Project 28 National Jet Fuels Combustion Program Area #4- Combustion Model Development and Evaluation

Georgia Institute of Technology

Project Lead Investigator

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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: Dec. 1, 2014-Dec. 31, 2017
- Task(s):
    1. Travel to NJFCP meeting. Funds only for travel for years 2 and 3 (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: Dec. 1, 2014-Dec. 31, 2018
    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

$350K from FAA and $350K cost share for year 1.
Subsequent years were funded primarily for travel to attend meetings twice a year. All research was funded by NASA under a separate NRA.

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)

The investigation team with specific tasks is as follows:

1. **Task 1:**
    - **Title:** Development of reduced kinetics for NJFCP Fuels

- **Lead:** Professor Tiangfeng Lu
- **Post Docs & Students:** Y. Gao, B. Majda, Y. Liu
- **University Affiliation:** University of Connecticut

2. **Task 2:**
   - **Title:** Network modeling and kinetics acceleration
   - **Lead:** Professor Wenting Sun
   - **Post Docs & Students:** S. Yang, X. Gao
   - **University Affiliation:** Georgia Institute of Technology
3. **Task 3:**
   - **Title:** LES of spray combustion in NJFCP test facilities
   - **Lead:** Professor Suresh Menon
   - **Post Docs & Students:** Dr. R. Ranjan, A. Panchal
   - **University Affiliation:** Georgia Institute of Technology

Project Overview

The overall objective of this activity is to establish a predictive capability to evaluate new aviation fuels in combustors for ASTM D4054 at operating conditions including lean blowout, cold start or altitude relights. The key objectives of this project are as follows:

- Establish a simulation strategy using Large-Eddy Simulations (LES) to capture fuel sensitivity in experimental screenings
- Collaborate with Area 2 to develop, optimize and evaluate efficient reduced chemical kinetics for use in LES
- Collaborate with Areas 3, 5 and 6 to perform LES investigation of the experimental rig for stable and LBO conditions

Task 1 – Development of Reduced Kinetics for NJFCP Fuels

University of Connecticut

Objective(s)

The objective of this research activity is to develop, optimize and evaluate reduced chemical kinetics models for use in LES of spray combustion in NJFCP test facilities. Additionally, for FY 16-18 only travel funds are provided to attend NJFCP program reviews in May and December. All research is funded by a NASA NRA.

Research Approach

Model Reduction for Cat A & C fuels

Skeletal and reduced models for Cat A and C fuels, including Cat A2 (POSF10325), C1 (POS11498, beta version) and C5 (POSF12345) have been developed based on the detailed HyChem models from Area 2 of the NJFCP program. The reduced models are validated over a wide range of parameters for ignition, extinction and flame propagation. The hybrid modeling approach with lumped fuel cracking reactions assumes that the intermediates of the fuel cracking are in quasi-steady state as demonstrated in [1, 2], resulting in highly compact detailed-lumped models for high-temperature real fuel oxidation. The detailed-lumped models consist of more than 100 species while the reduced models consist of less than about 30 species.

Procedurally, the DRG-based methods, including DRG [3-6] and DRG-aided sensitivity (DRGASA) [7, 8], are first employed to remove unimportant species and reactions based on reaction states sampled from auto-ignition and perfectly stirred reactors (PSR). The H radical is selected as the starting species in the graph searching in DRG. After the skeletal reduction of DRG, the skeletal mechanism is further reduced by using DRGASA with ignition delay and extinction residence time of PSRs being the target parameters. The skeletal models are then reduced using the linearized quasi steady state approximations (LQSSA) [9]. Global QSS species are identified and approximated with algebraic equations, which are analytically solved using a graph-based method to ensure high accuracy and robustness [9].

The reduction covered a wide range of parameters: pressure from 0.5 to 30 atm, initial temperature from 1000 K to 1600 K for auto-ignition, inlet temperature 300 K for PSR, and equivalence ratio from 0.5 to 1.5. A worst-case error tolerance of 20% was set for the target parameters in DRGASA. The sizes of the detailed-lumped, skeletal and reduced models are summarized in Table 1. The performance of the reduced models is demonstrated with Cat A2 in Fig. 1 for ignition delay, laminar flame

speed, and extinction of premixed and non-premixed counterflow flames for different flame conditions. Similar performances were observed for the reduced models for Cat C1 and C5.

Extended validation was further performed for Cat A2 for PSR at both lean and rich extinction conditions as shown in Fig. 2. The important reaction pathways controlling lean blow-out (LBO) are identified using bifurcation analysis [10] as shown in Fig. 3. It was found that LBO at the investigated conditions is primarily controlled by reactions involving small molecules, such as H, OH, CO and HCO. These reaction rates need to be accurately computed for accurate prediction of LBO.

High-Performance Model-Specific Solvers for Jet Fuels

Analytic Jacobian was developed for Cat A2, C1 and C5 for efficient time integration of chemistry using implicit ODE solvers, for which the Jacobian evaluation and factorization are typically the most time-consuming components. Analytic chemical Jacobian evaluation can reduce the computational cost to a level comparable to that for a single rate evaluation. As such the computational efficiency of implicit solvers can be significantly improved. The strategy to couple implicit solvers with the analytic Jacobian is applicable for simulations with arbitrarily large integration time steps.

Dynamic adaptive hybrid integration (AHI) [11] was further developed in addition to the analytic Jacobian technique by only solving the fast species and reactions implicitly, while treating the slow variables and source terms explicitly. The size of the implicit core to be solved in AHI can thereby be significantly reduced and the computational efficiency can be improved.

For simulations with integration time steps smaller than about 20 ns, non-stiff reduced models based on the dynamic chemical stiffness removal [12] are developed for Cat A2, C1 and C5, such that explicit solvers for time integration can be employed to achieve high efficient in high-fidelity DNS and LES of compressible flows.

The performances of implicit solvers with analytic Jacobian, AHI, and explicit solvers with dynamic chemical stiffness removal are compared in Fig. 4 for mechanisms of different sizes, including the skeletal and reduced Cat A2 models. Speedup factors close to or larger than an order of magnitude are achieved using analytic Jacobian, AHI and dynamic chemical stiffness removal.

Table 1. Size of the detailed-lumped, skeletal and reduced models for Cat A2, C1 and C5.

