Inserting Nonlinear *N*-Material Coupling PDF Information into Turbulent Mixing Models

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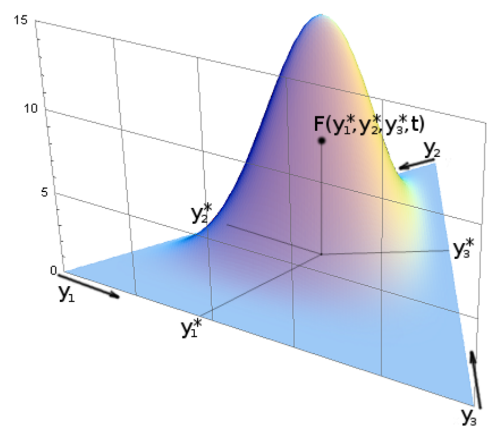
We are developing a new statistical theory for the prediction of multi-material mixing in variable-density turbulent flows for species of vastly different densities, e.g., hydrogen and iron. In practical turbulent flows all the relevant scales cannot be resolved and only the statistics can be economically predicted. Current statistical moment models, developed by averaging the Navier-Stokes equation, are consistent with a Gaussian mixing process, i.e., the passive-scalar ink-mixing-in-water problem. Such models are valid for unimodal Gaussian probability distribution functions (PDF) for dilute species' mass fractions and are popular in flows where the density fluctuations are small. We synthesize the Navier-Stokes averaging methods with the Master Equation methods of statistical physics [1] for a mixing process that predicts a variety of PDFs seen in experiments. Using a Master Equation that predicts a valid PDF ensures a physically realizable mixing process (satisfying proper bounds on the statistical moments) and ensures nonlinearly coupled mass fraction fluctuations. These results are required by first principles and cannot be accounted for by averaged Navies-Stokes methods.

At the level of engineering problem solution our work produces a first-principles (statistically speaking) prediction of coupled multi-species mixing for existing models such as BHR, implemented in LANL's RAGE code. In a bigger picture scientific sense we have made two important contributions to the prediction of variable-density mixing: (1) A new mathematical infrastructure that enables the coupling of species fluctuations during the mixing process – a phenomenon missed in Navier-Stokes-averaged methods. (2) We have made some key primary steps toward stochastic Lagrangian Monte Carlo algorithms that allow the prediction of the material-field PDFs and species reaction rates that avoids the theoretical pitfalls and calibrations of moment closure modeling. In the long term this work sets the groundwork for future numerical simulations using Lagrangian particle methods for turbulent flows in high-energy-density hydrodynamics, combustion, global security, as well as atmospheric, climate, and fusion energy sciences.



Joint PDF (vertical axis) of mass fractions for three materials in a control volume. Conservation of mass requires $\sum y_\alpha = 1$. The allowed sample space is bounded coupling all material mass fractions. This can only be ensured by such a PDF. The implications of this result are detailed in [2].

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References

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