A SEMI-LAGRANGIAN SCHEME FOR FLUID MIXING IN LAMINAR MICROFLOWS

Takuya Matsunaga*, Koichi Nishino2 and Seiichi Koshizuka1

1 Department of Systems Innovation, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan, matsunaga@mps.q.t.u-tokyo.ac.jp
2 Department of Mechanical Engineering, Yokohama National University, 79-1 Tokiwadai, Hodogaya-ku, Yokohama-shi, Kanagawa 240-8501, Japan, nish@ynu.ac.jp

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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 $\text{Pe} > 10^5$ 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.
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.

REFERENCES


