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Lamellar modelling of mixing processes in chaotic flows

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The development of CFD techniques and the rapid increases in computational speeds is making increasingly complex flows accessible to simulation. However, for processes with fast kinetics and slow rates of diffusion (which are often mixing sensitive), simulation of the detailed concentration distributions associated with the mixing processes is often intractable or limited to situations where the mixing is poor. A Eulerian approach may be considered, where the convection diffusion equations are solved to find the concentration distribution. For systems with rapid mixing however the length scales of concentration fluctuations will rapidly fall to below the mesh size and the simulation will become highly inaccurate. Alternatively a Lagrangian approach may be used, where the boundary between two segregated fluids is followed in the absence of diffusion processes. In this case the length of the boundary will grow exponentially, leading to excessive memory requirements. Consequently 'micromixing' models are often used where the length scales are estimated from turbulence parameters.

In this study we present a new Lagrangian approach using stretch rates to determine the local lamellar structure, and from this the local micro-scale concentration distribution can be accurately calculated. To achieve this the deformation of an element of fluid moving in the flow is calculated and the orientation of maximum stretching rate of the fluid element is determined. This orientation corresponds to the local orientation of the lamellar structure at the fluid element location. A small fluid line perpendicular to this lamellar structure is then simulated backwards in time to the initial conditions. From the initial distribution of the segregated fluids and the stretch rates, the local lamellar structure at the fluid element location can be accurately calculated. Using a one dimensional simulation of the convection diffusion processes along the line across the lamellae, the concentration variation in this lamellar structure can also be calculated with a high degree of accuracy.

This approach has been developed by considering two-dimensional deterministic chaotic flows. For these flows the method has been shown to predict the local lamellar structure with a high degree of accuracy. Current work will evaluate the approach for CFD simulations of unsteady laminar flows. Further work will be needed to broaden the applicability to three-dimensional flows, direct numerical simulations of turbulent mixing, and to model diffusion and reaction processes.

Keywords: Chaotic advection, lamellar modelling, mixing, micromixing.