	A2		C1 (beta)		C5	
	Species	Reactions	Species	Reactions	Species	Reactions
Detailed	112	790	112	794	112	790
Skeletal	38	185	37	210	38	185
Reduced	29		27		29	

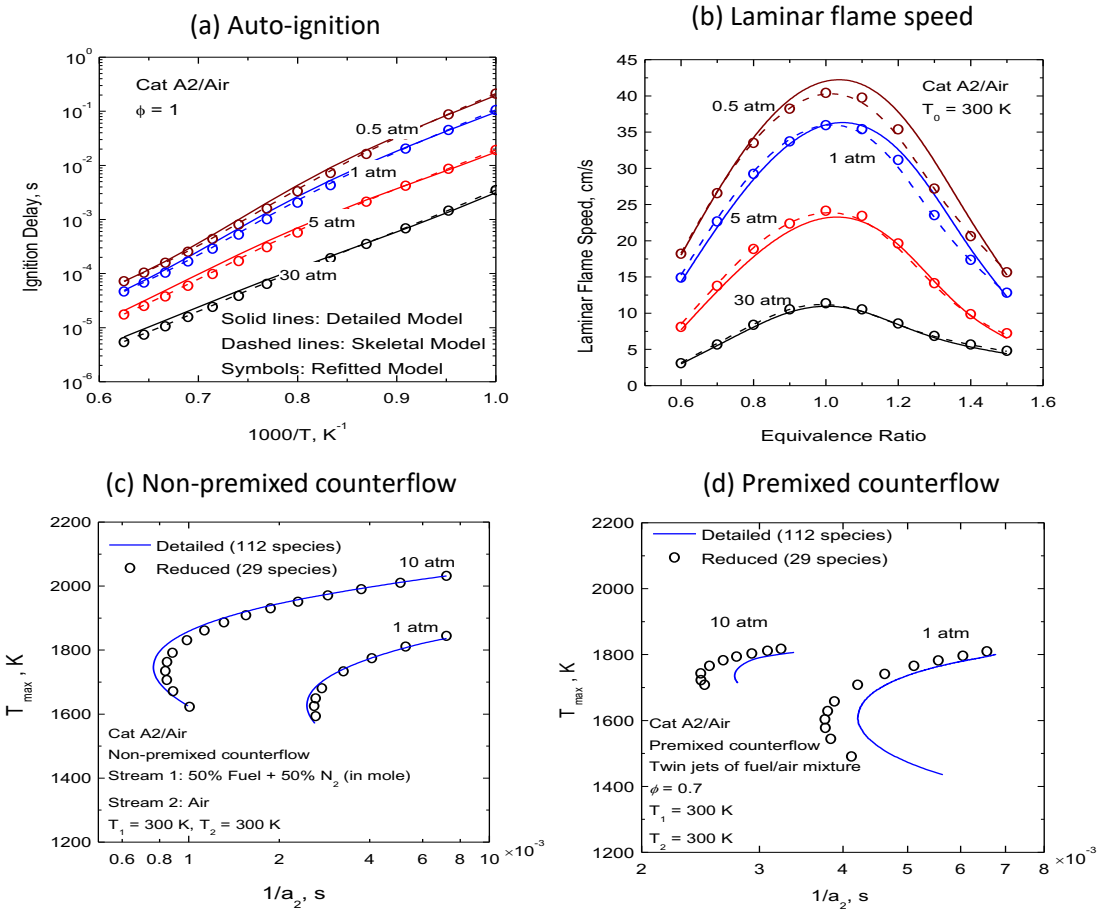

Figure 1. Validation of the reduced model against the detailed model for Cat A2 for a) ignition delay, b) laminar flame speed, c) extinction of non-premixed counterflow flames, and d) extinction of premixed counterflow flames.

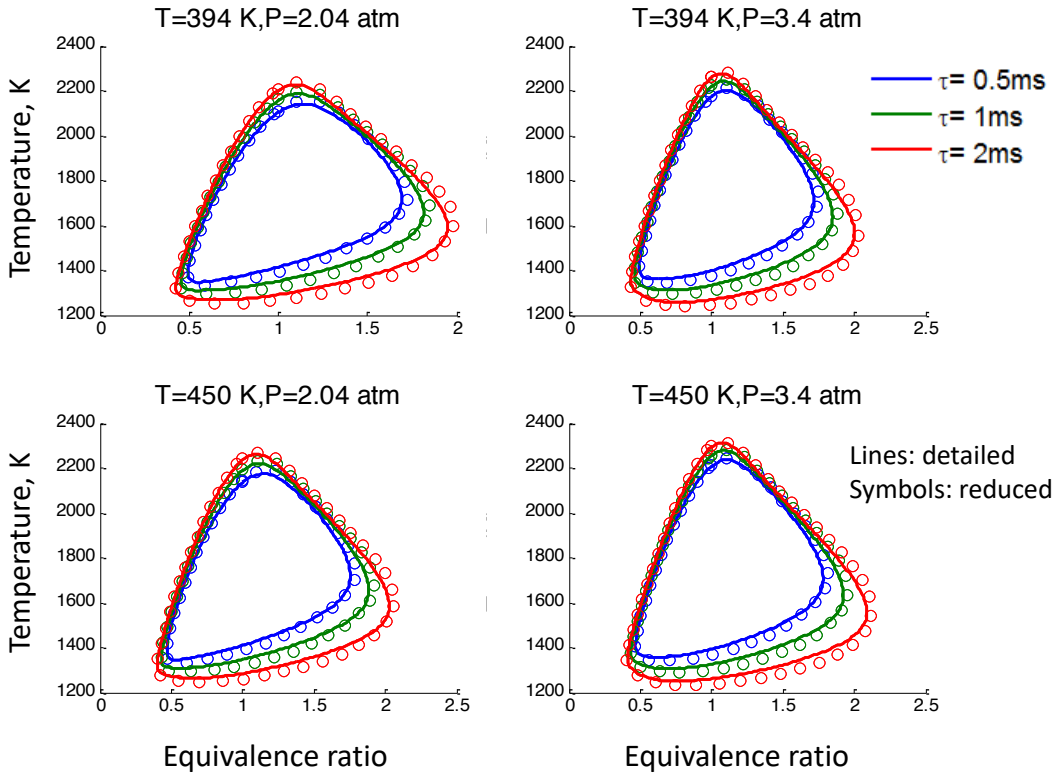

Figure 2. Extinction of Cat A2/air in PSR at different inlet temperatures, pressures and residence time.

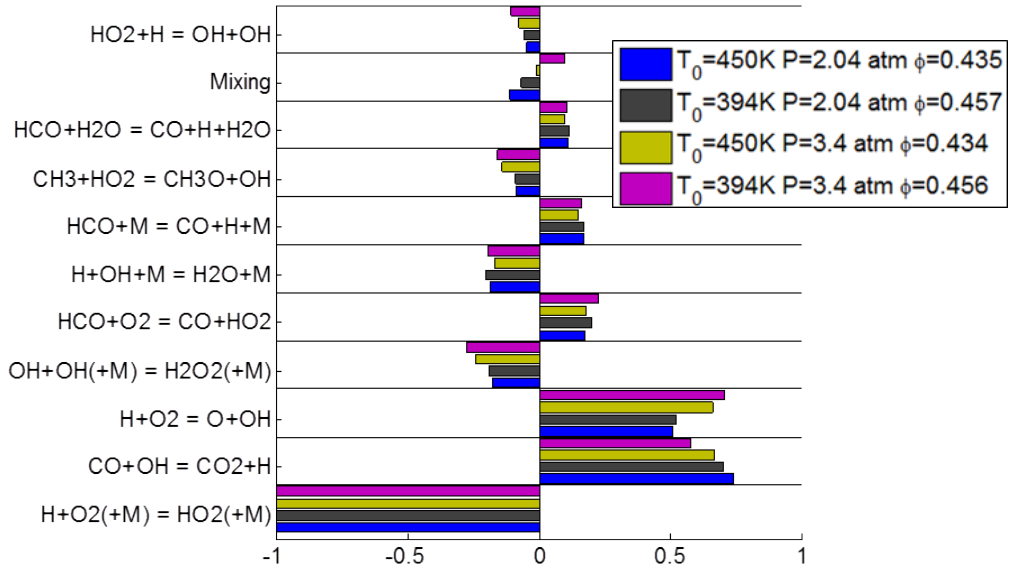

Figure 3. Controlling reactions identified using bifurcation analysis at the lean blow-out conditions in Figure 2.

