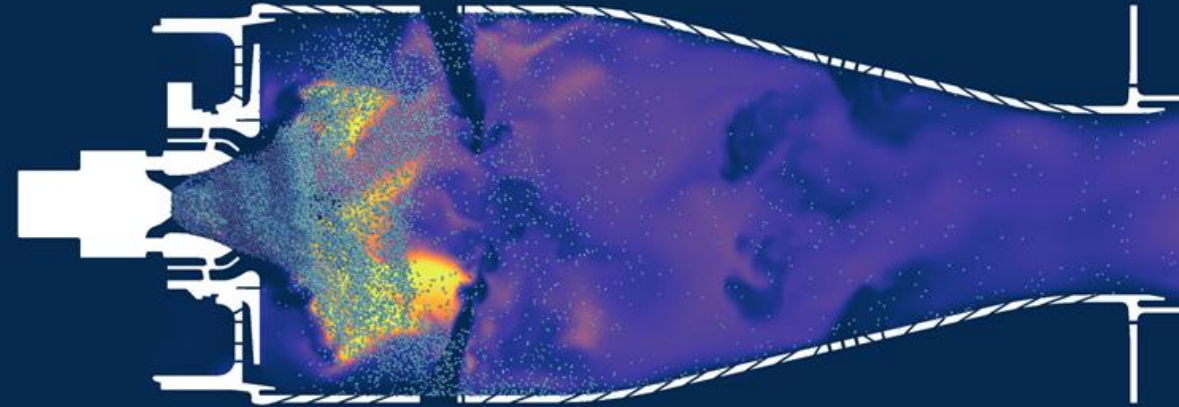


IEA AMF SAF webinar
April 29th, 2026

ASSESSING FUEL PROPERTY IMPACTS ON COMBUSTOR PERFORMANCE FOR AVIATION FUELS



DEBOLINA DASGUPTA

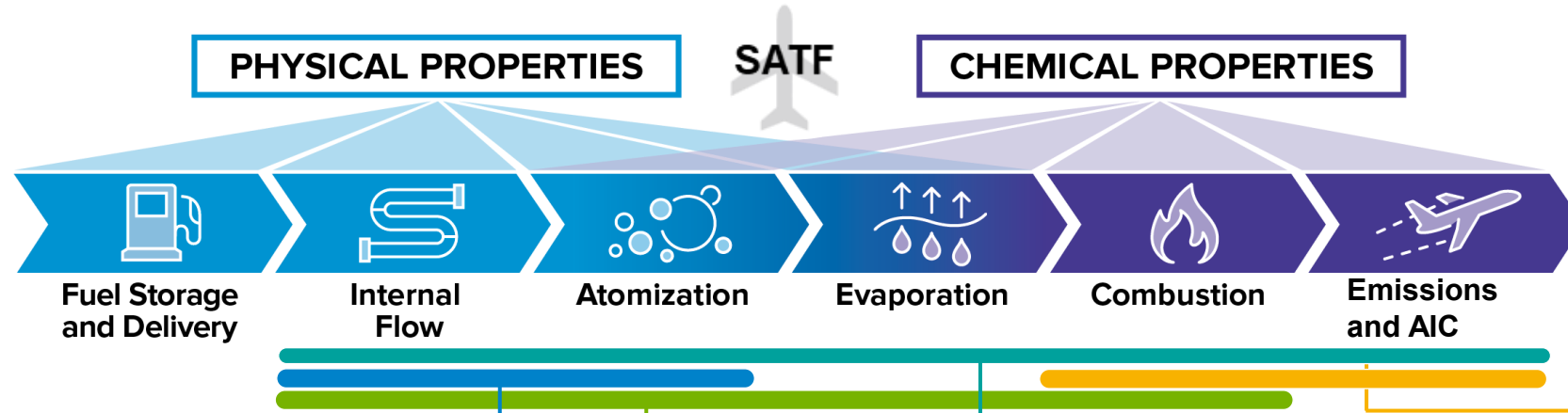
Senior Research Scientist

ACKNOWLEDGEMENT

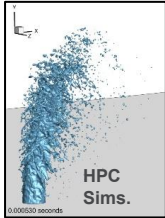
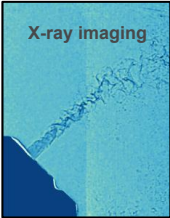
- Work is funded by Department of Energy Transportation Technologies Office, Technology Manager: Kevin Stork, Program Manager: Gurpreet Singh
- Convergent Science Inc. for licenses
- Simulations were performed on Computing resources provided on Bebop and Improv, a high-performance computing cluster operated by the Laboratory Computing Resource Center at Argonne National Laboratory

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MOTIVATION: OPEN QUESTIONS

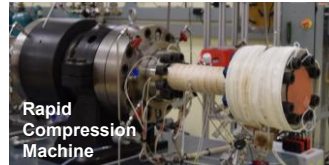
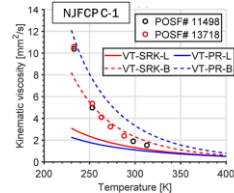


MULTIPHASE FLOWS



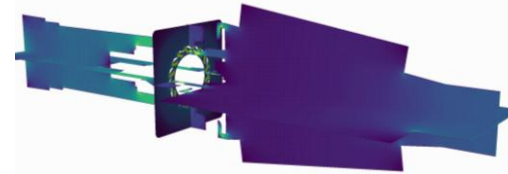
- Impact of fuel properties on spray behavior
- Change in behavior with different operating conditions
- Generation of high-quality data for model validation?

REAL FLUID BEHAVIOR AND CHEMISTRY DYNAMICS



- Development of engineering models for real fluid modeling applicable for the flight map.
- Development of surrogate to mimic the multi-component fuel and predicting properties accurately
- Data generation for validating chemistry models for new fuels

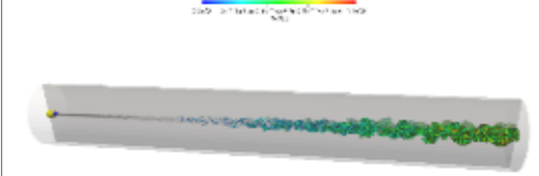
HIGH-FIDELITY SIMULATIONS



Mid-size combustor CFD simulation

- Influence of fuel properties on combustor performance
- Accurately capture the physics and understand the change in figures of merit such as lean blow out and ignition change with fuels
- Utilization of data from high-fidelity simulations to develop improved sub-models

