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A SEMI-LAGRANGIAN SCHEME FOR FLUID MIXING IN LAMINAR MICROFLOWS

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Numerical simulation of fluid mixing is of primary importance for many microfluidic devices. However, the current computations still encounter severe difficulties in the accurate prediction of high-Péclet (Pe) fluid mixing problems. The main error factor in the conventional grid method (*e.g.,* finite volume method) is the numerical diffusion, which causes significant overestimation of molecular diffusion with insufficient grid resolution. The criterion of the grid size becomes extremely large in high-Pe conditions, and it is quite difficult to obtain the accurate solution for Pe $> 10^5$ using the conventional grid method even with a cluster.[1]

In this study, we developed a novel semi-Lagrangian method for accurate simulation of fluid mixing in laminar flows. The method assumes that the concentration of chemical species can be treated as a passive scalar governed by the advection-diffusion equation, and the velocity field is given. Its discretization scheme, which we call the trajectory-based fractional discretization scheme[2], consists of a grid-based expression of a Laplacian with a spatial interpolation and a Lagrangian expression of convective transport by backward tracer particle tracking as illustrated in Fig. 1.

The proposed method is validated through two different test cases. One is the parallel two-fluid mixing in the two-dimensional uniform flow. In this problem, the analytical solution is given and the computation error can quantitatively be checked. As a result of this two-dimensional test, the present method is shown to provide accurate solution without numerical diffusion for any grid orientations with low grid resolution. Fig. 2 shows the absolute mixing index (MI)[3] error with respect to the analytical solution, where A and B indicate different grid orientations. Its accuracy is comparable with that of finite volume method using optimum grid system, and the order of convergence is 2.

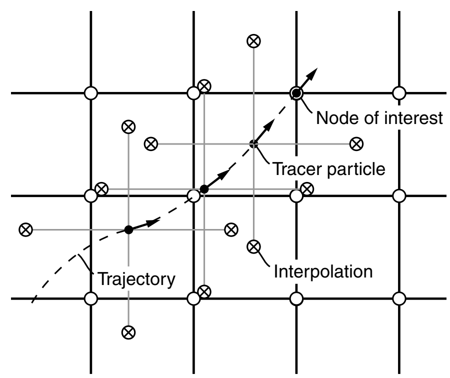

Figure 1: Schematic of the trajectory-based fractional discretization scheme

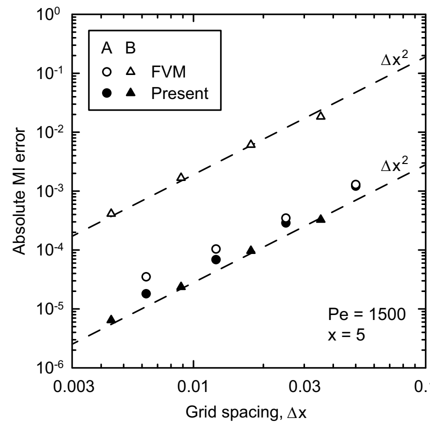

Figure 2: Absolute MI error with respect to the analytical solution for parallel two-fluid mixing

The other test is the three-dimensional engulfment flow mixing at Re = 200 in the T-shaped micromixer[4]. In this problem, we carried out reference simulations using the backward random-walk Monte Carlo method[5]. That is because the Monte Carlo method is a powerful computation technique that can simulate fluid mixing behavior very accurately without numerical diffusion by means of calculating a large number of particle trajectories according to the stochastic equation including the Wiener process. In this three-dimensional test, the present method is shown to provide accurate results comparable well to those obtained using the Monte Carlo method. Moreover, the Monte Carlo method requires a severely long computation time, whereas the present method achieves equivalent accuracy in a shorter computation time.

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