Project 028 Combustion Model Development and Evaluation

Georgia Institute of Technology, University of Connecticut

Project Lead Investigator

Suresh Menon
Hightower Professor of Engineering
School of Aerospace Engineering
Georgia Institute of Technology
270 Ferst Drive, Atlanta, GA 30327
404-894-9126
suresh.menon@ae.gatech.edu

University Participants

Georgia Institute of Technology

- P.I.(s): Suresh Menon, Professor; Wenting Sun, Associate Professor
- FAA Award Number: 13-C-AJFE-GIT-018
- Period of Performance: Oct. 1, 2016-Sept. 30, 2017
- Task(s):
    1. Travel to NJFCP meeting. Funds only for travel (S. Menon, PI)
    2. Development of dynamic adaptive chemistry solver and demonstrate the algorithm in different flame configurations, travel to meeting (W. Sun)

University of Connecticut

- P.I.(s): Tianfeng Lu, Associate Professor
- FAA Award Number: 13-C-AJFE-GIT-018
- Period of Performance: October 1, 2016 - September 30, 2017
    3. The task of UCONN in the NJFCP program is to develop reduced chemical kinetic models for jet fuels that can be employed in efficient large eddy simulations.
    4. The technical aspects of the UCONN task is to cover the travel expenses of the UCONN team to present the results from the NJFCP program in the conferences and program review meetings.

Project Funding Level

The Georgia Tech award is $6000 for S. Menon (PI), FY 2017 for travel
The Georgia Tech award is $39,999 for W. Sun, FY 2017 for travel and partial student support.
The UCONN subaward is $5000 for FY2017 for travel support

Investigation Team

The Georgia Tech team includes: Suresh Menon (PI) (travel funds only),
Wenting Sun (co-PI), Suo Yang (graduate student), Xiang Gao (graduate student)
Tianfeng Lu (co-PI, UCONN), Yang Gao (graduate student), and Ji-Woong Park (graduate student)

Project Overview
This project is developing computational tools to evaluate alternate fuel combustion in a spray combustion system. Reduced reaction kinetics from UCONN is being used for LES of reacting flows to investigate performance of various fuel mixtures. Funding for PI and Co-PIs are for travel to FAA meetings. One of the co-PI (W. Sun) has some additional funds to support a graduate student.

Task #1: Development of Reduced Kinetics For NJFCP Fuels
University of Connecticut

Only travel funds are provided to attend NJFCP program reviews in May and December 2017. All research is funded by a NASA NRA.

Task #2: Network Modeling and Kinetics Acceleration
Georgia Institute of Technology

Travel funds are provided to attend NJFCP program reviews in May and December 2017. Some additional funds provided for student.

Task #3: LES of Spray Combustion In NJFCP Test Facilities
Georgia Institute of Technology

Only travel funds are provided to attend NJFCP program reviews in May and December 2017. All research is funded by a NASA NRA.

Objective(s)
The primary objective for PI and Co-PI is to provide funds to travel to NJFCP and ASCENT project reviews and also to allow students to attend these reviews. The objective of the research for one of the co-PI (W. Sun) is to develop a Dynamic Adaptive Chemistry (DAC) Algorithm to employ different reduced kinetic models at different grid points to reduce the computation time in LES and DNS.

Research Approach
Primarily travel funds for all PI.

W. Sun: Research Description: Due to the increasing demand for combustion-based energy and concerns on its environmental impacts, high-fidelity simulation of turbulent combustion becomes a highly-important tool for combustor design. For any practical simulation method, the key is to provide quantitative solutions with minimal empirical constants. Large-eddy simulation (LES) has drawn significant attention during the past three decades, and its predictive capability is continuously increasing. In LES, the energy-containing large-eddy motions are resolved with sufficient grid resolution, while motions of scales smaller than the grid sizes, i.e. subgrid-scale (SGS) motions, are modeled. The chemical reaction rates are highly-nonlinear functions of species concentrations and temperature, which heavily depend on the turbulent mixing. On the other hand, chemical reactions also release heat and subsequently affect species concentrations and temperature, which in turn change the turbulent mixing. Chemical reactions occurring at different time scales may interact with eddies of different length/time scales, which further complicates the physiochemical processes. Therefore, turbulence/chemistry interaction is considered the most challenging problem in turbulent combustion modeling.