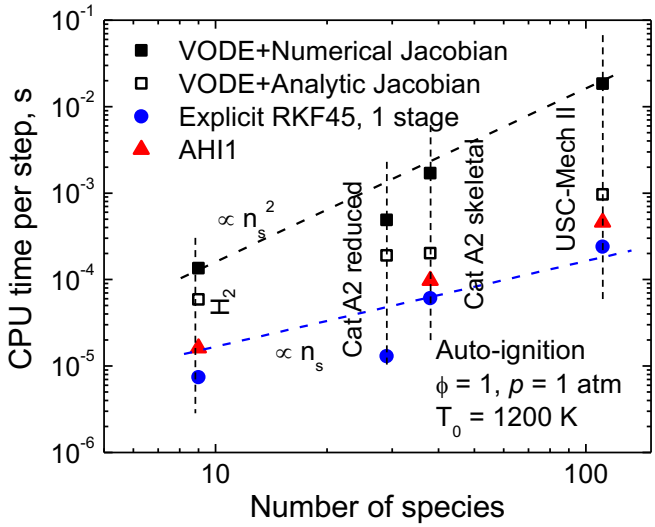

Figure 4. Averaged computational cost per integration time step in auto-ignition using different solvers and mechanisms of different sizes.

Milestone(s)

None

Major Accomplishments

The accomplishments of the current year's research activity with their impact on the rest of the project are as follows:

- **Development of reduced chemical kinetics models for Cat A2 and C5:** Based on the detailed-lumped models from Area 2, we developed a 38 species skeletal and 29 species reduced kinetics, which were used in the LES of spray combustion under Task 3 for stable and LBO conditions.
- **Comprehensive validation of the newly developed reduced models:** We performed a comprehensive validation of the new models by considering variety of combustion physics such as auto-ignition, perfectly stirred reactors (PSR), flame speed, extinction of premixed and non-premixed counter-flow flames, etc. The developed models are accurate enough to capture wide variety of combustion physics of interest such as LBO, cold restart, altitude re-lightning etc. Additionally, these models can capture the effects of fuel sensitivity, which is an essential element of the current research effort.
- **Development of efficient approaches for handling chemical kinetics in LES:** In LES with finite-rate chemical kinetics, use of a skeletal or reduced chemical kinetics lead to excessive computational cost associated with the chemical kinetics. Therefore, novel approaches have been developed to alleviate this excessive computational cost. This has been achieved by developing analytical Jacobian and non-stiff routines, which can be used for LES under Task 3. Additionally, having a mixture-averaged transport in a LES is also expensive, when the number of species is large. Therefore, reduced transport models of 15 species group has been generated, which can be used in LES instead of the expensive 29-species based transport for the reduced models, with a similar level of accuracy. The efficient approaches developed in this research effort will reduce the cost of large-scale LES and they will allow OES to simulate these problems without sacrificing the accuracy.

Publications

Yang Gao, "Model Reduction and Dynamic Adaptive Hybrid Integration for Efficient Combustion Simulations," Ph.D thesis, University of Connecticut, 2017.

Outreach Efforts

None

Awards

None

Student Involvement

- Y. Gao
- B. Magda
- Y. Liu

Plans for Next Period

None

References

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12. T. F. Lu, C. K. Law, C. S. Yoo, and J. H. Chen, "Dynamic stiffness removal for direct numerical simulations," *Combustion and Flame*. 156, 1542-1551 (2009).

Task 2 – Network Modeling and Kinetics Acceleration

Georgia Institute of Technology

Objective(s)

The objectives of this research activity are as follows:

- **Develop a dynamic mechanism reduction approach for LES Modeling:** The focus of this research effort was to develop a novel approach to perform a dynamic mechanism reduction for LES by identifying the reactor models such as mixing zone, flame zone etc., so that efficient computation of the chemical kinetics can be performed while using a chemical kinetics with large number of species.
- Travel funds are provided to attend NJFCP program reviews in May and December for FY 16 and 17. Some additional funds provided for student support in FY17.

Research Approach

Dynamic Adaptive Chemistry for LES Modeling

The developed algorithm CoDAC last year was further successfully implemented into a turbulent jet flame (Sandia Flame E). Detailed results were obtained for Sandia Flame E. Figure 1 below shows the snapshots of the spatial distribution of number of active species and number of active reactions, generated from the local PFA mechanism reduction (threshold=2%) of CoDAC method. Outside the jet brush, only 2 species (preselected seed species: fuel and oxidizer) and none of the reactions

are selected, because no chemical reactions occur there. Near the highly distributed turbulent partially premixed flame, a large number of species and reactions are selected, which is close to the full mechanism (20 species and 84 reactions). There is a large buffer zone between above two regions, which has intermediate number of selected species and reactions. The reduction of number of species and reactions in most spatial locations is responsible for the acceleration of chemistry calculation from the DAC method. Due to the highly efficient correlation techniques, the PFA mechanism reduction time is more than 500 times smaller than the chemistry calculation time, and only occupies 0.135% of the total computation time. Therefore, the computational overhead of CoDAC is negligible.

The computation time distribution is shown in Figure 2. The Frozen case (multi-species transport equations without chemical kinetics source terms) serves as the theoretical upper limit for the computation speed of all FRC models. From FPV case to Frozen case, the number of equations rises from 7 to 24 by a factor of 3.4. For this reason, the total computation time increases by a factor of 2.7, which is even better than the ideal linear computational complexity. The time for preconditioning matrix inversion increases by a factor of $11.2 \approx 3.42$, which is much better than the theoretical cubic computational complexity. This super-scaling maybe due to the relatively small size of chemical kinetics mechanism used in this study. The chemistry calculation is very expensive and dominates the total computation time. With respect to the conventional FRC model using DVODE, the new FRC model using ODEPIM and CoDAC significantly accelerates the chemistry calculation by a factor of 8.6 and reduces the total computation by a factor of 6.4. The chemistry time, however, still occupying 70% of the computation time in the new FRC model, which is the largest portion of the total computation time. In contrast, preconditioning matrix inversion only accounts for 7.4% of the total computational time. Therefore, the reduction of computational time in this part is not a high priority. In summary, the computation time of the new FRC model is within 3 times of that of the Frozen model without chemistry, within 8 times of that of the FPV model, and 6.4 times faster than the conventional FRC model.

Figure 3 below shows the time-averaged temperature distributions of Sandia Flame D and E, calculated by FRC-LES and FPV-LES approaches. Both flames have relatively simple flow characteristics, and the chemical reactions interlink to the local strain in both inner and outer shear layers. At approximately $x/d = 40$, intense flame regions can be observed in both flames, where the mixing and combustion are close to complete such that peak temperatures are achieved there. Due to the higher flow velocity in Sandia Flame E, the flame is either pushed further downstream (FPV) or detached from the centerline (FRC). So, the topologies of the results from the two models become different for Sandia Flame E. Besides this difference, both FRC and FPV models present a similar simple diffusion flame, and agree with Nd:YAG laser beam images.

