OPTIMAL SUB-MODEL SELECTION BASED ON STOCHASTIC MODELING OF PARTIALLY STIRRED REACTOR MODEL

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Abstract
Reactor-based models are well-suited turbulence-chemistry interactions sub-grid scale closures for Large Eddy Simulation (LES) due to their ability to account for finite-rate kinetics. However, a single timescale is usually employed to describe the whole spectrum of intrinsic timescales of chemistry, as in the Partially Stirred Reactor (PaSR) model. To tackle this limitation, a method leveraging Direct Numerical Simulation (DNS) data for the local selection of the chemical timescale formulation has been proposed. Although efficient, the method lacks generalization due to the elevated cost of covering different combustion scenarios with DNS.
In the present work, we investigate the stochastic modeling of Partially Stirred Reactors to generate valuable data for the chemical timescale classification. The objective is to improve combustion models predictive capabilities in LES of hydrogen combustion, a promising alternative to non-renewable fuels.

Introduction
Hydrogen's high energy and zero carbon emissions make it a promising clean fuel, but its fast kinetics and gas properties pose challenges to its integration in combustion systems. Computational Fluid Dynamics (CFD) can accelerate innovation to transition to a net-zero emissions economy. In particular, Large Eddy Simulation (LES) balances cost and accuracy by resolving large-scale turbulence and modeling sub-grid effects. The Partially Stirred Reactor (PaSR) model, commonly used as turbulent combustion closure for its ability to include finite-rate chemistry effects, accounts for subgrid-scale interactions as a ratio of characteristic timescales for mixing and chemistry. Péquin et al. [1] explored the use of supervised learning to locally select sub-models formulations in the PaSR model. The method, relying on Direct Numerical Simulations (DNS) data of turbulent combustion, is prone to limited generalization capabilities due to the elevated cost of exploring combustion scenarios with DNS. Building on these insights, we investigate the stochastic modeling of Partially Stirred Reactors [2] to generate valuable data at a lower cost

and aim at improving the PaSR model predictions in LES by locally selecting the optimal chemical timescale formulation. This approach is designed not only to reduce the dependency on expensive high-fidelity simulations but also to improve its robustness and adaptability range across a wider range of combustion regimes, including complex and high-pressure hydrogen environments.

Methodology

1. Partially Stirred Reactor (PaSR) closure

In the LES context, the filtered reaction rate of the *i*-th species $\bar{\dot{\omega}}_i$ is computed based on the mass exchange between the subgrid reactive fine structures and their inert surroundings, $\bar{\dot{\omega}}_i = \kappa\, \dot{\omega}_i(\tilde{\phi})$, where $\dot{\omega}_i(\tilde{\phi})$ is the laminar finite rate (LFR) source term of species *i* calculated at the filtered LES thermo-chemical state space. The cell reacting fraction κ provides the volume fraction occupied by the subgrid fine structures as a ratio of characteristic timescales for chemistry τ_c and mixing τ_m,

$$\kappa = \frac{\tau_c}{\tau_c + \tau_m}.$$

Four different formulations, i.e., Chomiak's (Ch.), Slowest Formation Rates (SFR), Fastest Formation Rates (FFR), and Jacobian-based (Jac.), can be employed for the modeling of τ_c. Using a single formulation for τ_c throughout the computational domain was found sub-optimal [1] and motivates this study.

2. Optimal local timescale formulation

Following [1], a local optimal formulation can be determined by minimizing the point-wise heat release rate-based Euclidean distances, d, between a target value, $\dot{Q}^{target}$, and different model responses, $\dot{Q}^{PaSR}$, while changing the τ_c formulation,

$$d = \sqrt{\left(\dot{Q}^{target} - \dot{Q}^{PaSR}\right)^2}.$$

3. Stochastic modeling

To provide the target value of the heat release rate and the thermo-chemical state space on which to compute the model responses, we perform simulations of stochastic Partially Stirred Reactors instead of relying on filtered DNS data. The reliability of this method has been demonstrated through comparisons with DNS results [2]. The stochastic modelling of Partially Stirred Reactors is achieved by solving the transport equation for the single-point joint scalar Probability Density Function (PDF) [3]. Molecular mixing, of characteristic time τ_m, is modelled using the Kernel Constraint Model (KerM) [2]. The solution to the PDF equation, and the target value of the heat release rate, are obtained from the time-integration of ordinary differential equations (ODE).

Results

The stochastic PaSR simulations are performed using 1000 particles for a 30% H_2 / 70% N_2 mixture. A total of 15 different mixing timescales $\boldsymbol{\tau_m}$ are used to generate a dataset (15000 observations) that spans the thermochemical space between chemical equilibrium and extinction. Euclidean distances $\boldsymbol{d}$ are calculated for each model

response at a point-wise level before being summed over the 15000 observations. Figure 1a) presents these total errors. The optimal total error (Opt.) is obtained by summing the lowest error at each observation among the model responses. The Jacobian-based and FFR formulations provide the best results, with each exhibiting around 20% deviation from the optimal case.

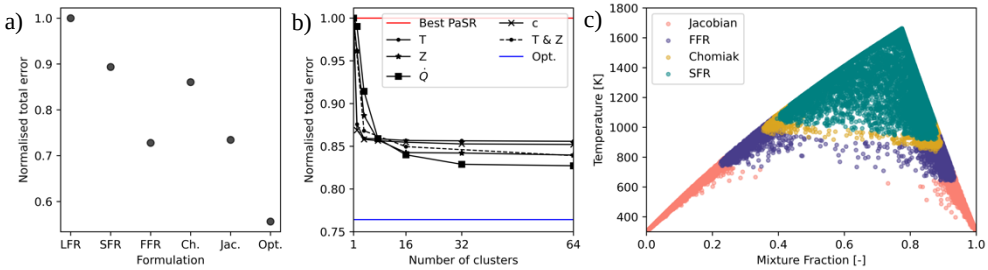

Figure 1. Normalised total errors for the dataset (a) of single timescale formulation PaSR models and optimal value; (b) of clustered PaSR solutions; (c) dataset clustered based on progress variable c, in T-Z space.

To further reduce modeling errors, the dataset is clustered on N_c number of clusters based on key thermochemical variables (temperature T, mixture fraction Z, heat-release rate, progress variable c based on H_2O, or a Z-T combination). Figure 1b) shows the performance of these clustering strategies with varying cluster counts. Clustering significantly improves model accuracy compared to using a single formulation globally, reducing the normalized total error by more than 15% with respect to the best PaSR model employing a single timescale formulation. Figure 1c) presents the 16-cluster solution based on progress variable where each cluster is colored according to its optimal timescale formulation. A clear stratification of formulations can be observed with the SFR definition dominating in high-temperature regions, largely independent of mixture fraction. The Chomiak formulation, by contrast, is only optimal for a limited subset of particles. FFR and Jacobian-based formulations are picked away from stoichiometric conditions.
The results show that the proposed approach significantly improves PaSR performance in stochastic modeling, reducing errors without relying on DNS data. Its effectiveness across combustion regimes and consistency with DNS-based trends highlight its potential for practical applications.

References

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