

Investigation of turbulent reacting mixing processes at high Schmidt numbers in a coaxial jet mixer using OpenFOAM

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Abstract

Turbulent mixing of fluids plays a dominating role in a large number of engineering devices such as combustion chambers, burners, injection systems and heat exchangers. Especially in the context of chemical applications exploration of physical mechanisms of mixing processes is extremely important to control the chemical reactions. Solution of this problem is based on detailed analysis of both hydrodynamics in the mixing device and behaviour of chemical reactions. These two processes are strongly coupled.

The aim of this work is the investigation of hydrodynamic and chemical aspects as well as their interactions in turbulent reacting mixing processes at high Schmidt and Reynolds numbers. The mixing device is a classical coaxial jet mixer (see figure 1(a)) consisting of a nozzle of diameter d positioned along the centerline of a pipe of diameter D with the length L . It provides excellent mixing properties due to strong vortices appearing at the jet boundary as a result of the instability of the shear layer. From dimensions analysis it can be shown that the characteristics of the jet mixer depend for the isothermal case on the following parameters: the diameter ratio D/d , the Reynolds number related to the nozzle flow $Re_d = du_d / \nu$, the Schmidt number Sc and the flow rate ratio V_D / V_d , where the jet velocity (nozzle) exceeds the coflow one (pipe). Two following mixing regimes can be observed. The flow similar to a free jet (hereinafter called j-mode) appears if $D/d < 1 + V_D / V_d$ (see [2] and [3]). Otherwise if $D/d > 1 + V_D / V_d$ a strong recirculation zone is created just behind the nozzle (hereinafter called r-mode). The r-mode is often used to accelerate the homogenization of fluids because the recirculation enhances the mixing efficiency drastically so that the homogeneous state is already reached after some pipe diameters downstream of the nozzle. On the contrary the j-mode is more useful to control the progress of chemical reactions.

The mixing of scalars has already been thoroughly investigated both experimentally (LDV, PLIF) and numerically in a number of previous works published by the authors (see, for instance, [12], [5], [9] and [7]) and presented at THMT05 [11] and THMT09 [10] respectively. Despite of efforts in the development of new scalar mixing approaches in the last years, there are only few models available which can (accurately) predict the amount of molecular mixing at varying Schmidt numbers. However, no modeling is needed if using direct numerical simulations but all scales up to the batchelor scale ($\lambda_B = \eta Sc^{-1/2}$) where the molecular diffusion takes places have to be resolved. Considering flows at high Reynolds numbers and high Schmidt numbers ($Sc \sim 1000$ for water) a DNS becomes impracticable due to the necessary high grid resolution. In the present study large eddy simulations have been done using an extended dynamic mixed model (DMM) which was also applied to the scalar dynamics of the flow. The DMM contains a special clipping procedure based on Taylor series approximation to improve the stability of LES computations [6]. The simulations were performed in j-mode at $Re_d = 12000$, $Sc \sim 1000$ and $V_D / V_d = 5$. A simple irreversible neutralization reaction of acid and base was chosen as representative reaction case to investigate the turbulence chemistry interaction. The variation of the density and thermal effects can be neglected due to small inlet concentrations of reagents. The chemical closure is modelled in terms of an eddy dissipation concept which slows down the chemical reaction rate whenever it is faster than the micromixing rate.

Figure 1(b) shows the profile of the passive scalar (mixture fraction of acid and base) obtained from LES and experiment along the x-axis at the centerline of the pipe. As seen f remains constant in the initial jet region at $x/D < 0.6$. The interior of the jet contains only acid. The chemical reaction takes place on the boundary between the jet and the coflow. At $x/D > 0.6$ the mixing arrives the jet centerline and it is completed at $x/D > 7$ with the formation of a homogeneous mixture. LES prediction for f agrees well with measurements. However, the performed frequency analysis of the passive scalar (see figure 1(c)) doesn't show a k^{-1} spectrum in the viscous-convective sub range (defined by $1/\eta < k < 1/\lambda_B$) in the energy spectrum which is suggested by Batchelor's theory. Antonia and Orlandi [1] note that there is no consensus yet in the literature concerning Batchelor's spectrum in the viscous-convective range for weakly diffusive scalars at high Schmidt numbers.

Figure 1(d) shows the concentration of the reaction product along the centerline of the jet mixer in the j-mode. The LES results are compared with experimental data obtained using PLIF and titration method [4]. The chemical reaction

along the centerline starts to proceed in the region where the mixing caused by the strong vortices in the mixing layer arrives the centerline and the mixture fraction becomes less than one.

