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Modeling of an Ethylene Jet Flame in a Hot and Diluted Coflow: Assessment of Scenario and Model Uncertainties

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Flameless combustion, also known as moderate or intense low oxygen dilution (MILD), ensures high combustion efficacies with low pollutant emissions thanks to the dilution of reactants, usually achieved through recirculation of combustion products. The technology has been successfully applied in several processes and has been found to be able to handle a large variety of fuels, including low-grade fuels, industrial by-products and hydrogen.
Further development of this innovative combustion technology would benefit of Computational Fluid Dynamics (CFD) tools; however, modeling flameless combustion is much more challenging than conventional flames, because of the strong coupling between turbulent mixing and chemical kinetics. It is well known that chemical kinetics plays a fundamental role, even though there no common opinion on the degree a mechanism can be reduced. Some useful works may be found on flameless burners fed with methane, but there is lack of information on different fuels.
The present work describes the numerical modeling of an ethylene jet flame issuing in a hot coflow burner, which is fully characterized in literature and emulates flameless conditions [1]. The data-set is particularly appealing, as it provides a sufficient degree of physics coupling, i.e. mixing and chemical reactions, to characterize the MILD combustion regime, without the additional effects of very complex geometries and flow fields. This allows addressing with more confidence the effect of different modeling choices on the numerical results.
The investigation aims at validating different aspects of turbulent combustion modeling, through a Validation and Uncertainty Quantification approach (V/UQ). Recognizing the various potential sources of uncertainty for the case under investigation, a complete analysis is performed to characterize scenario and model uncertainties and to propose a validated modeling approach by means of a careful assessment of all uncertainty sources, including experimental ones.
The following sources of uncertainties are considered:

- Boundary conditions, such as turbulence levels of the inlet streams.
- Turbulence model formulation.
- Combustion model and role of finite rate chemistry.
- Chemical kinetics.

Special attention is devoted to the role of chemical kinetics and to the possible degree of reduction of comprehensive chemical mechanisms. To this purpose, different reduction techniques are assessed, including reduced mechanisms based on skeletal and reaction manifolds, as well as constrained equilibrium approaches [2]. For the latter, two approaches are benchmarked for the selection of represented and non-represented species: a Principal Component/Principal Variable Analysis of the correlation structure of the thermo-chemical state of the system [3], which allows identifying the most energy-carrying variables, and an approach based on the separation of slow and fast reacting species, based on the spectral decomposition of the isothermal Jacobian of the state-space source terms [4]. The ultimate objective of the present work is to determine reliable error

bounds on simulation results, processing the several sources of uncertainty affecting the model outputs. As a consequence, the methodology allows establishing which values of the input (scenario & model) parameters allow validating the numerical models, ensuring consistency between experiments and numerical simulations. This is performed simultaneously against all the parameters defining the multi-dimensional input parameter space, as looking at a prior at time could lead to misleading conclusions. Such a process can potentially lead to global inconsistency, indicating a lack information in both models and experiments.

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