SOOT AND EMISSIONS

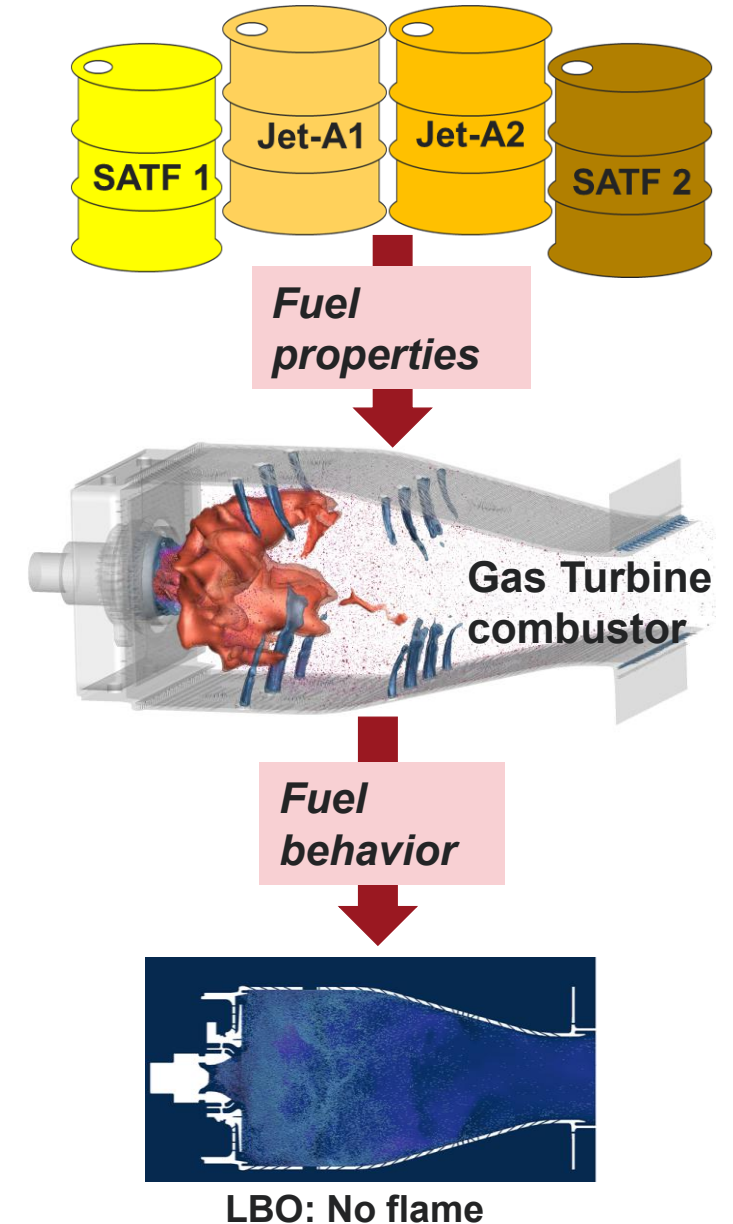


Soot interaction with atmosphere

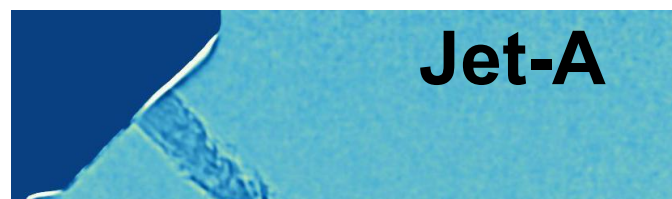
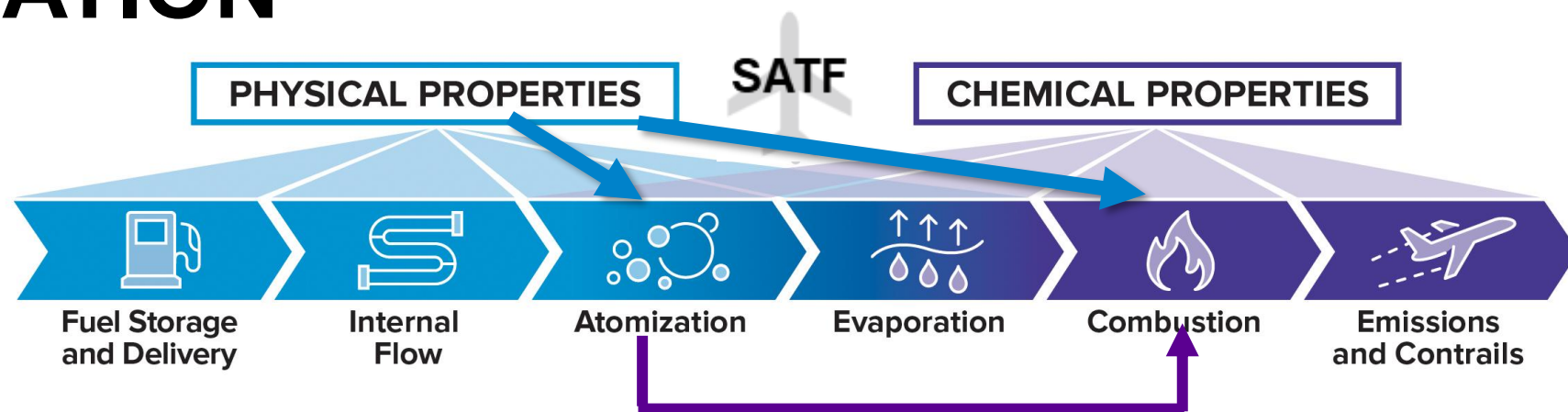
- Impact on emissions (soot, NOx, water vapor) with fuel changes
- Understanding the interaction between these emissions and the atmosphere
- Development of improved models that can support prediction of aviation induced cloudiness

RELEVANCE

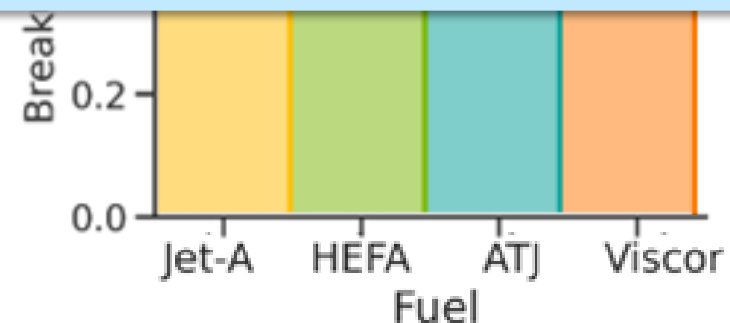
- Synthetic Aviation Turbine Fuels (SATF) possess properties analogous to Jet-A
- Between nominal Jet-A and C-category (alternate) fuels, 5 – 10 μm change in SMD are noted with property changes between -2% and +6% for density, +20% and +50% for dynamic viscosity, and -4% and +13% for surface tension [1, 2]
- Essential to compare their performance with Jet-A in engines as variations in fuel properties alter:
 - Combustion Dynamics,
 - Flame stability,
 - Combustor efficiency
- To measure the performance of these fuels, metrics are evaluated.
 - **Lean Blow Out (LBO):** minimum global equivalence ratio to sustain a flame