In contrast to time-averaged temperature distributions, the instantaneous temperature distributions of the two models are much more different, as shown in Figure 4. The topology difference between the results from the two models are much more obvious now: FRC predicts no flame near the center line, but FPV still predicts strong flame regions across the center line. In addition, FRC predicts intense flames wrapping around the vortices in the upstream region, which is not predicted by FPV. Particularly, results from FPV-LES approach agree with those from previous FPV studies. It is not obvious which one is closer to the experiment here, because a quantitative experimental measurement of instantaneous temperature distribution is not available. Therefore, even though both models could predict similar time-averaged statistics or spatial distributions, the prediction of unsteady/un-stationary evolution between FRC-LES and FPV-LES approaches could still be significantly different from each other. In view of the unsteady/un-stationary phenomena (e.g. ignition, extinction, combustion instability), such magnification of deviation between the two models becomes an important issue.

Both models predict very dynamic jet flow and flame structures and some levels of local extinction. Near the inlet, the broad pilot flame enhances the stability of the flame and results in minimal local extinction. In addition, turbulence intensity is very low in this region, and the flow field is close to laminar. This means that multi-species differential diffusion effect should be important, which cannot be captured by the FPV-LES approach if unity Lewis number assumption is enforced. For FRC, the piloted flame can survive further downstream to wrap around the vortices generated by shear layers. For FPV, however, the piloted flame distinguished much more upstream. In the downstream region, the outer co-flow and the inner fuel jet interact with each other in the high temperature region of the shear layer, which results more local extinction. In this region, the FPV-LES approach predicts relatively smaller regions with high temperature than the FRC-LES approach, and a completely different topology. Unlike Sandia Flame D, the large deviations between the two models are in both upstream and downstream regions. To better understand the deviations between the two models, detailed species distributions are investigated. Figure 5 compares the distributions of OH radical predicted by the two models. In the upstream region, FRC-LES predicts significantly more OH than FPV-LES. On the contrary, in the downstream region, FPV-LES predicts more regions with high OH concentration, although it is more distributed. However, in the downstream, FPV-LES actually predicts less

regions with high temperature. This contradicts with the general understanding that higher radical levels will result in a stronger heat release and a higher temperature.

To explain this observation, distributions of CO from the two models are compared in Figure 6. FPV-LES predicts both smaller peak CO level and smaller regions with high CO levels, in both upstream and downstream regions. $CO+OH=CO_2+H$ is one of the primary heat release reactions for methane flame. For this reason, CO oxidation becomes the rate-controlling step for the heat release in FPV-LES model, which also explains why it predicts significantly smaller regions with high temperature and partially explains its over-prediction of OH in the downstream region. The comparison of concentrations of major products (CO_2 and H_2O) between the two models (not show here for succinct) indicates that the FPV-LES approach predicts both lower peak product level and smaller regions with high product levels in the downstream region, which further confirms the above conclusion.

On the other hand, FPV-LES predicts smaller regions with high level of CH_4. Therefore, in the prediction of FPV-LES, part of the carbon element must be stuck at some intermediate species between CH_4 and CO, which mainly includes CH_2O and HCO. The conversion from HCO to CO is very fast, thus, only very low level of HCO can be accumulated in the flames (up to mass fractions of 10-5 level in this problem). In the generation of FPV table using 1D steady counter-flow configurations, the flame temperature is higher than the real unsteady conditions in turbulent combustion, thus $CH_2O+OH=HCO+H_2O$ tends to dominate the conversion from CH_2O to HCO. However, there are many holes in the intense flame regions with lower temperature of ~1200 K, in which $CH_2O+O_2=HCO+HO_2$ should dominate the conversion from CH_2O to HCO. With this intermediate-temperature, $CH_2O+O_2=HCO+HO_2$ is more likely to occur during the unsteady evolution. However, the steady FPV table cannot capture the flow unsteady evolution history of the flame, thus could easily overlook this important reaction. As a result, in those holes, carbon element in FPV case is partially stuck at CH2O and has difficulty to convert into HCO and CO. In this problem, CH_2O is accumulated up to mass fractions of 10-3 level.
The discrepancies between the two models could come from the different transport models, the FPV library, the unsteady evolution of filtered mixture fraction and progress variable in the FPV-LES approach, or some combinations of them. For this reason, in the following sections, predictions from the two models will be compared to experimental data in terms of (1) axial and radial distribution of both mixture fraction and progress variable, and (2) the conditional statistics in mixture fraction space.

Figures

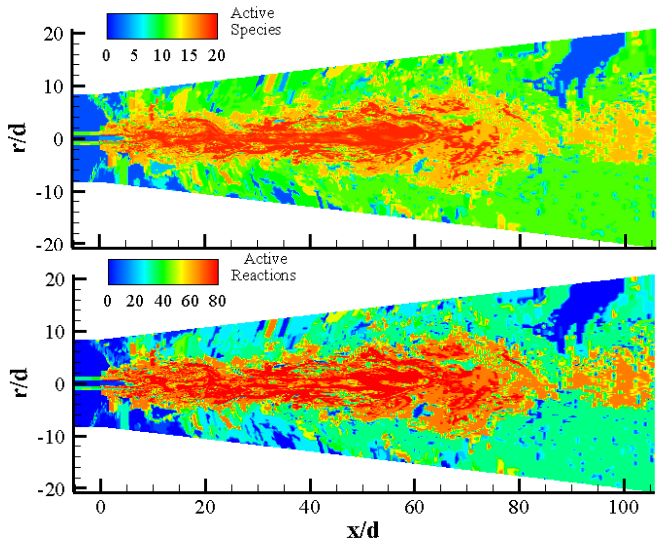

Figure 1. Instantons spatial distribution of numbers of active species (upper) and reactions (lower), generated from the CoDAC method with the FRC-LES approach

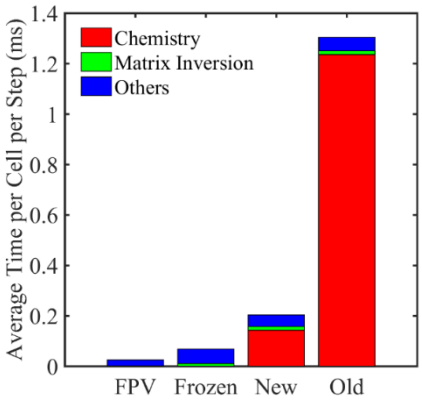

Figure 2. Average computation time distribution of the four models: FPV, Frozen (multi-species transport equations without chemical kinetics source terms), New (new FRC model using ODEPIM and CoDAC), Old (conventional FRC model using DVODE)

