

Narrative Report

PRF# 58173-DNI9

Project Title: A Computational study of the lean blow-off mechanisms for a bluff-body stabilized premixed flame

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Lean but stable combustors have received significant technological interest in gas turbine combustors, afterburners and industrial furnaces, due to the increasingly stringent emission requirements. Bluff-bodies are frequently employed to stabilize flames in premixed fuel-air streams, where lean blowoff is a safety and operational concern. The dynamic physicochemical events leading to lean blowoff are still not well understood, due to the highly-transient turbulent flow fields, the important role of finite-rate chemistry and their complex competition. The objective of the proposed research is to understand the intimate interactions between turbulence and chemistry, through computational studies that account for finite-rate chemistry using a reduced chemical mechanism with a mildly thickened flame (TF) model.

Over the past year, we focused on 1) selection of appropriate test cases and conduction of baseline large-eddy simulations; 2) examination of the details of flame sensors that are conventionally used with TF models. Large-eddy simulations of two bluff-body stabilized flames are conducted, including a stably burning turbulent premixed methane-air flame (flame CAM) and a turbulent premixed propane-air flame near blowoff (flame BEX). Baseline results are obtained using a transported probability density function model for flame CAM, and using a flame-resolved model for flame BEX. Both simulations employed reduced chemical mechanisms to describe the finite-rate chemistry, with 16 species and 31 species, respectively. Figure 1 shows the instantaneous iso-contours of temperature that represent the flame surfaces of the two flames. Both flames are under strong influence of turbulence, as evidenced by wrinkles on the flame surfaces. The velocity, temperature, as well as species profiles are compared against experimental data, to validate the numerical simulations. Good agreement is achieved for both flames. Subsequently, these baseline results will serve as benchmark for comparison with TF model that is developed in this project.

The TF model is then implemented in the in-house OpenFOAM-based LES solver. Most existing studies combine the TF model with one-step or two-step chemical mechanisms, and challenges remain when combining the TF model with reduced or detailed chemical kinetic models. In addition, the tight coupling between molecular diffusion and chemical reactions near blowoff can pose further challenge to the TF model. To advance the TF model towards these two directions, the details of the model formulation require further examination and modification. Year 1 of the project focuses on proposing an appropriate flame front sensor when combined with detailed chemistry, and year 2 will focus on appropriate model formulation for capturing extinction. A few flame sensors are proposed based on the physical intuition of the flame structures, and are compared among themselves and with existing models in literature. The proposed sensor based on formyl (HCO) performs the best for lean flames. Parametric studies are then conducted, to understand the performance the sensors under different equivalence ratios, temperature, and pressure.

A twin-premixed flame propagating against one another under homogeneous isotropic turbulence is constructed to verify and to assess the performance of the implemented TF model. The 16-species chemical mechanism is applied, and molecular diffusivity is considered by the mixture-averaged molecular diffusivity model. Direct numerical simulation of the target flame is first performed, serving as a benchmark case. An efficiency function that is required to recover the sub-grid flame wrinkling is also implemented. For LES, the performance of the models with and without the flame sensor, and with and without the efficiency function is compared. Figure 2 shows the integrated fuel mass fraction as function of time, which indicates the evolution of integrated heat release rates. The models with a dynamic HCO based flame sensor with efficiency functions best match the DNS, although the particular form of the efficiency function matters. Figure 3 further compares the iso-surfaces of the twin premixed flame, and case (e) ($F_{max} = 4$, efficiency function $\sim F^{0.337}$) is observed to recover the most sub-grid flame surfaces, compared to other combination of models (e.g., case (d) with $F_{max} = 4$, efficiency function $\sim F^{0.5}$). Models in case (e) will be employed in subsequent simulations of flame CAM and flame BEX.

During the first year of this grant, the PRF funds provided the PI and her lab a great opportunity to embark on an exploration journey of the critical problem of flame extinction. Supported by the PRF funds, the PI presented the simulation results to the international community during the International Premixed Turbulent Flame Workshop at

Dublin, Ireland, and attracted significant national and international invitation for collaboration, such as that from DLR Germany, from United Technology Research Center, and from researchers from Stanford University, Pennsylvania State University and University of Central Florida. The project also provides the postdoctoral researcher and the relevant graduate students significant training opportunities, in terms of understanding of the turbulence-chemistry interactions, numerical modeling, as well as professional development in presenting their findings through national conferences and journal publication. The project also synthesizes with other current activities and funded projects from the PI's lab, and fosters close collaboration with Prof. Baki Cetegen and Prof. Tianfeng Lu within UCONN.

