Mixing in Chemical Reactors

NETmix – A Novel Network Static Mixer and Reactor

KEYWORDS: Continuous processes / Mixing fundamentals / Flow Dynamics / Mutiphase flows/ Chaotic mixing

NETmix is a mixing technology conceived and developed at LSRE-LCM, and patented in 2005. This technology brings new solutions to processes depending on mass and heat transfer rates and control. NETmix was used in the continuous production of nanocrystalline hydroxyapatite with high-throughput, continuous production of carbon dioxide hydrates, and in several areas at LSRE-LCM, namely on several nanomaterials continuous productions (MOFs, magnetite, calcium carbonate), encapsulation and emulsification, water treatment by ozonation, electrochemical reactions, and for photocatalysis applications.

This technology was orginaly studied regarding its ability for single phase flow mixing and heat transfer. In the period of this report, the studies on single-phase flow focused on the dynamic features of mixing and its interplay with NETmix's topology. Heat transfer was also further studied. The main focus was on developing and validating CFD models for multiphase flows in NETmix and their application to the characterization of these flows.

Introduction

NETmix is a network mixer based on cylindrical mixing chambers interconnected by prismatic channels. Each mixing chamber is fed by two inlet prismatic chamber and splits the outlet flow by two prismatic channels. An image of a NETmix with inlet channels alternately fed by water and tracer is shown in Fig 1. Mixing in NETmix is based on the impingement of jets issuing from the prismatic channels. Inside the chambers, the jets are engulfed by dynamic vortices at a mixing rate that can be quantified using Lagrangian techniques. At LSRE-LCM, some Lagrangian methods have been studied to benchmark mixing: Lagrangian Mixing Simulation (LMS) and Batch Lagrangian Mixing Simulation (BLMS). Furthermore, dynamic systems analysis has also been thoroughly applied to the single-phase flow in NETmix, comprising spectral analysis with Fourier Transform, Proper Orthogonal Decomposition (POD), phase diagrams and Lyapunov exponents. All these tools have been applied to build further knowledge into mixing in NETmix and also to assess the issue of the reactor geometry.

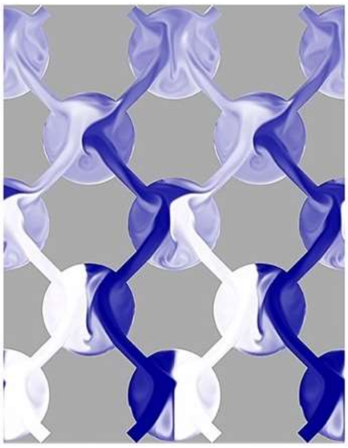

Fig 1.CFD simulation of mixing of a blue tracer in a NETmix reactor.

Many applications that were tried for NETmix are based on two-phase flows, most noticeably the continuous production of carbon dioxide hydrates, which is currently being exploited for industrial processes. Other multiphase applications include ozonation and emulsification processes. These technologies motivated the fundamental study of two-phase flows in NETmix.

Current Development

From the first works with static mixers at LSRE-LCM, it was known that operation at chaotic flow regimes required that a stream with a Reynolds number above 100 interact with an opposite stream in a space that allowed an expansion rate larger than 4. So, NETmix chambers were made with diameters generally larger than sixfold the inlet channels, but a thorough study on this dimension was missing. The NETmix design was optimised regarding the chamber diameter to channel width ratio, D/d. Because mixing in NETmix is quite efficient at chaotic flow regimes, tracer simulations always show high degrees of homogeneity, which makes it challenging to distinguish the mixing efficiency of several scenarios. The study of the impact of geometry on mixing was then based on Lagrangian methods and the assessment of the flow dynamics.

Fig. 2 shows the probability that a batch of particles injected from one inlet channel exits from the same or the opposite side outlet channel – BLMS. Results from the BLMS show that the best performance in NETmix occurs for 6.65≤D/d≤6.85, where the flow is equaly redistributed by both channels after mixing.

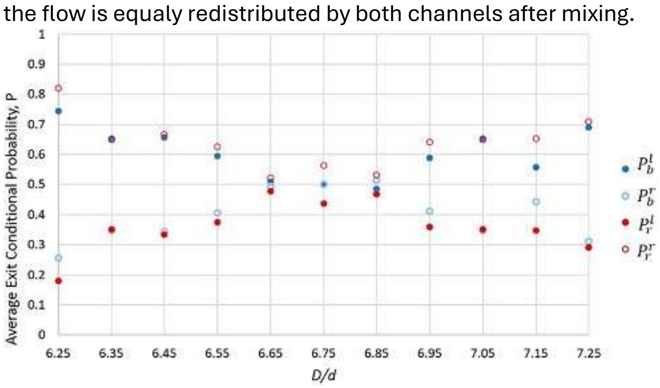

Fig 2. Effect of NETmix geometry on mixing.

Over the studied range of NETmix' geometries, a thorough analysis of the dynamic flow behaviour was made. This analysis considered phase diagrams (see Fig.3), Fourier transforms and Lyapunov exponents. A major finding from this study is contrary to the general belief that increasing turbulence enhances mixing. In NETmix, chaotic regular flows with more regular periodicity outperformed more turbulent ones. This is clear from the shape of the attractors in Fig. 3 and the mixing performance in Fig. 2.

