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Mixing and reactions: The case of Taylor dispersion in a tube

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The progression of reactions in systems where mixing occurs has been the subject of investigation for decades; however, there is still much that is unknown about such systems. One area of particular interest to us is the influence of the initial configuration of a system as it evolves in time. Many (if not most) investigations of mixing are formulated at the *long time* limit, which requires that a certain amount of relaxation of the system has occurred. Although this is an interesting regime that has relevant to, for example, reactions occurring in the subsurface, it does not describe the initial phases of mixing well.

In this work, we examine how the initial configuration of a system can influence the mixing and reaction process evolution. Such *early time* conditions have relevance to many systems. For example, in industrial processes the basic design constraints of mixing facilities essentially requires that the mixing regime is dominated by early time behavior (e.g., the effective reaction rate for multi-component injections into tubular, packed bed, or fluidized bed reactors would all generally depend strongly on the initial configuration of the chemicals introduced).

Because mixing is exceptionally complex, we have chosen to examine a two-component mixing and reaction process within a tubular reactor. This choice is motivated in part by the simplifications that this geometry allows, and in part because of recent successes we have had in better understanding the early time dispersion process (pre-asymptotic Taylor dispersion) in such systems. The results of this work will focus primarily upon (1) development of the effective mass transport equations (resulting in an explicit representation of convection, effective dispersion, and the effective reaction rate), and (2) presentation of a closure scheme for this problem, and an prediction of the effective rate of reaction via numerical computations. In particular, we will discuss the need to search for effective empirical dynamical scaling laws even in the presence of a fully-predictive theory. The need for empirical models arises because, in this particular case, the process of upscaling does not reduce the *complexity* of the problem to the extent that would be the most useful for applications.

References

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