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Progress and Challenges for High-Fidelity Simulations of High Schmidt-Number Fields

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Simulations of gas-phase combustion benefit from the fact that the Schmidt number Sc=ν/D is almost unity, so that the smallest scalar scales are similar to the smallest velocity scales (of turbulence), i.e. the Batchelor η_B scale is almost identical to the Kolmogorov micro length η_K. A small deviation from this rule occurs for flames, where the inner flame structure and intermediate species may occur in thin layers – an issue that is normally well represented by flamelet models.

A very different challenge occurs, however, in flows carrying nano-particles, which is usually simulated and modelled as a Eulerian phase. These small particles are still large compared to molecules, and thus their diffusivity will be many orders of magnitude lower than that of the gas-phase. As a result, mixing is very slow and structures will be observed that are far smaller than Kolmogorov-eddies, following a scaling law of $\eta_B = \eta_K\,(\nu/D)^{-1/2}$. Given that nano-particles can experience Schmidt-numbers in the range of 10^4, resolving the scalar field would require a 100-fold mesh refinement over the resolution needed for a flow-field DNS. (A similar problem occurs for the mixing of liquids – which, as a result, is rarely simulated by CFD-type methods.)

For a non-reacting flow, the impact of the slow mixing is normally quite limited, even though the performance of a mixer might be over-estimated by simulations that do not apply a sufficiently resolved grid. The situation is very different, however, for reacting flows – where the presence of a very high concentration of a reactant or of nano-particles can have strong effects on either product formation or on the rate of particle aggregation and growth.

To yet resolve mixing at such high Schmidt numbers, different strategies have been explored. Where a global refinement can rarely be afforded, an adaptive local mesh refinement at the mixing layer is often feasible, even though the refinement will also lower the global time-step width. An alternative description is due to particles [1], where the scalar field is represented by notional particles that follow the flow and diffuse (disperse) based on a Wiener term. Such a description can be very accurate but suffers from the need for a very great number of numerical particles that cover the entire computational domain. A third option is a decomposition method [2], where the low wave-number content of the scalar field is described by finite volumes, but the high wave number content is described by "correction particles" that are only required in the thin mixing layers but nowhere else.

Our presentation will aim to a) present the problem of high-Schmidt number, to b) discuss the potential impact on simulations and experiments, and to c) derive strategies for dealing with the high Schmidt number mixing.

References (if needed)

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[2] Leer, M., Pettit, M. W. A., Lipkowicz, J. T., Domingo, P., Vervisch, L., Kempf, A. M. (2022). A conservative Eulerian-Lagrangian decomposition principle for the solution of multi-scale flow problems at high Schmidt or Prandtl numbers. J. Comput. Phys. 464, 111216.