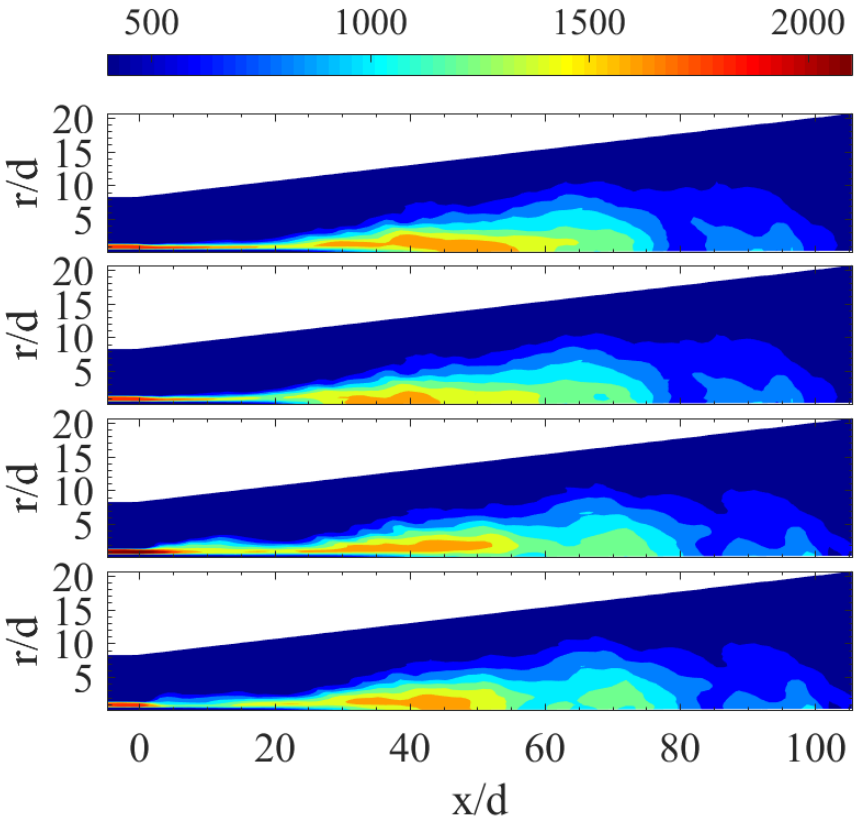

Figure 3. Time-averaged temperature distributions. From upper to lower: Sandia Flame D from FRC-LES; Sandia Flame D from FPV-LES; Sandia Flame E from FRC-LES; Sandia Flame E from FPV-LES

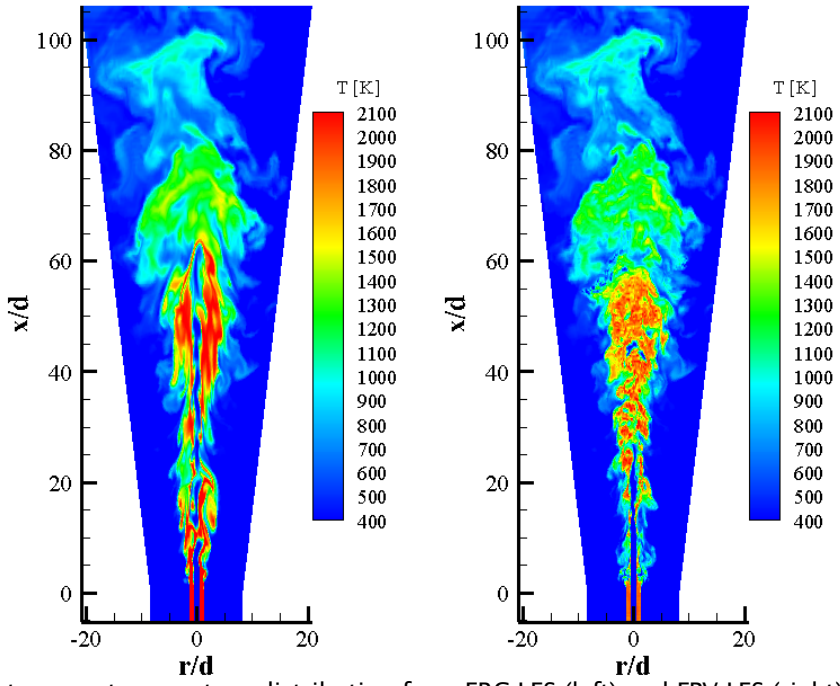

Figure 4. Instantaneous temperature distribution from FRC-LES (left) and FPV-LES (right) at a same time

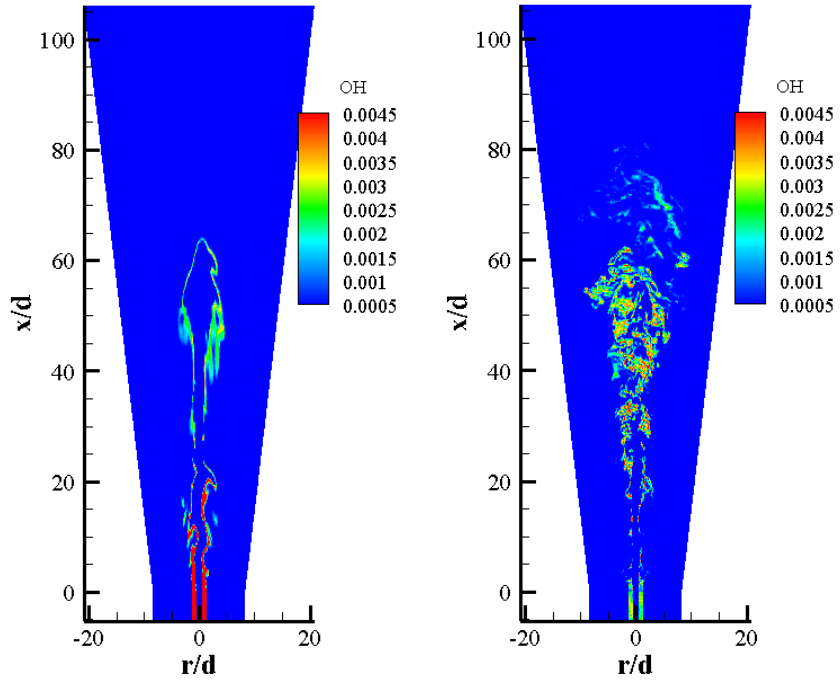

Figure 5. Instantaneous YOH distribution from the FRC-LES (left) and the FPV-LES (right) at a same time

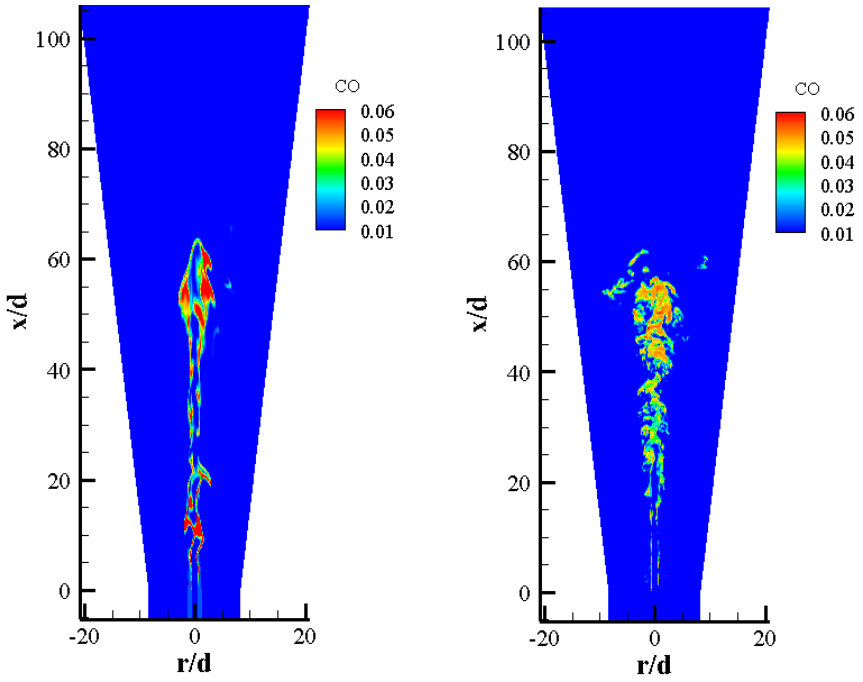

Figure 6. Instantaneous YCO distribution from the FRC-LES (left) and the FPV-LES (right) at a same time

