Project 028 Area 4: Combustion Model Development and Evaluation

Georgia Institute of Technology

Project Lead Investigator

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University Participants

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- P.I.(s): Suresh Menon
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- Task(s):
 - 1. Development of reduced kinetics for NJFCP Fuels
 - 2. Network modeling and kinetics acceleration
 - 3. LES of spray combustion in NJFCP test facilities

Project Funding Level

\$350K from FAA and \$350K cost share.

Investigation Team

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:
 - 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.

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-lumped 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 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 mechanisms 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 1 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 the 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 is improved.

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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 Fig. 2.

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

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 counterflow flames, etc. The developed models are accurate enough to capture wide variety of combustion physics of interest such as LBO, cold restart, altitude relightning 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 an 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

N/A

Outreach Efforts

N/A

<u>Awards</u> N/A

Student Involvement

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- Y. Gao
- B. Majda
- Y. Liu

<u>Plans for Next Period</u>

In future, the research effort will focus on the following tasks:

- Develop and optimize reduced kinetics and transport for Cat C1 fuels.
- Develop a robust and generalized strategy for different NJFCP fuels.
- Perform comprehensive validation of the fuels for wide range of combustion physics such as LBO, cold start and altitude re-lightning.
- Deliver the reduced models to be used for LES and to the OEMs.
- Develop a dynamic strategy for computational acceleration for all NJFCP fuels.

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Task 2 - Network modeling and kinetics acceleration

Georgia Institute of Technology

Objective(s)

The objectives of this research activity are as follows:

- Develop a reactor network model for assessment of chemical kinetics: This task was aimed to use preliminary LES results obtained from Task 3 to develop a reactor network model for assessment of the newer chemical kinetics model developed under Task 1 for different NJFCP fuels.
- 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.

Research Approach

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Assessment of Reduced Kinetic Mechanism Using Reactor Network Model

In this task, reactor network model was developed based on LES modeling (from Prof. Menon's group) to assess detailed and reduced kinetic mechanism generated by Prof. Wang's group at Stanford and Prof. Lu's group at UCONN. The schematic of the combustor in LES and corresponding reactor network model is shown in Fig. 1. The reactor network model was developed based on the simulation conditions of LES which is used to model Area 3 and Area 6 combustors. As demonstrated in Fig. 1, LES combustor simulation results were employed to extract information of volume, residence time, temperature, and pressure. The reactor network model was then formed by a serious of Perfect Stirred Reactor (PSR) and Plug Flow Reactor (PFR). These reactors model mixing zone, flame zone, recirculation zone and post-flame zone, respectively with identical residence time and temperature/pressure conditions in LES simulation. Therefore the chemical effect and accuracy of the reduced kinetic mechanism can be evaluated by comparing results from reduced and detailed kinetic mechanisms.

The results from reactor network model for CatA2 model are summarized in Fig. 2. From Fig. 2 it can be seen the reduced kinetic mechanism of CatA2 can accurately reproduce the detailed mechanism for major species. There is deviation on the prediction of minor species, such as H_2O_2 , but the deviation of minor species does not affect the prediction of heat release prediction. This rationales the applicability of the reduced kinetic mechanism.

Based on the results from reactor network model, detailed reaction pathway analysis was conducted and an automated program has been developed. The reaction pathways of CatA2 in different regimes are shown in Fig. 3. In Fig. 3, the darkness of arrows indicate the intensity reaction flux of reaction pathways. Darker color means faster conversion. The direaction of arrows indicate the direction of conversion. It can be seen that in the mixing zone of the combustor, fuel starts to decompose owing to the presence of H and OH from the recirculation zone. In flame zone, the dominate reaction pathway of jet fuel is pyrolysis into small hydrocarbons, majorly C_2H_4 and then oxidizes to CO and CO_2 . The reaction pathways in the recirculation zone and post flame zone are the regions where CO burns out. Results from Fig. 3 also indicate different reaction pathways in different regions, therefore it is highly possible to use different submechanisms in different region to accelerate computation efficiency.

Dynamic Mechanism Reduction for LES Modeling

In different regions of combustor and at different time steps, the dominate chemistry is different. The reactor network model shows that in the post flame region, CO to CO_2 conversion dominates the chemical reaction while fuel pyrolysis and initiation reactions are negligible there. Therefore, using a global reduced kinetic mechanism is not efficient in the whole LES simulation regime both spatially and temporally. On-the-fly mechanism reduction [Sun, et al 2010; Sun, et al 2015; Yang, et al 2015] can be applied in LES modeling to further reduce the cost of computation.

In this task, the globally reduced CatA2 skeletal mechanism with 38 species (from Prof. Tianfeng Lu's group) is used. It is noteworthy that it is not necessary to do mechanism reduction every time step and every grid point, so a local vector \Box is used to determine whether new local reduced mechanism is needed or not at a specific grid point.

Λ -	$\left[\frac{T-T_{o}}{T-T_{o}}\right]$	$\ln \chi_{O_2} - \ln \chi_{O_2,0}$	$\ln \chi_{fuel} - \ln \chi_{fuel,0}$	
Δ-	T_o	' $\ln \chi_{O_2,0}$ '	$\ln \chi_{fuel,0}$	

Where T is temperature of the flow. \Box is mole fraction of species. Subscript 0 means initial condition. This local vector \Box is calculated in simulation and compared with the value from last time step. If \Box is smaller than a specific value, the locally reduced mechanism from last time step can then be used without new reduction. Otherwise, Path Flux Analysis method (PFA) [Sun et al. 2010] is used at local temperature and pressure condition to generate a new locally reduced mechanism for calculation.