NETmix is a technology stemming from fundamental research at LSRE-LCM, which experienced a fast industrial uptake. The industrial dissemination raised a large number of technical challenges that were not considered initially, for example the two-phase flow regimes for each set of operational conditions.

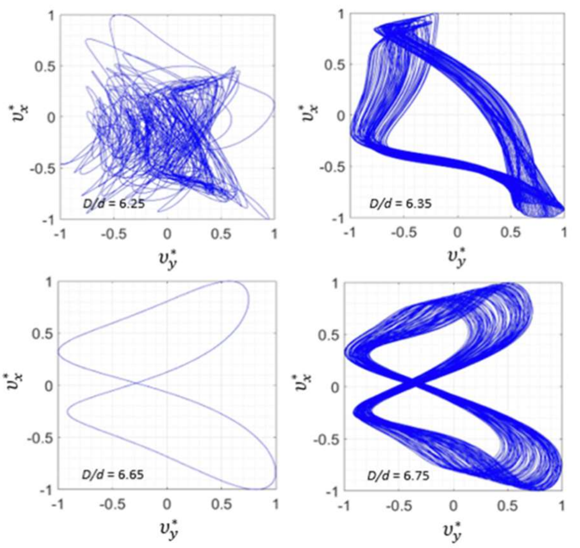

Fig 3. Phase diagrams of normalized velocity components for four NETmix' geometries.

During the period of this report, CFD models for the simulation of the two-phase flow were assessed and validated experimentally. The two-phase flow CFD models were based on the reduced geometry model Network Unit Block (NUB), which enables the simulation of very wide networks by setting periodic boundary conditions in the side walls of a single column of mixing chambers. The walls of the network elements play a key role in the flow regimes. So the Volume of Fluid model (VOF), which has interface reconstruction between phases, was the one that provided more knowledge on the flow, although at the expense of further computation hours in HPC clusters. Methods were assessed and developed to benchmark mass transfer in the two-phase flows. One method was based on the computation of shear rates in one of the phases, which are related to enhanced diffusion. Fig. 4 shows shear rate maps in one phase from a CFD simulation with VOF. The benchmarking of the best operational and design parameters resort to interfacial area generation rate, cumulative shear rate over the phases interface, or mean bubble diameter. Several operational parameters were simulated, such as Reynolds number, surface tension, and contact angle.

Although the reduced geometry NUB was used in the two-phase flow studies, each parameter studied in a CFD simulation with VOF took from one week to one month in a computational cluster. For this reason, and to make CFD simulation compatible with engineering practice, the model geometry was further decreased imposing further periodic conditions in addition to the side ones, now between the inlets and outlets – LoopNUB model. This poses new problems, for example how to set the flow rates of each phase. Methodologies were developed to address these issues, and the LoopNUB model was validated. The LoopNUB enables to address more complex situations for multiphase flows, namely the simulation of 3D geometries with heat transfer.

Future Perspectives

LoopNUB enables the complete descriptions of complex flow in NETmix (e.g. multiphase with heat transfer). This model will be further developed for additional cases of industrial relevance, e.g.: combustion, and electrochemical reactions.

Large heat transfer rate in NETmix and good control of mixing, make it a promising technology for lean combustion. Some cases were simulated in Joana Matos thesis, and in the short term they will be tested experimentally.

Research will be made to introduce mechanistic models that enable a more realistic simulation of mass transfer in multiphase flows.

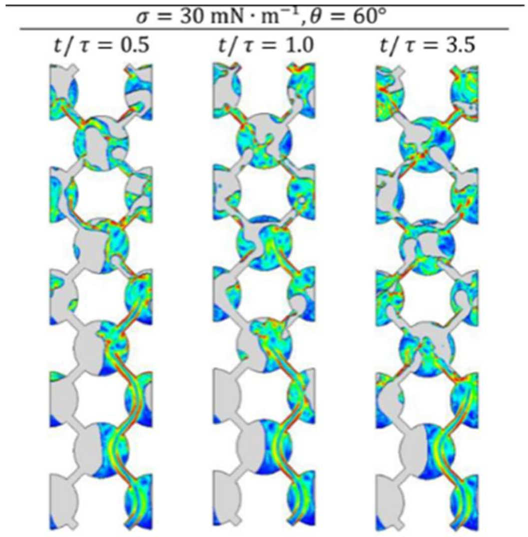

Fig 4. Maps of the shear rate in one phase for NETmix multiphase flow.

Related Sustainable Development Goals

Outputs

PhD Theses

[1] Joana Matos Silva, Mixing and Controlled Combustion in NETmix, PDEQB, FEUP, 2022

[2] Isabel Sousa Fernandes, Multiphase Flow in NETmix: mixing studies and applications, PDEQB, FEUP, 2023

Master Dissertations

[1] Sofia Brandão, Oscillatory NETmix Reactor: Fundamental studies on oscillatory NETmix reactor, MEQ, FEUP, 2022

Patents

[1] Lopes et al., Network heat exchanger device, method and uses thereof, 2018

Selected Publications

[1] J. Matos et al., Frontiers in Chemical Engineering 3, 771476 (2021)

[2] I.S. Fernandes et al., Chemical Engineering and Technology 44, 2002 (2021)

[3] I.S. Fernandes et al., Chemical Engineering and Processing - Process Intensification 194, 109580 (2023)

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