Milestone(s)
Project completed

Major Accomplishments
The accomplishments of the current year's research effort with the impact on the rest of the project are as follows:

- Detailed analysis of Sandia Flame E results were conducted to evaluate the performance of the algorithm in terms of computation time. Simulation results were also compared with results without using DAC to assess the accuracy of the DAC algorithm for both major species and minor species.

Publications
Suo Yang, "Effects of detailed finite rate chemistry in turbulent combustion," Ph.D thesis, Georgia Institute of Technology, 2017

Outreach Efforts
None

Awards
None

Student Involvement
Suo Yang, Xiang Gao

Plans for Next Period
Project is complete

References

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3. Yang, S., Yang, V., Sun, W., Nagaraja, S., Sun, W., Ju, Y., (2015) Parallel On-the-fly Adaptive Kinetics for Non-equilibrium Plasma Discharges of C2H4/O2/Ar Mixture. *AIAA SciTech 2015*, *(submitted)*

Task 3 – LES of Spray Combustion in NJFCP Test Facilities

Georgia Institute of Technology

Objective(s)

The objective of this research activity is to establish a simulation strategy using LES to capture fuel sensitivity in experimental test facilities. In particular, the focus of the current year's effort is to perform a baseline validation of the numerical framework for two of the NJFCP fuels, namely Cat A2 and Cat C5 by matching experimentally stable conditions and to demonstrate that the method can predict lean blowout and can capture fuel sensitivity.

Simulations were conducted initially for Area 6 and Area 3 rigs during Year 1 but subsequent work was funded by NASA and FAA support during FY16 and FY17 was focused on travel funds to attend the FAA meetings. Results reported below were obtained during Year 1 effort funded by FAA and current results are substantially different but are reported under NASA funding separately.

Research Approach

Numerical Methodology

We use the well-established Eulerian-Lagrangian (EL) formulation [1] to perform LES of spray combustion in NJFCP test facilities. In the EL method, a Lagrangian tracking of the dispersed phase is performed and the gas phase is modeled using the conventional Eulerian framework [2]. The coupling between the dispersed phase and the gas phase is specified through inter-phase exchange source terms that appear in the mass, momentum and energy transport equations. A detailed description of the governing equations, turbulence closure and numerical method is provided elsewhere [1, 3]. Here, we briefly summarize the numerical method used in this study.

The gas phase is simulated using a second-order accurate (in both space and time) finite-volume solver for the unsteady Favre-filtered, multi-species, compressible Navier-Stokes equations [3]. A hybrid scheme, which dynamically switches between a second-order-accurate central scheme and a third-order-accurate MUSCL (Monotone Upstream-centered Schemes for Conservation Laws) scheme [3] is used in this study. The subgrid-scale (SGS) momentum and energy fluxes are closed using a subgrid eddy viscosity model, which is obtained using the local grid filter Δ and the subgrid kinetic energy k_{sgs}, for which an additional transport equation is solved [4]. The dispersed phase is simulated using the Lagrangian tracking method [5], which solves for the individual droplet evolution in space and time within the gas phase. The time advancement of the Lagrangian equations are performed through a fourth-order-accurate explicit Runge-Kutta scheme [1]. The closure of the subgrid-scale turbulence chemistry interaction is attained through the quasi-laminar formulation.

LES of Area 3 Rig

The simulation parameters for the Area 3 rig for the gas and spray phase are summarized in Table 1 and Table 2, respectively. The focus of this research effort was to perform a validation of the numerical methodology by simulating the Area 3 rig matching the experimental test conditions corresponding to the stable combustion configuration. Afterward, the same configuration and numerical methodology is used to study fuel sensitivity and LBO. Here, we describe the results for the stable combustion with two different fuels, namely Cat A2 and Cat C5. The experimental data is only available for Cat A2 fuel.

Figure 1 shows the instanteneous contours of the temperature field for in the central and axial planes of the combustor. We can observe a high temperature region in the core of the vortex bubble. This central recirculating region with high temperature products and radicals acts an aerodynamic flame holder leading to stable flame on the periphery of the vortex

bubble in its updstream part. Figure 2 shows the instanteneous OH mass fraction on the same planes. Note that OH mass fraction is typically considered as an indicator of the flame location. We can observe that simiar to the temperature contours, the OH radical is present in the core region with flame anchoring occurring on the periphery of the central vortex bubble. Figure 3 shows the spray droplets colored by their temperature along with the flame identified by the temperature iso-surface (T 1800 K). We can clearly observe lower temperature particles near the location where they are being injected in the domain and the higher temperature particles near the flame where they eventually get evaportated.

Figure 4 shows comparison of the time averaged velocity components with the experiments. Overall the results show a reasonable agreement with the experiments, and the trends appear to be captured by the simulations. Note that the experimental profiles shown in this figure are only available for Cat A2 stable configurations. In addition to Cat A2 simulation results, Figure 4 also includes results for Cat C5 cases (A3-$C5_1^S$ and A3-$C5_2^S$) for stable conditions. Here, Case A3-$C5_1^S$ uses chemical kinetics for C5 with A2 as the liquid fuel, whereas Case A3-$C5_2^S$ uses chemical kinetics and fuel corresponding to C5. These cases were considered to demostrate sensitivity of the fuel on the results. We can observe that the results for the velocity components only show minor sensitivity. However, the radial profiles of the temperature shown in Figure 5, show differences among the three cases, where the central core appears to be colder in the case employing C5 as the liquid fuel.

Based on the results presented here, we can conclude that the LES framework employed in this research effort is adequate to capture the dynamics of unsteady spray-flame-trubulence interaction, which is essential to study the combustion physics such as LBO, cold restart and altitude relightning for the present NJFCP program.

Tables

Table1. Gas phase simulation parameters for the Area 3 rig.

Parameter	Value	Source
Outlet/reference pressure	50 Psi	Experiment
Inlet mass flow rate	53 g/s	Experiment
Inlet temperature	350 F	Experiment
Bulkhead temperature (Isothermal walls)	530 F	Experiment

Table 2. Details of the spray parameters for the Area 3 rig.

