Finite volume scalar mixing simulations with a lattice-Boltzmann Navier-Stokes solver

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Mixing is a common operation carried out in the oil, chemical and petrochemical industries. It may be used to achieve a degree of homogeneity as in blending or to promote heat and mass transfer. The focus of this work is on scalar mixing in liquid systems. The challenge is in the prediction of turbulent scalar mixing in complex geometries (e.g. mixing time or solubility of salts in a stirred tank).

The single-phase flow is solved with a lattice-Boltzmann numerical solver[1], which provides a discretized solution to the momentum balances. The scalar convection-diffusion equation is solved with an explicit finite-volume method on the lattice-Boltzmann grid.

Prediction of scalar mixing in liquid systems (e.g. blending of two miscible liquids) by means of a finite volume formulation is a challenge in itself. Despite their unconditional stability, various schemes (e.g. first order upwind[2], hybrid[2], power-law[2]) for discretizing the convection term are notorious of their generation of false diffusion, which may exceed the molecular diffusion in liquid systems (that can have Schmidt numbers up to $Sc=10^3$, i.e. a scalar diffusivity that is much lower than the viscosity) by some orders of magnitude. Next to the first order power-law and second order QUICK[3] schemes, a high-resolution TVD[4] scheme was explored in a direct simulation of cavity flow. The latter scheme greatly reduced false diffusion and remains stable.

In strongly turbulent flow the smallest scales need to be modeled to keep the computational cost at an acceptable level. We use the well-known Smagorinsky[5] subgrid-scale model, which is embedded in the lattice-Boltzmann scheme. The Batchelor scale (which is the smallest scale of scalar transport) is typically 30 times smaller ($Sc=10^3$) than the Kolmogorov scale, and hence it is expected that the influence of the scalar subgrid-scale fluctuations on the resolved-scale scalar field is larger than the influence of the subgrid-scale velocity fluctuations on the resolved-scale velocity field. From this, it is reasonable to take a turbulent Schmidt number to be smaller than unity (we chose 0.7).

Two LES flow cases have been considered: a plane channel and a mixing tank. In channel flow, results with the various scalar transport discretization schemes will be compared and numerical diffusion effects will be highlighted. In a mixing tank we need to deal with complexly shaped boundaries. Results with stair-stepped walls, as well as with a ghost-cell technique that models the boundaries that are not aligned with the grid more accurately will be discussed.

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