The discrepancy between simulations and measurements can be explained by two following reasons. First it should be noted here that the comparison between measurements is reasonable at the distance larger than $x/D > 1$. The measurements at the initial distance $x/D < 1$ are not quite reliable due to a well-known drawback of the titration method used in the experimental setup. The method holds true well provided that the product concentration exceeds a certain threshold resulting in a rapid change of the pH value of the water solution. Below this threshold the measurements are not sensible to the product concentration variations. This is the case at the small distances x/D . Within this region the numerical results might be more accurate than the experimental ones. Second, the reason for the discrepancy can be drawbacks of the micromixing model used in calculations. The analysis of experimental data revealed a relatively large discrepancy between the product directly measured and the product calculated using the mixture fraction at resolution of 300μ . It means that the micromixing effects are not negligible and can be essential although the reaction is very fast.

For identification of possible additional involved structures the flow domain has been analysed with the help of the proper orthogonal decomposition (POD) applied to the velocity and pressure fields. To reduce the complexity of the calculations the method of Sirovich [8] was used. A typical isosurface of the POD pressure mode for the jet mixer is shown in figure 1(c). It shows the characteristic rollup in the shear layer between the jet and coflow up to the point of the jet's breakup. These vortical structures appearing chaotically in time and in the space are manifested themselves as the big recirculation zone in the time averaged velocity field.

The results of the presented study demonstrate that the OpenFOAM package is a very attractive tool for simulation of mixing, homogenisation and reacting turbulent flows in chemical engineering applications.

Key words: LES, turbulent mixing, Schmidt number, chemical reaction

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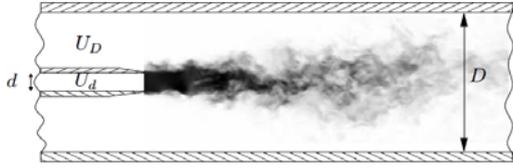


Fig 1 (a)

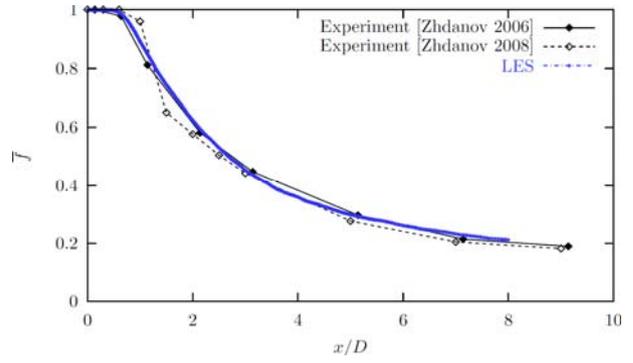


Fig 1 (b)

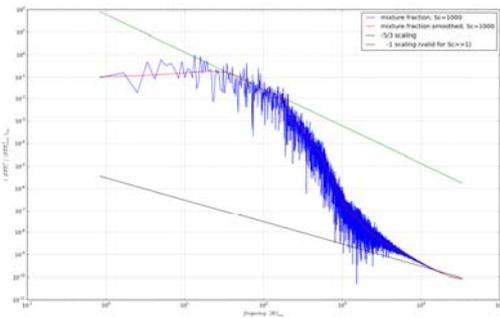


Fig 1 (c)

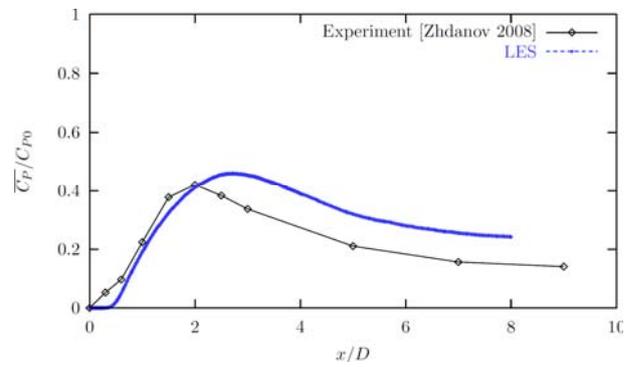


Fig 1 (d)

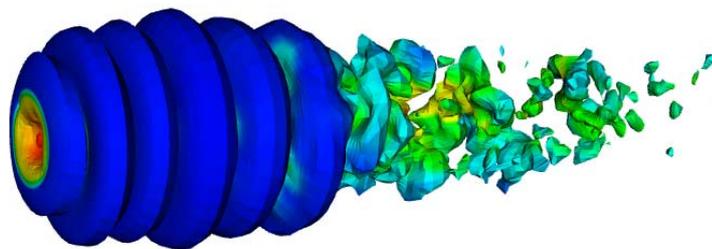


Fig 1 (e)