Injector type	Pressure blast	Experiment
Pressure drop across nozzle	40 Psi	Experiment
SMD	27 μm	Rizk scaling
Mass flow rate (stable)	1.3 g/s	Experiment
Mass flow rate (LBO)	1.14 g/s	Experiment
Injection temperature	100 F	Experiment
Particles distribution	Log normal	Simulation
Injection	Hollow cone with cone angles 50° and 90°	Estimated from number density obtained from experiments

Table 3. List of LES cases indicating their current status.

Case	Fuel	Kinetics	Condition	Rig	Status
A3-A2^{S}	Cat A2	Cat A2	Stable	Area 3	Complete
A3-C5$_1^{S}$	Cat A2	Cat C5	Stable	Area 3	Complete
A3-C5$_2^{S}$	Cat C5	Cat C5	Stable	Area 3	Complete
A3-A2^{B}	Cat A2	Cat A2	LBO	Area 3	Underway
A3-C5^{B}	Cat C5	Cat C5	LBO	Area 3	Underway
A6-A2^{S}	Cat A2	Cat A2	Stable	Area 6	Underway
A6-C5^{S}	Cat C5	Cat C5	Stable	Area 6	Future work
A6-A2^{B}	Cat A2	Cat A2	LBO	Area 6	Future work
A6-C5^{B}	Cat C5	Cat C5	LBO	Area 6	Future work

Figures

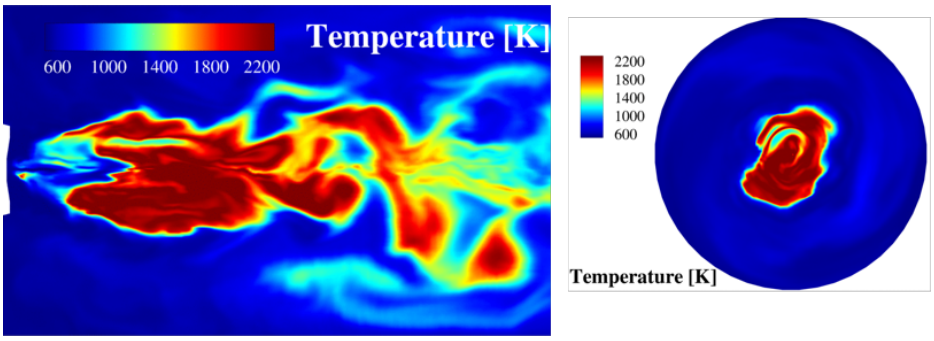

Figure 1. Temperature contours for LES of experimentally stable configuration with CatA2 kinetics.

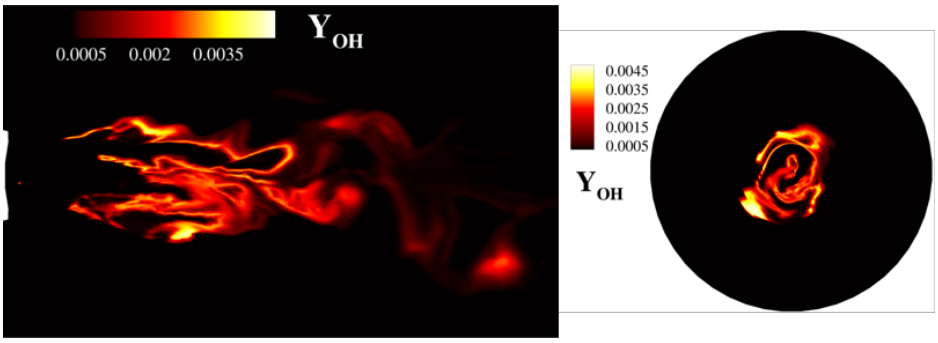

Figure 2. OH mass fraction contours for LES of experimentally stable configuration with CatA2 kinetics.

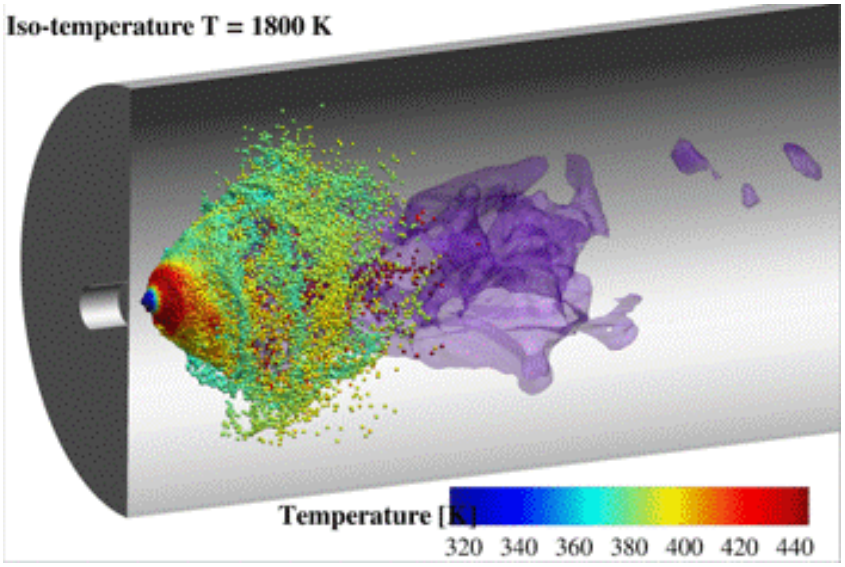

Figure 3. Spray particles (colored by temperature) and flame (identified by temperature iso-surface) visualization in LES of experimentally stable configuration with CatA2 kinetics.