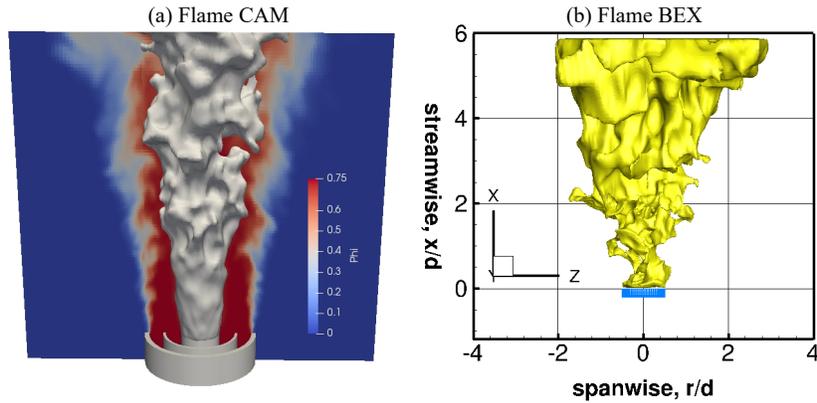


Figure 1 Iso-contours of temperature corresponding to (a) Flame CAM and (b) Flame BEX.

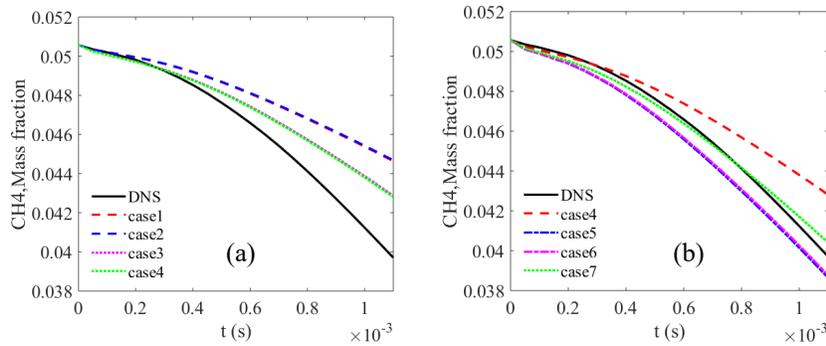


Figure 2 Total mass fraction of CH_4 versus time for different cases using detailed chemistry with 16 species.

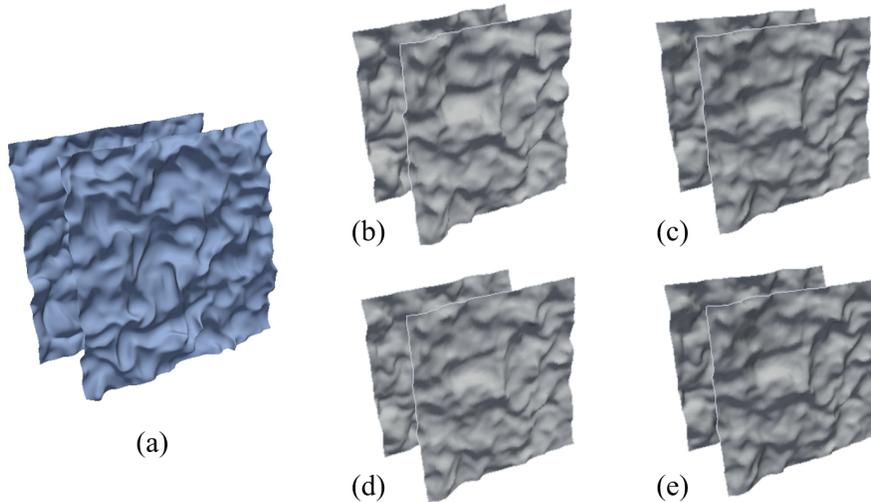


Figure 3 Iso-surface of fuel mass fraction ($Y_{CH_4} = 3\%$) for (a) DNS, (b) case4, (c) case 5, (d) case6, and (e) case7 at the same instant of time 0.004 s ($0.36\tau_f$).