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Optimal Sub-model Selection Based on Stochastic Modeling of Partially Stirred Reactor

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Accurate characterization of turbulence-chemistry interactions is essential for the development of predictive combustion models, particularly in hydrogen-fueled systems where fast reaction kinetics and shorter ignition delay times pose additional challenges. Reactor-based models like the Partially Stirred Reactor (PaSR) are commonly used in Large Eddy Simulations (LES) to account for finite-rate chemistry, but typically rely on a single global chemical timescale, which limits their accuracy across complex and spatially varying combustion regimes [1]. Previous approaches [2] that leverage Direct Numerical Simulation (DNS) data to select local chemical timescale formulations have demonstrated improved predictive capabilities through a priori assessment but remain impractical for broader application due to their high computational cost and limited operational range.

To address this limitation, the present work proposes the use of stochastic PaSR [3] modeling to generate data at a lower cost but still physically consistent for training a model that selects optimal chemical timescales *on-the-fly* based on local thermochemical conditions. The selection will be performed via clustering and a posteriori error minimization, with the aim of integrating the method into an LES framework for turbulent non-premixed hydrogen combustion. This approach is expected to reduce reliance on DNS data, improve generalization across different combustion scenarios, and enhance the robustness of PaSR closures in practical CFD applications. The planned work will evaluate the feasibility and performance of this methodology in capturing key combustion features while maintaining computational efficiency.

References

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