MOTIVATION

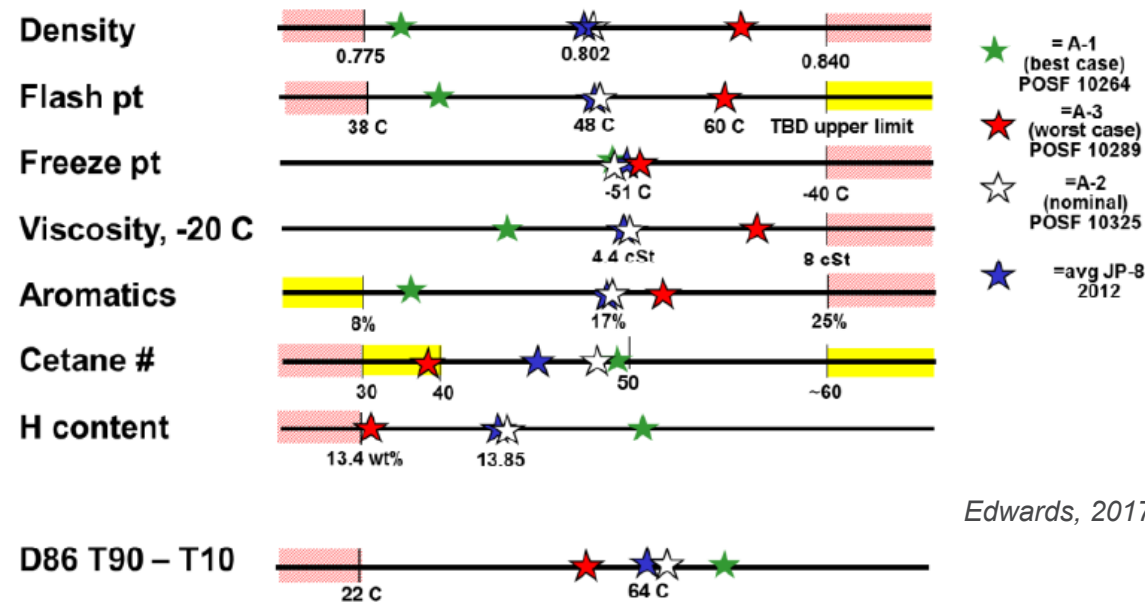


How does change in fuel properties impact the flame behavior at stable and off-normal conditions?



MOTIVATION

Drop-in fuels



Edwards, 2017, AIAA SciTech Forum, AIAA 2017-0146

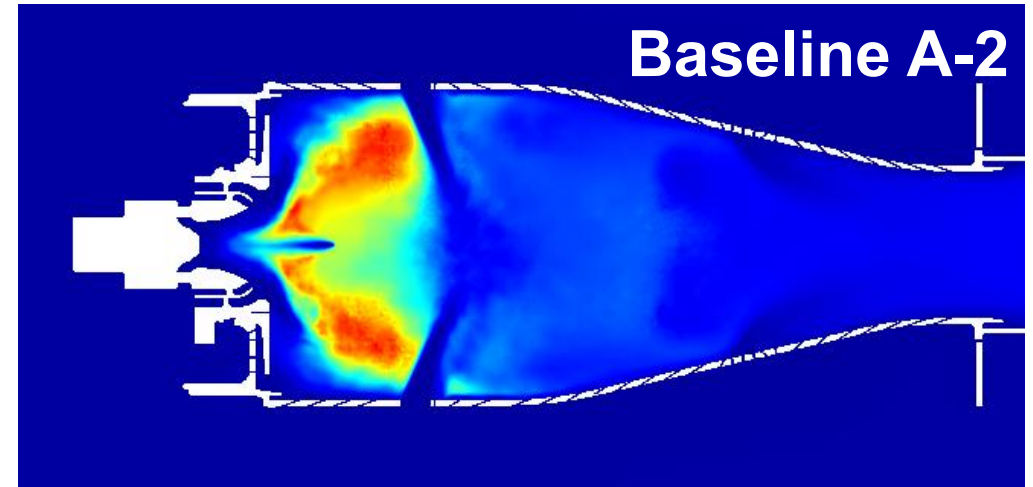
Figure 1. Property Range of the Category A Conventional Fuels with Respect to Allowed Limits (Red Established, Yellow Proposed)

- Limits on properties to be defined as drop-in fuels
- Property variation considered here include:
 - Density: $\pm 3\%$
 - Kinematic Viscosity: $\pm 3\%$
 - Heat of combustion: $\pm 3\%$

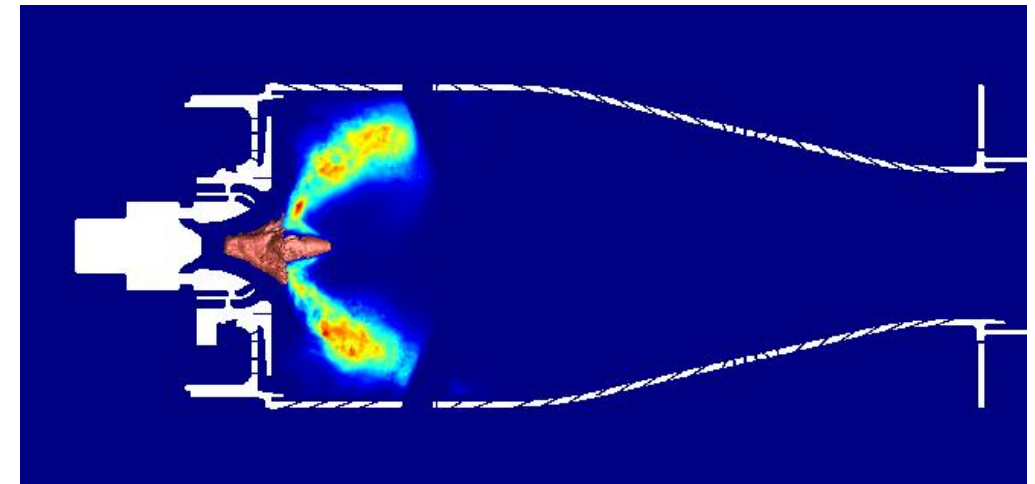
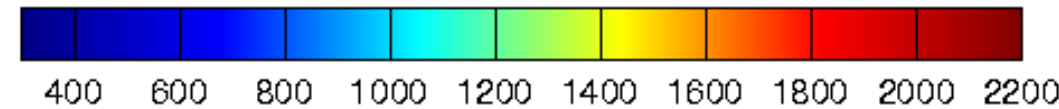
RESULTS: BASELINE A-2

Temperature and OH Contours

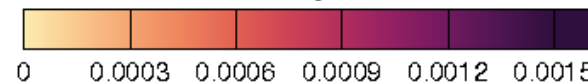
- Stable condition for A-2
 - $\Phi_{\text{global}} = 0.096$
- For the baseline A-2 case, the high temperature regions can be seen for a typical flame.
 - There is a slight asymmetry in the two branches of the M-flame, with a greater downstream penetration of the top branch.
 - This can be seen with the slightly higher temperature pocket downstream of the dilution air compared to the lower branch.



