chi_i = \cos\left(\frac{1}{3}\cos^{-1}\left(1 + 4\chi_{i-1}^3 - 6\chi_{i-1}^2 - \frac{2^{1-n_{me}} r_s^{a_o}}{r_s+1}\right) - \frac{2\pi}{3}\right) + \frac{1}{2},$$

where r_s is the flow rate ratio, $i = 1\ to\ 2^{n_{me}+1}$, $a_0$is 0 if i is even or 1 if i is odd, $\chi_0 = 0$, and n_{me} is the mixing element. This work was developed during a placement of Margarida Brito (PhD student) at the University of Manchester from April

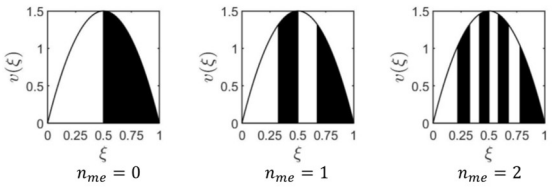

Fig 1. Production of unequal thickness strips due to the presence of a parabolic-like velocity profile in the channel of the SR mixer for different mixing elements, n_{me}.

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Mixing was analysed in CIJs from LMS, which uses particles to track the flow front between two fluids. The line formed by an ensemble of particles enables the calculation of the instantaneous rate of interfacial area generation between the fluids and the computation of segregation scales. LMS uses the Eulerian velocity field from 2D CFD simulation, which has a spatial resolution determined from the flow dynamics, for the simulation of mixing at scales that are several orders of magnitude below the CFD grid-scale. Fig 2. shows the injection of particles in CIJs for Re=600. Since only the interface between the two fluids is simulated, the LMS is orders of magnitude faster than the flow field simulation. This work applies LMS to 2D CFD simulations of the flow in CIJs for Re = 100, 300 and 500. LMS shows that the interfacial area generation is exponential for chaotic flow regimes (Re = 300 and 500) and linear for steady flows (Re = 100). Moreover, LMS can simulate segregation scales smaller than 10^{-8} m, i.e., LMS result spans and overcomes the entire range of spatial scales that have physical meaning.

LMS was adapted considering the diffusive scales, and the

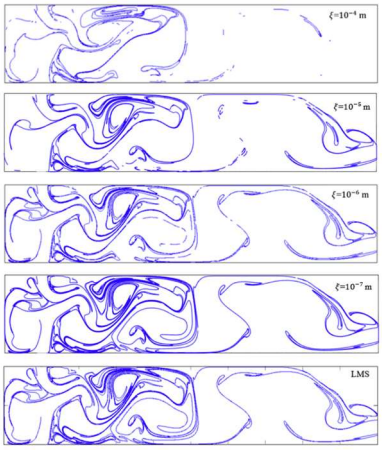

Fig 2. LMS and DLMS simulations of 2D CIJ reactors at Re=600 for a minimium striation thickness of $\xi = 10^{-7}$m to 10^{-4}m.

method Diffusive Lagrangian Mixing Simulation (DLMS) was introduced. In DLMS, the interface is only generated if the local segregation scale is above a threshold value, below which the contacting front between fluids is ruptured. The elimination of particles in diffusion-dominated regions makes DLMS more realistic, and the computation is faster than in LMS. To develop and illustrate the application of DLMS, 2D CFD simulations of the flow in CIJs reactors are used. The comparison between DLMS and LMS results is shown in Fig. 2 for the same flow condition, Re=600.

POD is applied to the flow in CIJs, aiming to extract average and coherent flow structures, enabling better insight into a mixer thoroughly studied from dynamic analysis tools and mixing simulation. This research explores the range of applications of POD in chaotic flows. It also explores the application of POD for flow data compression, which enables the usage of large data sets on post-CFD simulation mixing studies, e.g. with Lagrangian methods. Fig.3 shows the flow reconstruction from different modes and the original flow field. This research was developed in collaboration with Professor Alain Liné from INSA-Toulouse and Professor Cláudio Fonte from the University of Manchester.

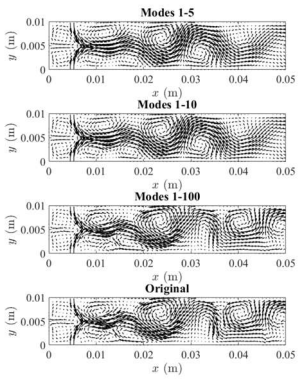

Fig 3. Reconstruction of flow for five residence times using 5 modes, 10 modes and 100 mode. The original flow field is also displayed.

Mixing mechanisms in CIJs were also studied from experimental flow visualisation. Reactive PLIF methods for micromixing visualisation studies were also tested and optimised from an acid-base reaction with fluorescein and Fenton's reaction, with rhodamine-B as a reaction-sensitive tracer. Both test reactions were studied in stopped-flow Acid-Base Reaction system

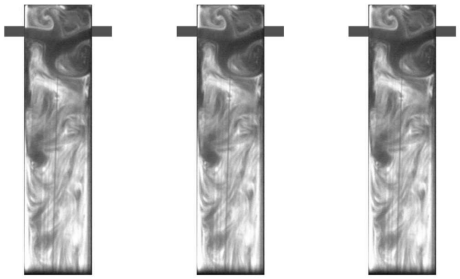

Fig 4. PLIF image obtained from acid-base reaction system and oxi-RPLIF method at Re=125 and Re=150, respectively.

equipment to define suitable operational conditions, namely the chemical composition of the inflow streams, the concentration of reagents and fluorophore, and suitable excitation light wavelength. Fig.4 shows the PLIF images from fluorescein test reaction systems. The mixing dynamics and the reaction course were visualised from the acid-base reactive PLIF images. For the Fenton reactive PLIF method, the streams are initially dyed with a tracer, and the reaction is assessed from the vanishing of the tracer and then the decrease of its emission intensity. So, this method also enables the assessment of the chemical reaction rate throughout the mixing chamber.

Nevertheless, the vanishing of the fluorescence does not give a clear visualisation of the chemical reaction and the generation of the interfacial area between the two fluid streams. This feature is handy in chaotic flow regimes where mixing occurs by interfacial area generation, and so the fluorescein method was preferred for the CIJs study. This research was a collaboration with Professor Isabel Nunes from the University of Aveiro.

Future Perspectives

In the future, LMS will be applied to further cases, namely NETmix and T-jets. POD will be further applied to NETmix and oscillatory flow reactors. Artificial intelligence algorithms will also be explored to predict the POD modes, enabling flow reconstruction and the simulation of the extended range of mixing conditions. Sofia Brandão, PhD student, will perform these studies, supported by FCT scholarship 2023.00452.BD.

Related Sustainable Development Goals

Outputs

PhD Theses

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

Selected Publications

[1] Brito M.S.C.A., Processes, 10, 1260 (2022);
[2] Ribeiro J.P. et al., 10, 1916 (2022);
[3] Brito MSCA et al., Chemical Engineering and Processing - Process Intensification, 170, 108714 (2022);
[4] Matos M.M. et al., Chemical Engineering Research and Design, 163, 307-319 (2020);
[5] Torres P. et al., Chemical Engineering & Technology, 42, 1709-1716 (2019);
[6] Matos J. et al., Chemical Engineering Science, 192, 199-210 (2018).

Team

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