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Incomplete Mixing and Reactions - A Lagrangian Approach in a Pure Shear Flow

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Incomplete mixing of reactive solutes is well known to slow down reaction rates relative to what would be expected from assuming perfect mixing. As reactions progress in a system and deplete reactant concentrations, initial fluctuations in the concentrations of reactions can be amplified relative to mean background concentrations and lead to spatial segregation of reactants. As the system evolves, in the absence of sufficient mixing, this segregation will increase, leading to a persistence of incomplete mixing that fundamentally changes the effective rate at which overall reactions will progress. On the other hand, nonuniform fluid flows are known to affect mixing between interacting solutes. Thus a natural question arises: Can non-uniform flows sufficiently enhance mixing to suppress incomplete mixing effects, and if so, under what conditions? In this work we address this question by considering one of the simplest possible flows, a laminar pure shear flow, which is known to significantly enhance mixing relative to diffusion alone. To study this system we adapt a novel Lagrangian particle-based random walk method, originally designed to simulate reactions in purely diffusive systems, to the case of advection and diffusion in a shear flow. To interpret the results we develop a semi-analytical solution, by proposing a closure approximation that aims to capture the effect of incomplete mixing.

The results obtained via the Lagrangian model and the semi-analytical solutions consistently highlight that if shear effects in the system are not sufficiently strong, incomplete mixing effects initially similar to purely diffusive systems will occur, slowing down the overall reaction rate. Then, at some later time, dependent on the strength of the shear, the system will return to behaving as if it were well-mixed, but represented by a reduced effective reaction rate. If shear effects are sufficiently strong, the incomplete mixing regime never emerges and the system can behave as well-mixed at all times.