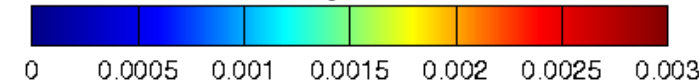
Temperature [K]



$Y_{\text{CH}_2\text{O}}$ [-]



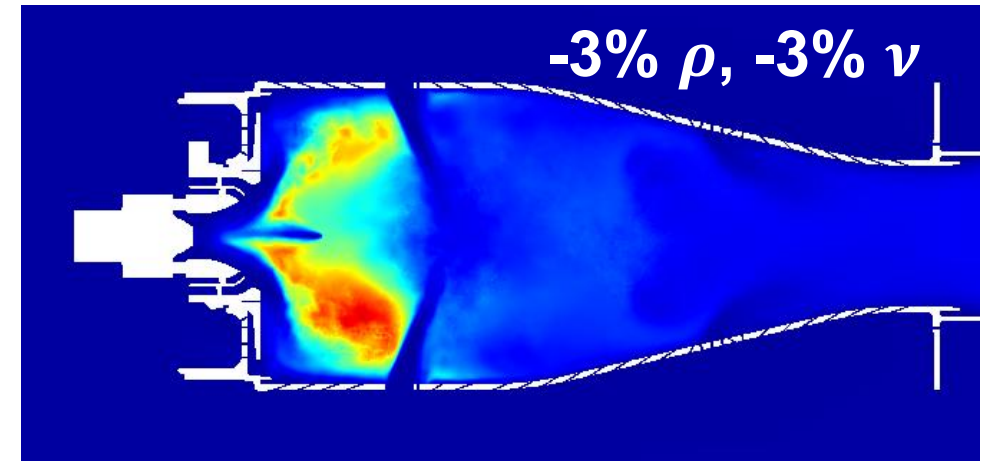
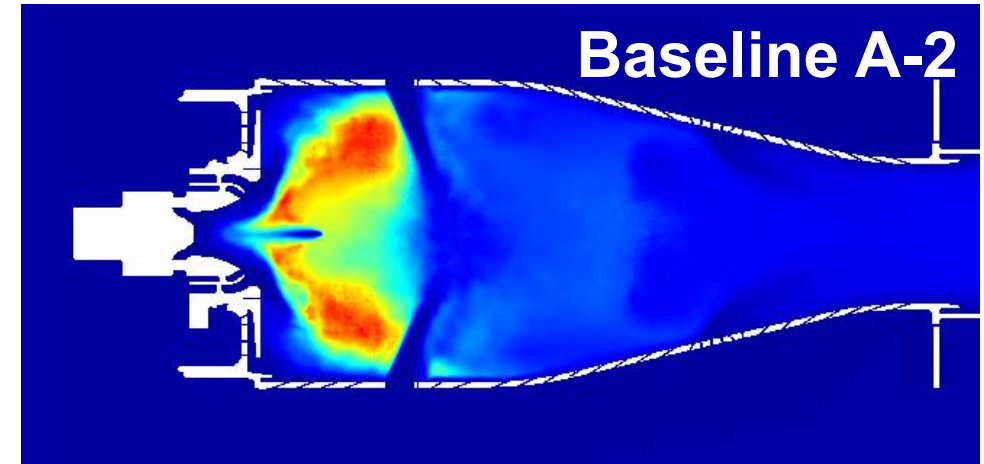
Y_{OH} [-]



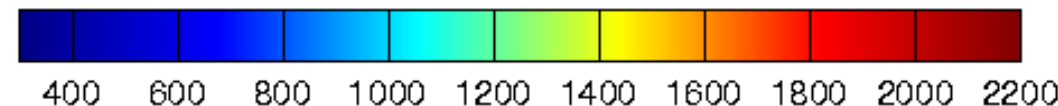
RESULTS: COMBINATIONAL CHANGES

Temperature Contours

- With a reduction in density and kinematic viscosity, enhanced asymmetry is seen
- Higher temperatures in the lower branch compared to the upper branch.
- A reduction in the density and more prominently the kinematic viscosity leads to changes in secondary atomization leading to smaller droplets.
- A potential reason to observe the enhanced flame asymmetry could be the asymmetry in fuel vapor distribution pronounced by the flow-field.



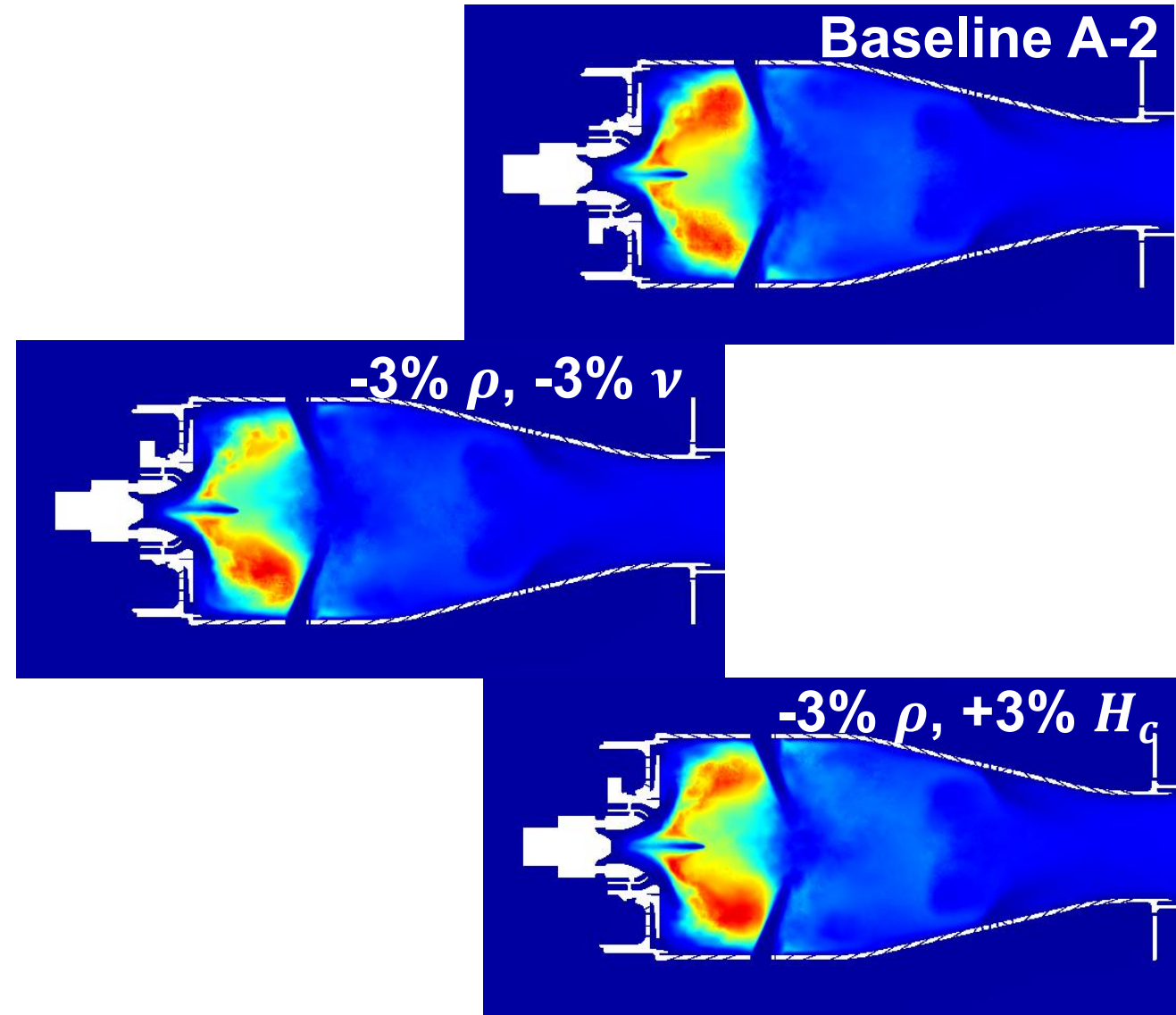
Temperature [K]