The on-the-fly adaptive kinetics (OAK) was tested using a 3D premixed turbulent flame code provided by Prof. Menon's group. This turbulent flame mode is the core module for the LES code used to simulate Area3 and Area6 combustors. Computation was conducted using full skeletal mechanism with 38 species and OAK method. The results of OH mass fraction are than compared for accuracy as shown in Fig. 4. Figure 5 further compared the PDF (Probability Density Function) of reaction rates of fuel and OH.

The CPU time was then compared for calculation with CatA2 skeletal mechanism with and without OAK. The comparison is shown in Fig. 6. As shown in Fig. 6, OAK can significantly decrease the computation cost on chemistry by almost 28 times.

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The time used for mechanism reduction (PFA) is negligible. The total computation time is shortened by factor 7 and the most time consuming part is the calculation of transport properties after using OAK. Therefore, the adaptive property methodology was extended to the calculation of transport properties. If new locally reduced mechanism is needed in the calculation, the transport properties will be calculated. Otherwise, transport properties from last time step will be used without new calculation. The results using both adaptive kinetics and transport property (OAK+CoTran) are also compared and shown in Fig. 4 and 5. It can be seen from Fig. 4 and 5 that nearly identical results were obtained from three methods with max deviation less than 0.5%. The comparison of CPU time shown in Fig. 6 clearly indicates that with adaptive kinetics and transport, the computation time of transport property is almost negligible and the total computation time of turbulent flame can be decreased by factor 17.

Figures



Figure 1. (top) LES simulation results of combustor (bottom) reactor network model developed based on LES simulation geometry and conditions



Figure 2. Comparison of reactor network modeling results between detailed CatA2 kinetic mechanism (dashed line) and skeletal kinetic mechanism (solid line); red: flame zone, black: mixing zone, blue: recirculation zone, green: post flame zone.





Figure 3. Reaction path flux analysis for CatA2 in the flame zone



Figure 4. Profiles of OH mass fraction of premixed Cat A2 turbulent flame (left) with skeletal mechanism, (middle) with OAK, and (right) with OAK and transport adaption



Figure 5. PDF of reaction rates of fuel and OH of premixed Cat A2 turbulent flame (left) with skeletal mechanism and (right) with OAK





Major Accomplishments

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

- **Development of a reactor network model**: In this research past LES data was used to segregate the combustor into different zones so that the chemical kinetics effect and accuracy of the reduced kinetic mechanism can be evaluated by comparing results obtained from reduced and detailed kinetic mechanisms. This framework allowed to establish that the developed reduced kinetics models under Task 1 are appropriate enough to capture the combustion physics of interest to the NJFCP program.
- Development and validation of on the fly adaptive kinetics: A typical combustor can be segregated into different zones as mentioned above and within each of such zones, only some of the species are active. This lead to development of an approach "on-the-fly adaptive kinetics" (OAK), which lead to reduction in the overall computational cost. The method was validated by comparing results obtained by considering all the species in a conventional manner, thus establish that the approach will help reducing the computational cost of LES of large-scale combustors.

Publications

N/A

Outreach Efforts

N/A

<u>Awards</u> N/A

Student Involvement

N/A

Plans for Next Period

In future, the research effort will focus on the following tasks:

• Perform extensive validation of the OAK approach by considering LES of flame turbulence interaction in canonical premixed and non-premixed configurations.





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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.

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 similar 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-C5¹^s and A3-C5²^s) for stable conditions. Here, Case A3-C5¹^s uses chemical kinetics for C5 with A2 as the liquid fuel, whereas Case A3-C5²^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

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

Table1. Gas phase simulation 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 2. Details of the spra	/ parameters for the Area 3 rig	
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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	Cat C5	Cat C5	Stable	Area 3	Complete
A3-A2 [₿]	Cat A2	Cat A2	LBO	Area 3	Underway





A3-C5 ^в	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 ^в	Cat A2	Cat A2	LBO	Area 6	Future work
A6-C5 ^в	Cat C5	Cat C5	LBO	Area 6	Future work

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

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-C5¹^s and A3-C5²^s) and experiment (A3-A2^s).



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x = 34 mm

Radial profile of temperature

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

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

N/A

Outreach Efforts

N/A

<u>Awards</u>

N/A

Student Involvement

• A. Panchal

Plans for Next Period

In future, the research effort will focus on the following tasks:



- Implementation of efficient reduced kinetics and other acceleration techniques in the LES solver to speedup parametric studies.
- Collaborate with Area 5, UTRC and OEMs to develop closures for spray combustion
- Develop efficient turbulence-chemistry subgrid closures for LES of spray capable of predicting fuel sensitivity to LBO and ignition.
- Area 3 rig will be simulated again with the new ari-blast injector used in the ongoing experiments for Cat A2, C5 and C1 fuels.
- Area 6 rig will be simulated for stable and LBO conditions for different fuels.

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