TITLE: **Enabling Advanced Modeling and Simulations for Fuel-Flexible Combustors**
AUTHORS: **Heinz Pitsch** (PI)
INSTITUTION: Stanford University, Department of Mechanical Engineering
Building 500, Stanford University, Stanford, CA 94305-3035
PHONE: (650) 736 1995
FAX: (650) 725 7834
E-MAIL: h.pitsch@stanford.edu
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1. ABSTRACT

Objectives

Gas turbines are known as the main source of electrical energy in the world. Diminishing resources and environmental challenges such as global climate change demand clean and efficient usage of coal as well as the utilization of renewable resources and "opportunity" feed-stocks such as biomass, petroleum coke, etc. These needs call for the development of advanced next-generation turbine technologies. One of the most important features of advanced turbines is the capability of operating robustly on fuels derived from gasification of coal and feed-stocks. One has to design and develop integrated gasification combined-cycle power plants, which can have high thermal efficiency and near-zero NO_x emissions. Such a goal can be met by the assistance of advanced simulations that are validated by reliable comprehensive experimental data.

The overall objective of the present project is to enable advanced modeling and simulations for the design and optimization of fuel-flexible turbine combustors. This goal will be accomplished by using high-fidelity extensively-tested LES software and state-of-the-art models for premixed turbulent combustion. In the recent past, we have developed many new modeling techniques related to combustion LES. Our innovative approaches include a completely consistent description of flame propagation; a coupled progress variable/level set method; fuel transport properties and heat losses at the boundaries and through thermal radiation. In addition, the accomplishments from the Coal Research Program, such as detailed chemical mechanisms at elevated temperature and pressure and relevant experimental data, will be utilized. During the project period, these techniques will be applied, assessed, and potentially improved or adapted for premixed and partially premixed gas-turbine combustion. As a result, the present work would help us greatly to understand the current industrial problems with predictive simulations, and make a significant contribution to the fulfillment of UCR program's goal of developing advanced turbine technology for clean and efficient use of coal and a diverse mix of energy resources.

Accomplishments achieved up to date

In the project, we are using a well-sophisticated semi-implicit finite-difference LES code developed in our group. The code solves the filtered Navier-Stokes equations in the low Mach number limit; it can have any high order of numerical accuracy in space discretization with a high computational efficiency. The solver has been extensively used to simulate combustion processes in several applications, for example, in combustors and industrial furnaces. Numerous physical-chemical and numerical models describing turbulent combustion have been proposed in previous works. For instance, Knudsen and Pitsch have developed a general flamelet-type transformation holding in the limits of both non-premixed and premixed burning recently. As a result, a model for distinguishing between premixed and non-premixed burning regimes has been derived. The proposed model has been validated, in particularly, by a presumed-PDF LES of a lean-premixed low-swirl burner that has been studied experimentally at Sandia CRF and LTH (Lund, Sweden). An instantaneous level-set representation of a low swirl premixed flame from the LES is shown in Fig. 1. Figure 2 presents time averaged mean velocity profiles and root-mean-square velocity profiles as a function of the burner radial coordinate. The experimental data are shown in each graph by the markers. The solid lines present the LES solutions. In general, LES predictions in Fig. 2 agree very well with the experimentally measured profiles, which justifies the approach used in the LES.

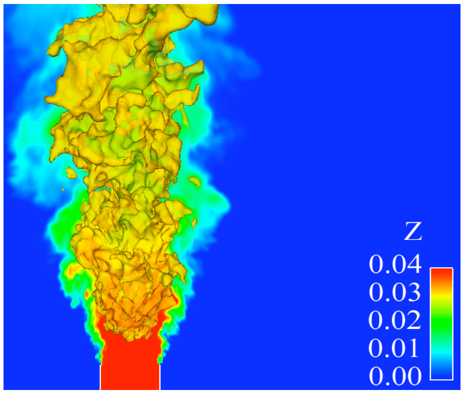

Fig. 1. Level-set representation of the flame front, colored by the mixture fraction Z.

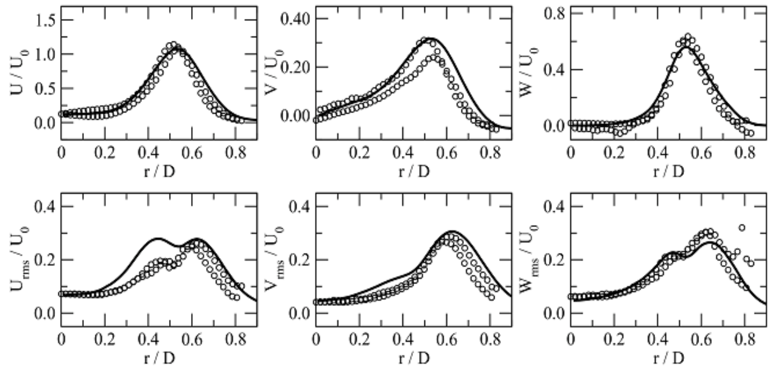

Fig. 2. Time averaged swirl burner velocity (top) and rms-velocity (bottom) profiles; Axial, radial, and azimuthal profiles are shown from left to right. Solid lines present the LES; experimental results are shown by markers.

Plans for the Remaining Period of Performance

The work planned for the remaining time of the project includes the following tasks:

1. ***Prediction of Flow Field and Inlet Boundary Conditions.*** We will simulate cold flows for the combustors from NETL and Sandia CRF and compare the simulation and experimental results. Then we will generate inlet flow boundary conditions for the chamber simulation by simulating flow in a nozzle with swirlers.
2. ***Study of fuel composition effect on laminar flame speed.*** We will create a table for a laminar flame speed as a function of fuel compositions, equivalence ratio, temperature and pressure. The table will be tested by modeling the Siemens flames and comparing to their experimental data on blowout and flashback.
3. ***Simulation of turbulent premixed burning in the modeled combustors.*** Various models for premixed combustion will be implemented and tested by performing the simulations of the modeled turbine combustors from NETL, Sandia CRF and Siemens, and comparing to their experimental data. We will also validate the simulations by comparison to the DNS performed in CCSE at Berkeley Lab. In the frame of this work, we will implement the wall heat transfer model and study the effect of the model on temperature distribution and pollutant emission. Also, the role of the fuel composition, non-unity Lewis numbers and other effects in blowout and flashback will be investigated. As a result, we will identify models' deficiency and make improvement.
4. ***Study of thermal radiation effect on flame propagation and NO concentration.*** A state-of-the-art radiation model we will implemented into the LES solver and validated on simple configurations. Then we will investigate the role of radiation in the modeled turbine combustors from NETL and Sandia CRF.
5. ***Simulation of real turbine combustor***. Finally, when all the models are tested and improved, a full-fledged combustion LES will be carried out for a real turbine combustor from Siemens to make practical predictions. We are going to perform this task at the end and after the project period.

2. LIST OF PUBLISHED JOURNAL ARTICLES, COMPLETED PRESENTATIONS AND STUDENTS RECEIVING SUPPORT FROM THE GRANT

Journal Article

- A General Flamelet Transformation Useful for Distinguishing Between Diffusive and Premixed Modes of Combustion, E. Knudsen & H. Pitsch, to be submitted.

Conference Presentations

- A Partially Premixed Combustion Approach for Presumed-PDF LES, E. Knudsen & H. Pitsch, SIAM 12th International Numerical Combustion Conference, Monterey, CA, Apr 1, 2008.