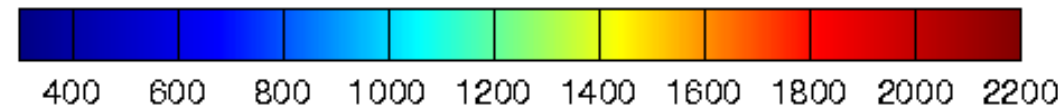
RESULTS: COMBINATIONAL CHANGES

Temperature Contours

- With a reduction in density and an increase in heat of combustion, broader and wider regions of high temperature are noted.
 - This can be attributed to the increased energy release per kg of fuel.
- It can also be noted that the flame is not as asymmetric as the reduced density and kinematic viscosity case.
 - This could be due to the higher temperatures leading to improved vaporization everywhere and the fact that density plays a less significant role in secondary atomization compared to kinematic viscosity.



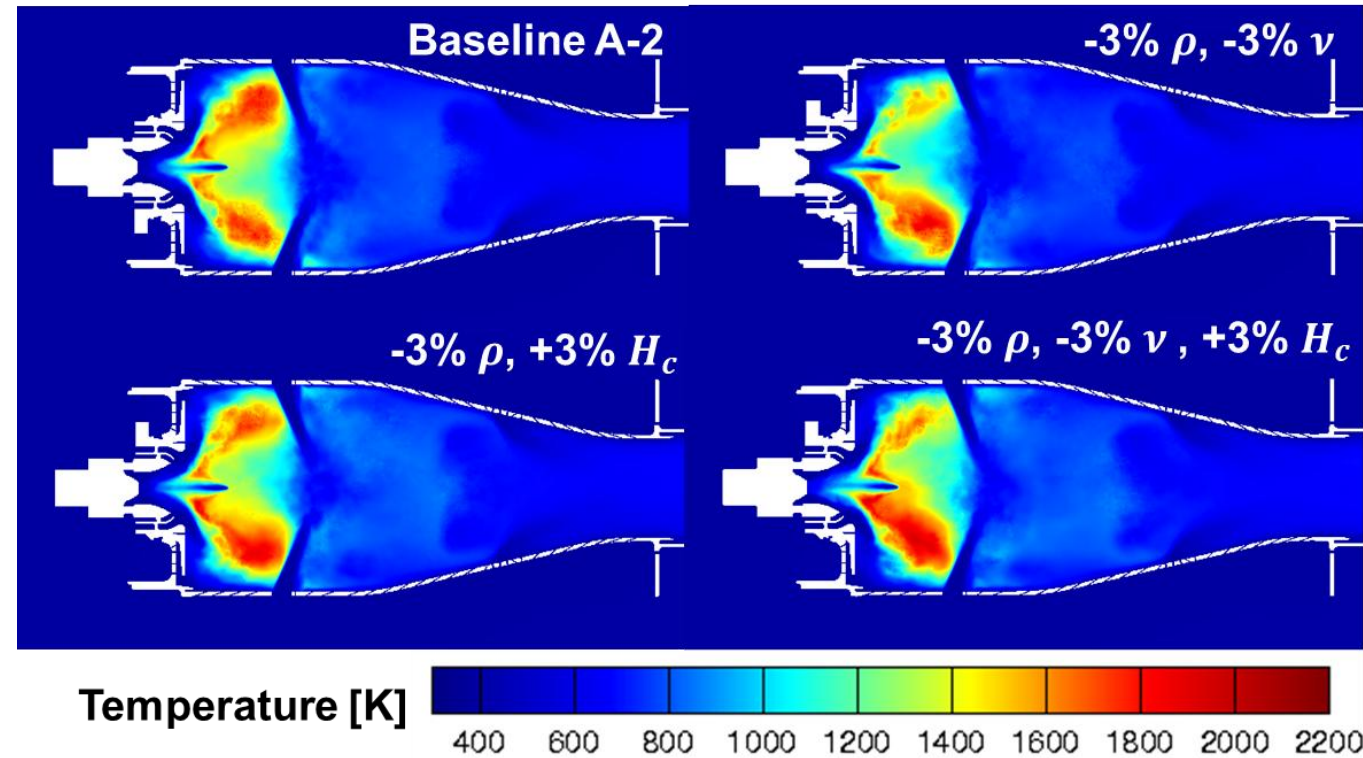
Temperature [K]