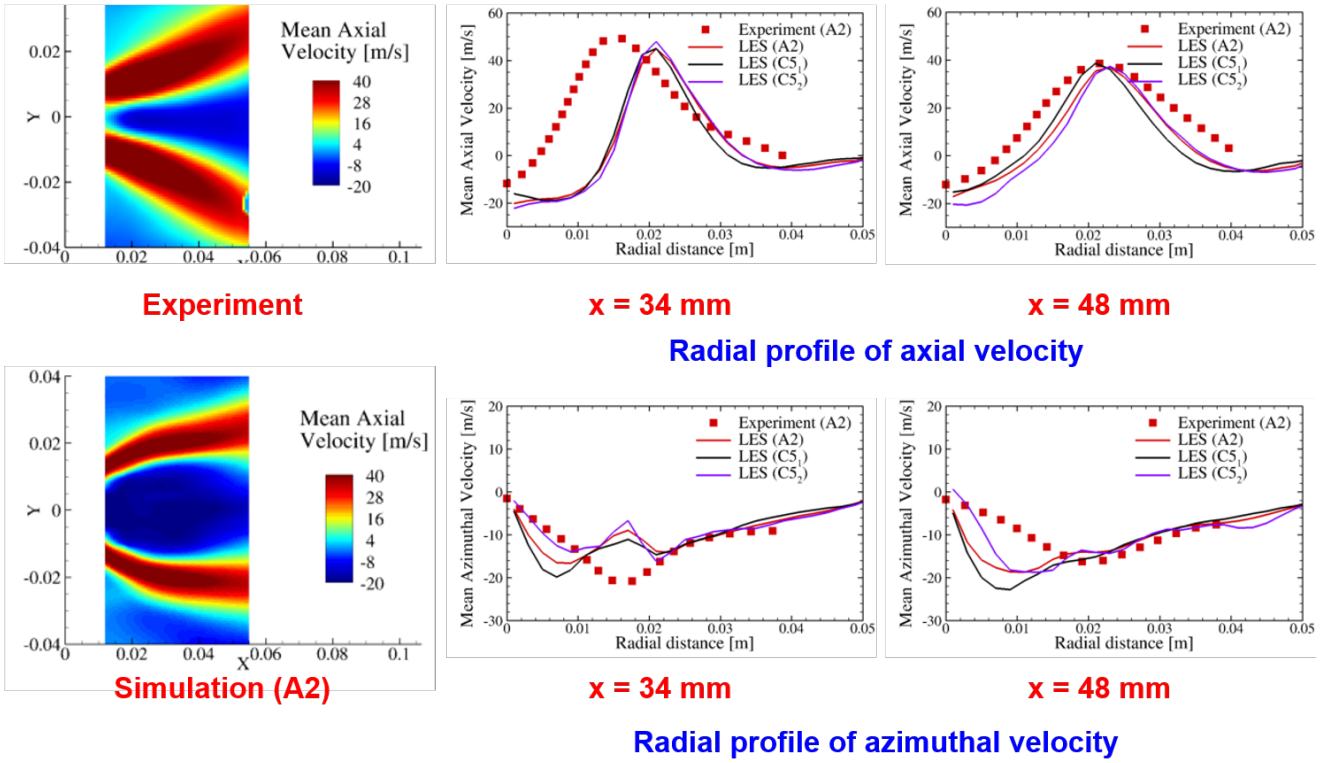

Figure 4. Comparison of time averaged velocity components obtained from LES (A3-A2^S, A3-C5$_1^S$ and A3-C5$_2^S$) and experiment (A3-A2^S).

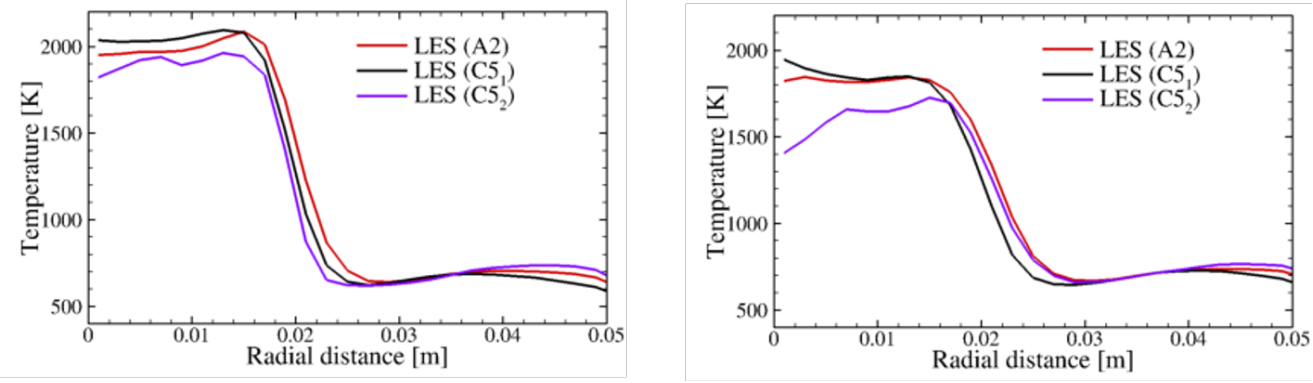

Figure 5. Comparison of the time temperature obtained from LES of different cases illustrating fuel sensitivity.

Milestone(s)

Project completed

Major Accomplishments

The accomplishments of the current year's research effort with the impact on the rest of the project are as follows:

- **Simulation of the Area 3 rig with Cat A2 fuel**: The simulation has been performed matching the experimentally stable conditions to validate the numerical methodology. It used the reduced chemical kinetics model developed under Task 1. The spray condition was partly estimated from the experiment and additional condition was prescribed through the Rizk's scaling law. Overall, the results show a reasonable agreement thus establishing the suitability of the numerical framework employed in this investigation.
- **Simulation of the Area 3 rig with Cat C5 fuel:** The simulation was conducted by keeping the same configuration as mentioned above and only changing the fuel. The change in the fuel was done in two sub-steps leading to two cases. In the first case, only the chemical kinetics was modified whereas in the second case both the liquid fuel and the chemical kinetics corresponded to the Cat C5 fuel. The results obtained from Cat A2 and C5 cases show fuel sensitivity, which is an essential element of the NJFCP program.
- **Simulation of the Area 3 rig under LBO conditions:** Additional set of simulations corresponding to LBO conditions is currently underway.
- **Simulation of the Area 6 referee rig:** The simulation of the Area 6 referee rig with effusion cooling holes and Cat A2 fuel is also currently underway.

Publications

[1] Yang, S., Ranjan, R., Yang, V., Menon, S., Sun, W., "Sensitivity of Predictions to Chemical Kinetics Models in a Temporally Evolving Turbulent Non-premixed Flame," Combustion and Flame, Vol. 183, 224-241, 2017.
[2] Yang, S., Ranjan, R., Yang, V., Menon, S., Sun, W., "Parallel on-the-fly Adaptive Kinetics in Direct Numerical Simulation of Turbulent Premixed Flame," Proceedings of the Combustion Institute, Vol. 36, Vol. 2, 2025-2032, 2017.
[3] Yang, S., Ranjan, R., Sun, W., Yang, V., and Menon, S., "Sensitivity to Chemical Kinetics Models in Time Evolving Turbulent Non-Premixed Flames," 10th U.S. National Combustion Meeting, College Park, MD, April 23-26, 2017.
[4] Rieth, M., Ranjan, R., Kempf, A., and Menon, S., "On the Comparison of Finite-rate Kinetics and Flamelet Based Subgrid Models for LES of Turbulent Premixed Flames," 10th U.S. National Combustion Meeting, College Park, MD, April 23-26, 2017.

[5] Milan, P., Ranjan, R., Panchal, A., and Menon, S., "Flame Dynamics Sensitivity to Turbulent Combustion Models in a Swirl Spray Combustor," AIAA-2017-5079, 53rd AIAA/SAE/ASEE Joint Propulsion Conference, Atlanta, GA, 10-12 July 2017.
[6] Ranjan, R., Panchal, A., Hannebique, G., and Menon, S., "Towards Numerical Prediction of Jet Fuels Sensitivity of Flame Dynamics in a Swirl Spray Combustion System," AIAA-2016-4895, 52nd AIAA/SAE/ASEE Joint Propulsion Conference, Salt Lake City, UT, July 25-27, 2016.

Outreach Efforts
None

Awards
None

Student Involvement
- A. Panchal

Plans for Next Period
There are no more plans for this project. For the following two years FY 16 and FY 17 all research was done under NASA funding and FAA provided only travel funds to attend appropriate meetings twice a year.

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4. Kim, Won-Wook, and Suresh Menon. "An unsteady incompressible Navier–Stokes solver for large eddy simulation of turbulent flows." International Journal for Numerical Methods in Fluids 31.6 (1999): 983-1017.
5. Faeth, Gerard M. "Mixing, transport and combustion in sprays." Progress in Energy and Combustion Science 13.4 (1987): 293-345.