

Flow and Mixing in a Novel Intensified Passive Mixer-cum-Reactor

Chirag Khalde¹, Ajinkya Pandit², Jitendra Sangwai¹, Vivek Ranade²*

1 Indian Institute of Technology, Madras. Chennai 600036; 2 Queen's University, Belfast, BT9 5AG

*V.Ranade@qub.ac.uk

Highlights

- Developed a novel intensified passive mixer-cum-reactor.
- Comprehensive computational model was developed to investigate flow and mixing.
- Mixing performance was found to depend mainly on number of threads & Reynolds number.
- The model and results will be useful to optimize design of mixer-cum-reactor.

1. Introduction

Significant efforts have been and are being spent on developing intensified tubular reactors for continuous manufacturing of fine and specialty chemicals [1, 2]. The developed designs can be broadly grouped into two classes: a) active: uses moving surfaces to enhance mixing (rotors, vibrations etc.) and b) passive: uses geometrical configuration to enhance mixing. Passive mixing devices have several advantages over active mixing devices. Several designs and geometric configurations involving folding structures, serpentine channels, splitting and recombining flows and obstruction have been used [3]. Many of these designs involve formation of secondary vortices which result in local variations in heat transfer and concentrations. In this work, we have developed and computationally investigated flow and mixing in a novel intensified mixer-cum-reactor. The new configuration is based on combination of two: 'Kutta condition' and 'Searle principle' and is schematically shown in Fig. 1. The configuration involves inserting multiple threaded members placed concentrically in a tube/ pipe. The number of threads, direction of threads, thread depth, clearance between threaded member and tube wall and distance between subsequent threaded members are the key design parameters. The nose and aft part of the threaded member is conical (the angle of the cone is one of the key design parameters). The fluid flowing through this apparatus experiences a pinching effect in the near-nose

region. Later, swirling effect is experienced in the clearance between the threaded member and the wall. Mixing in this region is enhanced due to shearing effect. In the aft region of the threaded member, the conical tail allows the flow to continue in a swirling path imparted by the threads. There is a smooth change in the direction of swirl in the laminating layers in the region between the two members of



Figure 1. Schematic of proposed intensified mixer cum

opposite threading. The design offers an easy to fabricate tubular reactors with intense mixing, heat and mass transfer capabilities. In this work, we present key flow and mixing characteristics of the proposed novel mixer-cum-reactor.

2. Methods

The flow and mixing characteristics of the passive reactor, containing two units of modified geometry, has been simulated. Based on initial investigations of mesh sensitivity, a highly refined 3D unstructured grids (~27 million cells) were generated in ICEMCFD. The governing equations for steady state incompressible laminar flow were discretized using second order upwind scheme and solved using commercial CFD software ANSYS FLUENT. Water was considered as a working fluid. For mixing study, steady state simulations were carried out using 'species transport' model using steady state flow solutions obtained earlier. Input of tracer was imposed on the half part of inlet, which has same water properties with mass diffusivity of $2 \times 10^{-9} m^2/s$. This study was carried out for three threading units at four different values of Reynolds number (Re = 100x; $1 \le x \le 4$) to understand their effect on mixing intensity and flow dynamics.



3. Results and discussion

After establishing converged flow field, tracer simulations were carried out. A sample of results in the form of contours of tracer mass fraction at the inlet (Fig. 2a) and outlet (Fig. 2b) as well as path lines of fluid particles colored with tracer mass fraction (Fig. 2c) are shown in Fig. 2. As fluid flows through the mixer, it is forced to follow the helical motion of the fluid streams resulting in enhancement in lamination (in the

threaded region) and engulfment (in the region between the members of opposite threading). The tracer contours shown in Fig. 2a and 2b clearly indicate the mixing effect and trails of the swirling effect induced in the flow. The swirling effect on the flow is generated not only in the aft, but also in the front side of the member. This effect can be attributed to the tendency of the fluid to divert itself towards the threading direction due to the generated pressure distribution. Thereby, fluid experiences swirling and impinging effect together at the near front nose region. No secondary vortices or dead zones are formed.

Mixing realized in the reactor was quantified by evaluating mixing intensity (I_M) profile along the reactor length. The mixing intensity was defined as:

$$I_{M} = 1 - \sqrt{\frac{\sigma^{2}}{\sigma_{\max}^{2}}}; \text{ where } \sigma^{2} = \frac{1}{|A|} \int_{A} (m - \overline{m})^{2} dA \qquad (1)$$

Extensive simulations were carried out to quantify influence of key design and operating parameters on mixing performance. The number of channels present in the design plays a pivotal role in deciding the mixing capability. A sample of simulated results is shown in Fig. 3. Improvement in I_M can be realized by increasing the number of channels (Fig. 3a). Influence of Reynolds number on I_M is more complex because of interaction between residence time and improved mixing rate. Increase in Re improves mixing but reduces residence time thereby providing less time for mixing to occur (Fig. 3b). Simulated results were critically analyzed to evolve guidelines for tailoring mixing in the proposed mixer-cum-reactor as desired.

4. Conclusions

The developed passive mixer-cum-reactor mixer looks promising for achieving enhanced mixing and heat transfer characteristics for single as well as multiphase flows. Secondary vortices or dead zones are avoided by the unique combination of swirl, change of directions and pinching effect. Another unique feature of the reactor is that it can also be configured in multi-stage units and can be easily scaled up/down.

References

- [1] Ranade, V.V., M.K. Sharma and A.A. Kulkarni, Chemical Engineering Journal, 278 (2015) 454-468.
- [2] R.P. Utikar, V.V. Ranade. ACS Sustainable Chemistry & Engineering, 5 (2017) 3607-3622.
- [3] C.Y. Lee, W.T. Wang, C.C. Liu, Fu, L.M, Chemical Engineering Journal 288 (2006) 146–160.

Keywords

Passive mixer-cum-reactor, no back flow, easy to assemble, intense mixing







Figure 3. Mixing intensity plots: (a) Variation in I_M with Re for different threading configurations; (b) Variation of I_M along the length of the reactor at different Re