RESULTS: COMBINATIONAL CHANGES

Temperature Contours

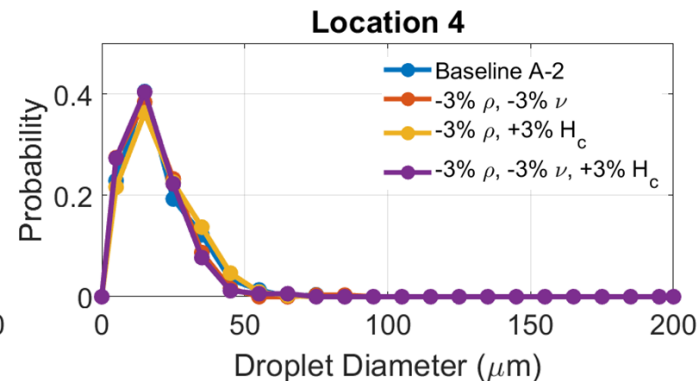
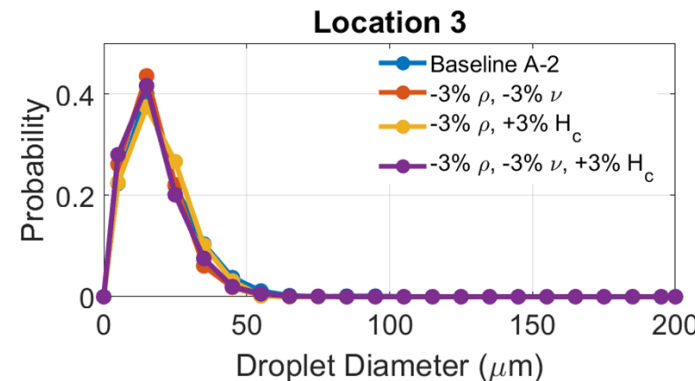
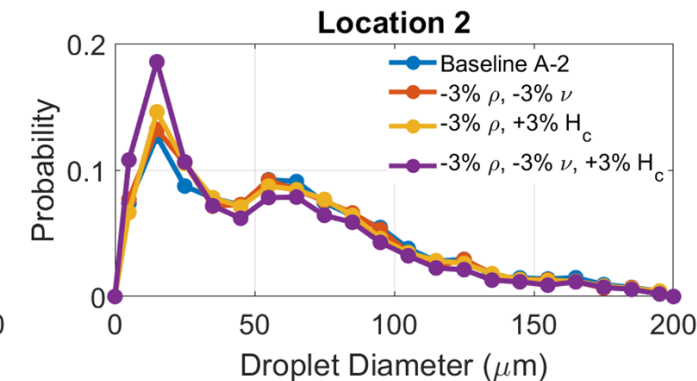
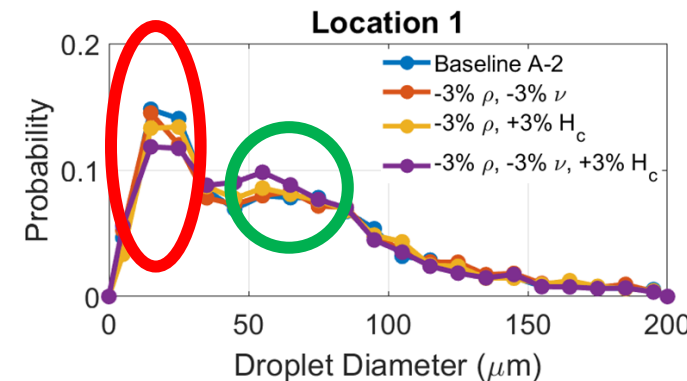
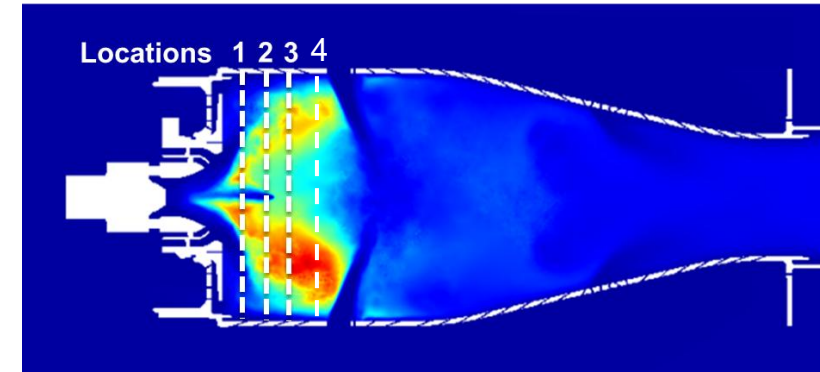
- With a reduction in density, kinematic viscosity, and an increase in heat of combustion:
 - The temperature distribution is more asymmetric compared to the previous case
 - Continues to have wider regions of higher temperatures.
- The asymmetry is similar to what was observed with the reduced density and kinematic viscosity.



