



## Numerical investigation of turbulent reactive mixing in a novel coaxial jet static mixer



Minmin Zhou<sup>a,b</sup>, Dehong Bai<sup>a</sup>, Yuan Zong<sup>a,\*</sup>, Ling Zhao<sup>a</sup>, Jeremy Nicholas Thornock<sup>b</sup>

<sup>a</sup> State Key Laboratory of Chemical Engineering, East China University of Science and Technology, Shanghai 200237, PR China

<sup>b</sup> Institute for Clean and Secure Energy, Department of Chemical Engineering, University of Utah, Salt Lake City 84112, USA

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### ABSTRACT

In the fast reaction category, the turbulent reactive mixing strongly affects the reaction products yield and distribution. The present work adopts a high-efficiency vortex structure induced by a novel static mixer – hollow cross disk (HCD) to enhance the turbulent reactive mixing within the tubular turbulent flow. Specifically, the direct quadrature method of moments (DQMoM) coupled with the interaction-by-exchange-with-the-mean model (IEM) is utilized to simulate the consecutive competitive reactions system in this tubular turbulent flow. In order to quantitatively evaluate the enhanced mixing effect of the HCD, the turbulent reacting flows in the Kenics static mixer and coaxial jet mixer have also been studied. A combining analysis of turbulent flow field and the chemical species distribution indicates that the turbulent mixing enhancement mechanisms of these two static mixers. The simulation suggests that the sinusoidal wave structure in the HCD generate an important flow structure-counter vortex pairs (CVPs), which increases the momentum exchange between the near-wall region and the flow core. Moreover, the spatial distribution of the mixture fraction and reaction product concentration in these configurations agrees well with its turbulent flow field characteristics. The improved turbulent mixing initially is located at the jet periphery when at  $0 < z/D < 2$ , which fits well with the HCD's longitudinal evolution of turbulent energy dissipation. Whereas at  $z/D > 2$ , CVPs of the HCD ameliorate the near-wall area's turbulent mixing and thus increase the reaction productivity and selectivity. Additionally, the effects of flow rate on segregation index are studied to suggest that the improvement of  $X_s$  for HCD is of about 35% relative to the original tubular flow.

### 1. Introduction

Mixing processes involving chemical reactions occur widely in many industrial applications, such as chemical engineering, pharmaceuticals and particle synthesis. Since the chemical reaction is a molecular-scale phenomenon, reactants, initially presented in separate solutions, can only encounter each other through the action of molecular diffusion [1]. According to the responsibilities of the three scales of turbulent mixing, mixing on small-scale can directly affect the reaction course which entails the engulfment and deformation of the eddies near Kolmogorov scale as well as molecular diffusion. While mixing mechanisms on larger scale, i.e. macro- and meso-mixing, which are responsible for breaking up the fluid elements and convecting them into the space of interest, have indirect influence by changing the environment for local mixing [2,3]. Therefore, it is possible to enhance chemical reaction selectivity by modifying the mixing conditions in many practical applications. This relationship is of particular significance for reactive turbulence flow [4]. When the time scale of the reaction (or

characteristic times) is of similar magnitudes of mixing, both mixing conditions and chemical kinetics determine the distribution of reaction products [5,6]. In this sense, the characteristics of reactive turbulence can be not only represented by its energy cascade, but also by the species distribution during the reaction. Specially, the macro-mixing process and meso-mixing process can be characterized by the mixture fraction and turbulence kinetic energy, respectively. And the local micro-mixing status is governed by the local turbulence energy dissipation rate and the species spatial distributions [7,8].

More generally, higher turbulence level and low viscosity solvent can promote rapid mixing. A wide range of static mixers and multi-functional heat exchangers/reactors (MHE/R) have been employed as turbulence promoter to enhance turbulence level and improve the mixing efficiency [9–11], such as twisted tape [12], winglet-type configuration [13], fins [14], nozzles [15]. The behind mechanisms have been reported to lead a more energetic efficient flow structure, which mainly promote secondary transverse flow and thus enhance the mass and heat transfer rate [11]. Recently, high-efficiency vortex (HEV)

\* Corresponding author.

E-mail addresses: [Minmin.Zhou@utah.edu](mailto:Minmin.Zhou@utah.edu) (M. Zhou), [zongyuan@ecust.edu.cn](mailto:zongyuan@ecust.edu.cn) (Y. Zong), [zhaoling@ecust.edu.cn](mailto:zhaoling@ecust.edu.cn) (L. Zhao).

static mixer has drawn so much interests for a better reaction control, improved selectivity, byproduct reduction and enhanced safety advantages [10,16–18]. Its intensification mechanisms stems from the artificially generated vortex structures which are caused by the pressure difference and the shear-instability-driven flows generated by Kelvin–Helmholtz instabilities [8,19]. Such vortex generators (VGs) have already been successfully applied to enhance the heat transfer in MHE/R [11,20–22].

In other aspects, some research show the turbulent mixing mechanism of these VGs that is much closed related with improving chemical reactions selectivity and yields [7,8,17,20]. Habchi's research [8,20] analyzed the fluid mechanisms or energy dissipation characteristics by numerical simulation methods to understand the mixing mechanism of static mixers. Other researches adopt the chemical probe method [23] to investigate turbulent reactive mixing of VGs [25]. The chemical probe method usually involves a competitive-consecutive or competitive-parallel reaction system. The representative example reaction systems are naphthol/sulphanilic acid [26] and iodide/iodate reaction system [23,27]. Such competitive reaction system usually includes a pair of competitive reaction. Commonly, a clear distinction of reaction rate constant is available between each reaction in the system. Thus, the local mixing can regulate the reaction course [24]. If local mixing is perfect, only the fast reaction occurs while the slower reaction hardly happens. On the contrary, when the mixing is slow and non-ideal, the slower chemical reaction takes place and the slow reaction products are formed, which are determined by the competition between local mixing extents with slower reaction kinetics. This present research designs a novel VG–hollow cross disk (HCD) and adopts the competitive-consecutive reactions system to explore the turbulent mixing performance of HCD.