The turbulent combustion models that have been developed for LES can be classified into two major categories: the finite-rate chemistry (FRC) models, and the flamelet generated manifold (FGM) models. The FRC models category includes the laminar chemistry model, the perfectly-stirred reactor (PSR) model, the partially-stirred reactor (PaSR) model, the linear-eddy model (LEM), the Monte Carlo method for Lagrangian filtered probability density function (FDF) transport equations, and the thickened flame model (TFM). The FGM models category includes the steady laminar flamelet model, the Lagrangian flamelet model, and the flamelet/progress-variable (FPV) model. Among FGM models, the steady laminar flamelet model provides the advantages of easy implementation and low computational cost. There are, however, limitations associated with this model. First, the mixture fraction essentially does not carry information about the chemical states. The model uses the filtered dissipation rate of mixture fraction as an additional parameter to account for the flame stretching effect. The dissipation rate, however, does not provide a unique mapping from mixture fraction to the corresponding reaction state. In order to overcome the drawbacks of the steady laminar flamelet model, the FPV model was proposed to incorporate a transport equation to track a progress variable. This model has been developed to account for low-level of extinction, re-ignition, and unsteady mixing effect to some extent. It, however, cannot handle multiple-feed streams unless adding a third parameter, which makes the look-up table very difficult to handle due to the large computer memory requirement and time to build up the table. In addition, the higher-dimension look-up table results in a more complicated data retrieval process and coarser table grid, which could introduce higher interpolation errors. Compared to the FGM models, the detailed chemical kinetics in the FRC models are computationally prohibitive for LES applications due to the large number of species and the stiffness resulting from a broad range of chemical time scales. In the present work, DAC is incorporated into a preconditioning scheme to allow an Eulerian FRC-LES approach in a fully-compressible flow CFD solver. The established FRC-LES framework is then used to investigate a low-Mach partially premixed turbulent flame (Sandia Flame D) as a benchmark case.

Milestone(s)
Attend FAA mid-year meeting in May and annual meeting in Dec 2017 as required

Major Accomplishments
UCONN team:

Reduced kinetic models for five jet fuels, namely Cat A1, A2, A3, C1 and C5, have been developed from Version 2 of the detailed HyChem models and validated for ignition delay, stirred reactor extinction, flame speed, and extinction of premixed and non-premixed counterflow flames. The reduced models have been delivered to the NJFCP numerical simulation teams. Note this work was done under NASA funding but provided to other researchers in this program.

Georgia Tech team:

Travel to ASCENT and NJFCP meetings to present progress (on work funded by NASA).

For W. Sun, additional funding from the ASCENT program has allowed to get the DAC implemented into Sandia Flame D. We developed a 20-species and 84-reactions methane/air kinetics model reduced from the GRI-3.0 as a kinetic model in computation since Sandia Flame D is a methane/air flame. Results shows that the DAC method provides effective local mechanism reduction with negligible computational overhead. In FRC-LES, the techniques of ODEPIM and DAC provide an acceleration of 8.6 times for chemistry, and 6.4 times for the total computation. This work laid the foundation in the application of DAC in more complicated problem such as gas turbine combustor simulation.

Publications
None

Outreach Efforts
None

Awards
None

Student Involvement
UCONN team:

Two graduate students (Yang Gao and Ji-Woong Park) are involved in the NJFCP project. The students are responsible for the development and validation of reduced jet fuel models and the compilation of a package to help integrating the reduced models to large eddy simulations. Yang Gao has graduated in October 2017.

Georgia Team:

S. Menon: Achyut Panchal (funded by NASA) and Dr. Reetesh Ranjan, Research Engineer will be attending the NJFCP review.

W. Sun: Two graduate students (Suo Yang and Xiang Gao) are involved in the NJFCP project. The students are responsible for the development of reduced kinetic models and conduct LES simulation with DAC for Sandia Flame D.

Plans for Next Period

Funds for FY 18 are being provided for the PI to travel to NJFCP meeting only at this time.