RESULTS: COMBINATIONAL CHANGES

Droplet distribution

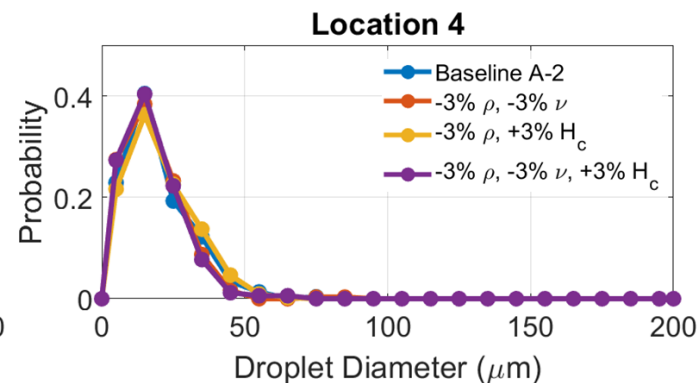
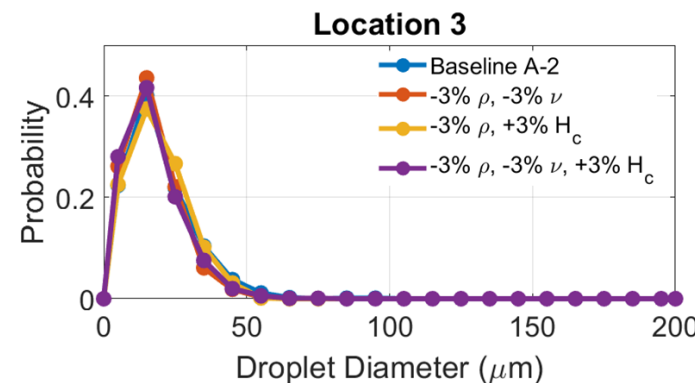
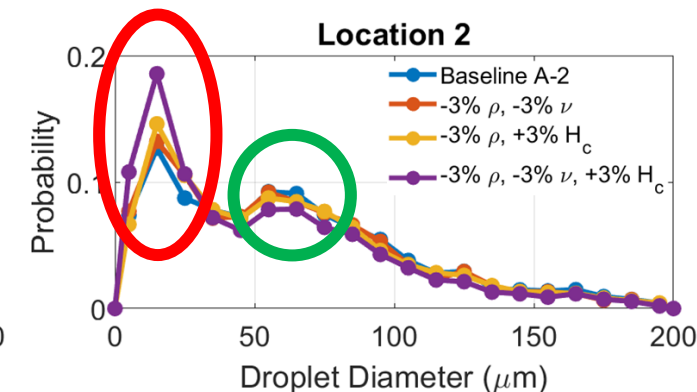
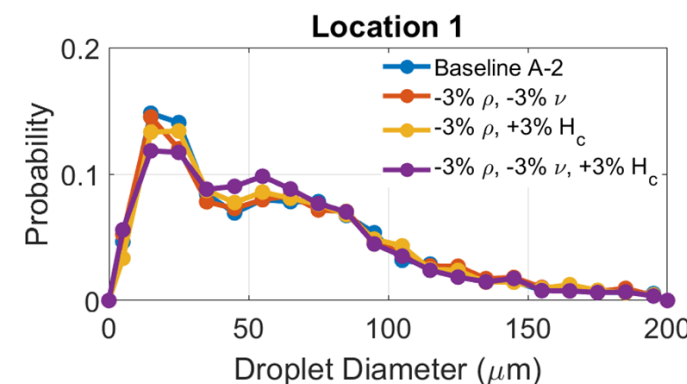
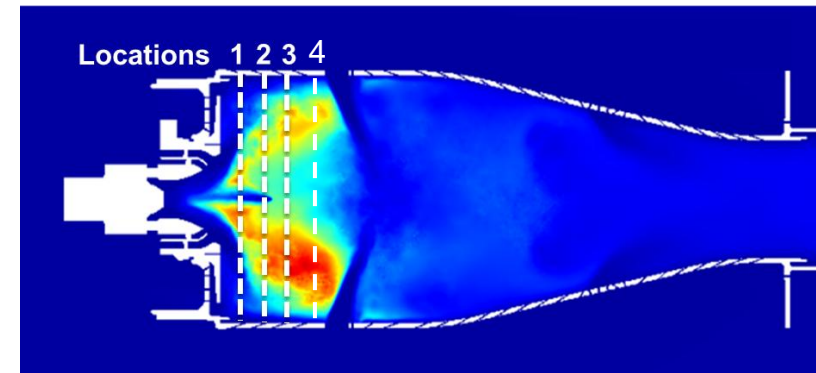
- The droplet distribution is not significantly impacted at downstream locations.
- However, differences are observed in distributions closer to the flame anchoring location.
- For the baseline A-2, at location 1, a first peak is seen at around 20 μm . A second peak is observed at $\sim 50 \mu\text{m}$.
- For all the combinational changes, the peaks are seen at similar values.



RESULTS: COMBINATIONAL CHANGES

Droplet Distribution

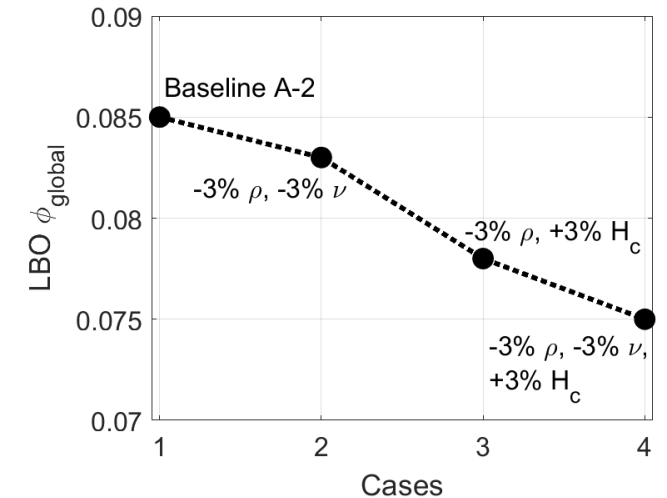
- At location 2, the probability of the peak at $\sim 20 \mu\text{m}$ increases.
 - This can be attributed to improved secondary atomization for the case where density and kinematic viscosity change.
 - A bigger change is seen with an increase in H_c due to improved vaporization.



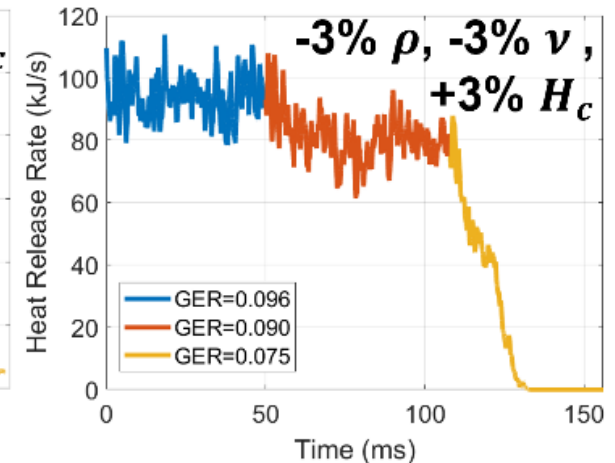
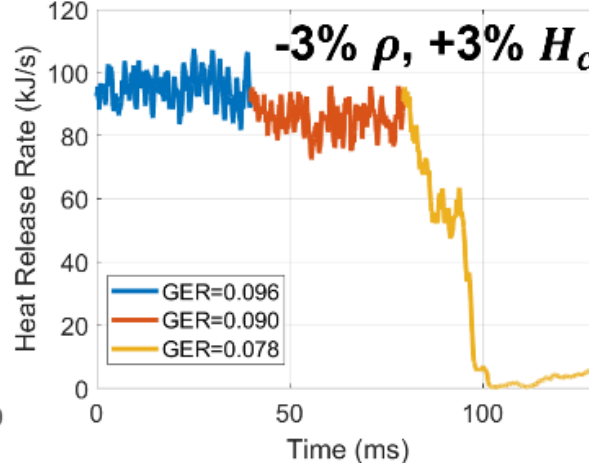
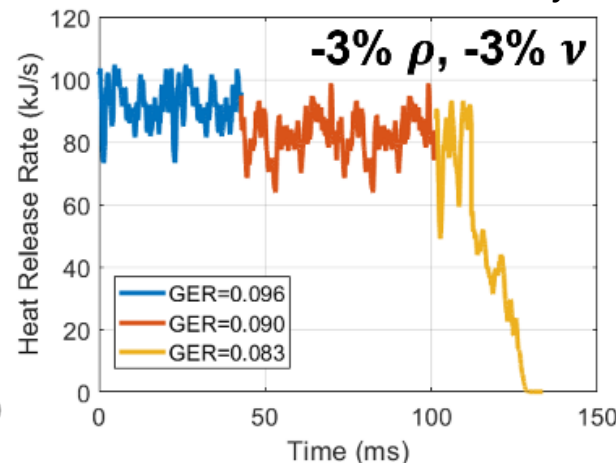
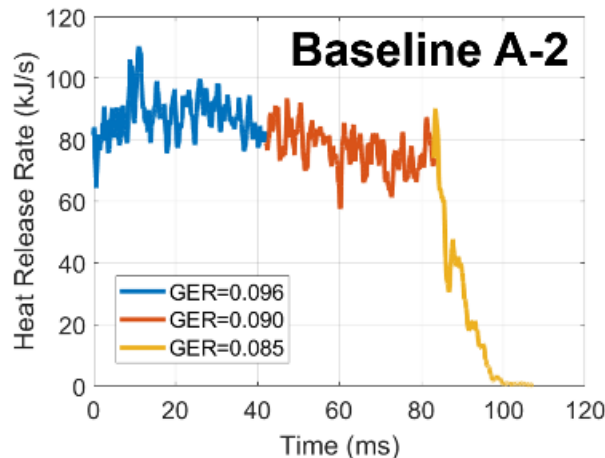
RESULTS: COMBINATIONAL CHANGES