The complexity of experimental measurements on the mixing of turbulent reacting flows impels numerical research on it. Current numerical methodology adopted for reactive turbulence flow is separating the velocity and scalar quantities into resolved and unresolved components. In order to close the solution of the reacting flows, the chemical source terms that appear in the scalar and energy transport equations should be modeled. Among the close models for the chemical source term, probability density function (PDF) method, coupling a transport equation of one scalar quantity, represents an alternative to simulate the reactive turbulence flow [28]. Due to the high dimension of the PDF equation by this method, Monte Carlo technique is usually required, which is computationally expensive even if the multi-processor computers are used [29]. The direct quadrature method of moments (DQMOM) is a evolution of the finite-mode PDF approach introduced by Marchisio and Fox [28,30] in the context of the population balance equation (PBEs), which is categorized as a presumed probability density function (PDF) approach. CFD model can use low-order moments to represent the PDF and also couples with the micro-mixing model to predict the turbulent reacting flows [31–33]. This method does not introduce significant statistical error and is amenable to the existing CFD code due to its computationally affordable cost [34,35]. In order to represents the exchange rate between the interested laminated structure with it surrounding fluid elements by either engulfment or a turbulent dispersion mechanism [36], interaction by exchange with the mean (IEM) model is adopted in the present work [37–39]. Because of its attractive features of this method, DQMOM-IEM method have been successfully applied for predicating turbulent reactive flows [36,34,31,32]. However, to the best of the knowledge, investigation of the turbulent reaction performance of multi-functional heat exchangers by CFD is still rare.

In the present work, a novel VG–hollow cross disk (HCD) is designed to enhance a reactive turbulent channel flow, which consists of a connected set of wavy faces of HCD located near the wall, which is expected to induce efficient flow structure in tubular reactor. In order to explore the performance of HCD as an internal for chemical reactor, it is necessary to characterize its mixing performance at different scales. The

DQMOM-IEM model is coupled with the commercial CFD code fluent, as a closure of the chemical source term so that the turbulent flow field and the chemical species distribution in the reactor can be analyzed. This paper is organized as follows. Section 2 introduces the key features of DQMOM-IEM for the turbulent reacting flows. Section 3 gives the numerical details of the computation model, as well as validation tests. Section 4 is divided into three sub-parts, i.e. momentum transport, turbulent reactive mixing and comprehensive performance. Section 5 draws the conclusions of the paper.

## 2. Theoretical background

### 2.1. Governing equations

The simulation of the three-dimensional turbulent flow field is based on the solution of Reynolds Averaged Navier–Stokes (RANS) equations for the incompressible flows, closed with standard  $k - \epsilon$  turbulent model. The general form of governing equation can be expressed by:

$$\frac{\partial(\rho\phi)}{\partial t} + \frac{\partial(\rho U_j \phi)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( D_\phi \frac{\partial \phi}{\partial x_j} \right) + S_\alpha, \quad (1)$$

where  $\phi$  is the averaged desired function for mass, momentum, energy, turbulent kinetic energy and dissipation rate of turbulent kinetic energy.  $D_\phi$  is the effective diffusion coefficient, and  $S_\alpha$  is a term accounting for different-nature sources.

### 2.2. Reactive mixing model

#### 2.2.1. Competitive-consecutive reactions

Bourne et al. [26] proposed a unique fast competitive-consecutive reacting system with naphthol (A), diazotised sulphanilic acid (B), 4-(4'-sulphophenylazo)-1-naphthol (P), and 2,4-bis(4'-sulphophenylazo)-1-naphthol (S), respectively. The reaction system comprises of two steps and the reaction kinetic can be described as follows:



$r_1$  and  $r_2$  are reaction rates for  $R_1$  and  $R_2$ , respectively. The reaction system is initiated by adding species A as the limiting reactant and species B is in stoichiometric excess to A. The primary products (4-(4'-sulphophenylazo)-1-naphthol) is formed first and then coupled with B to form side products (2,4-bis(4'-sulphophenylazo)-1-naphthol (S)) Given at  $T = 298 \text{ K}$  and  $pH = 10$ ,  $k_1 = 7.3 \times 10^3 \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}$  and  $k_2 = 3.5 \text{ m}^3 \text{ mol}^{-1} \text{ s}^{-1}$ , which is buffered in  $\text{Na}_2\text{CO}_3/\text{NaHCO}_3$  solution. The mixing efficiency is quantified by the segregation index,  $X_S$ , which is defined as [3]:

$$X_S = \frac{2C_S}{2C_S + C_P}, \quad (4)$$

where  $C_S$  and  $C_P$  refer to the concentration of species S and species P.  $X_S$  varies between 0 for perfect mixing and 1 for total segregated status. In the test condition, the injected species (A) will be instantaneously consumed by reaction  $R_1$  and then reaction  $R_2$  does not occur, which delivers null  $X_S$ . In this sense,  $X_S$  as the selectivity of reactions represents the amount of fluid in the partially segregated stage, which can reversely reflect the multi-scale mixing performance [40,41].

The reaction progress variables  $Y_1$  and  $Y_2$  for reaction  $R_1$  and  $R_2$  respectively, are defined the range of [0,1] and its value is related with the reaction rate constant. Combining the reaction progress variables ( $Y_i$ ) of each reaction with the mixture fraction can describe each reaction extent [28,31].  $\xi_{st}$  refers to the stoichiometric mixture fraction. Their definitions are given as follow:

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