Lean Blow Out

- For finding the Lean Blow Out (LBO) Global Equivalence Ratio (GER), the GER is reduced in steps starting from 0.096 GER.
 - For every step-down, the initial condition is the previous steps last time step.
 - Every GER operating condition is run for 30 ms (~2 flow-through times)
 - The heat release rate is continuously monitored. During the step-down process, beyond a certain GER, the heat release rate starts decreasing rapidly towards zero. This GER is the LBO GER.
 - After the 0.005 GER step-down, for the combinational change cases, additional simulations were run to delineate the LBO GER for each case
 - Every case is re-rerun with GER = 0.096, then GER = 0.09 and LBO GER



Heat release rate variation with time to identify LBO GER

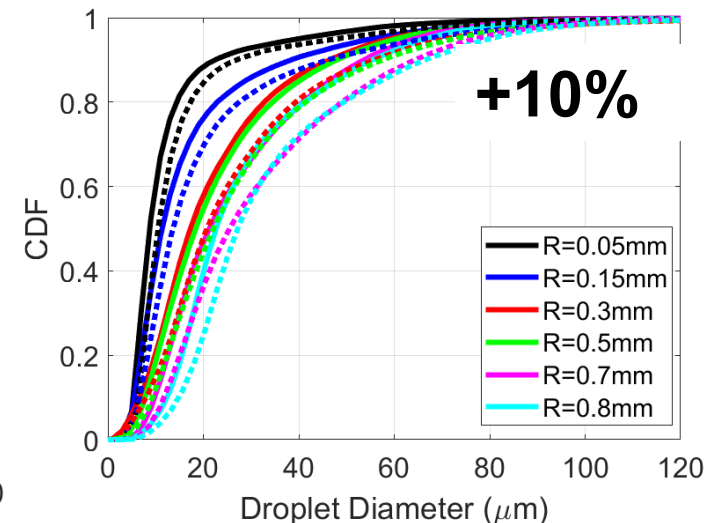
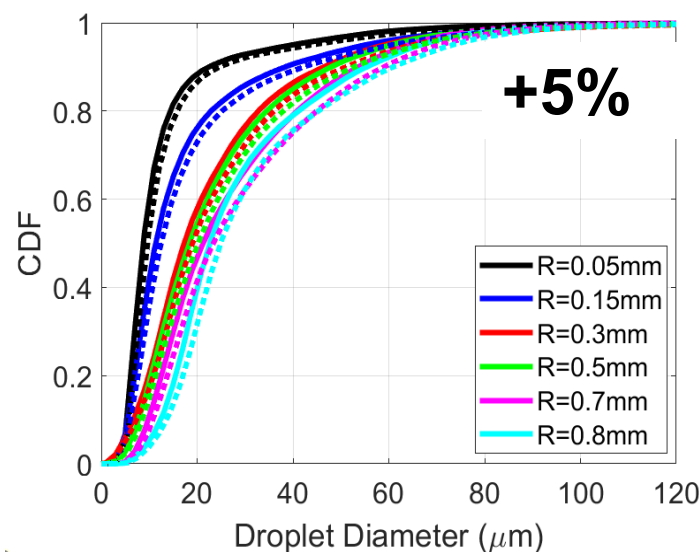
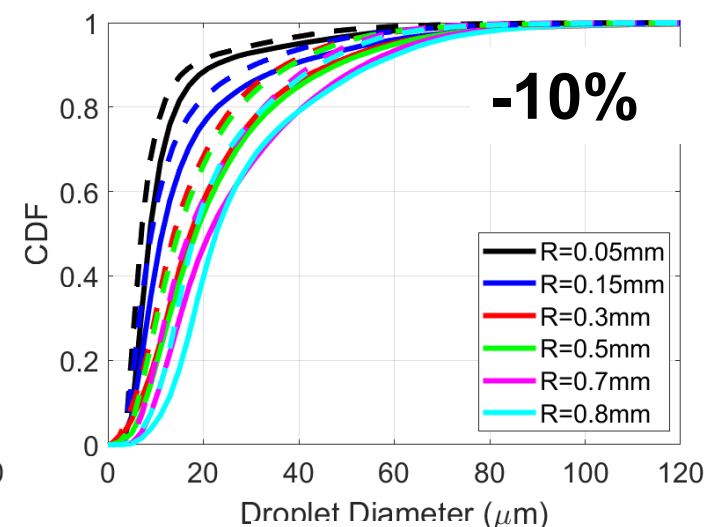
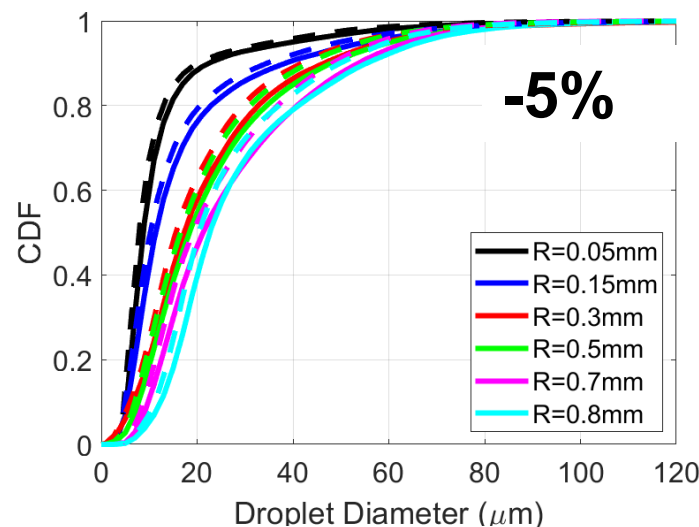


LBO equivalence ratio for combinational changes

CFD MODEL DEVELOPMENT

Droplet size initialization for the current study

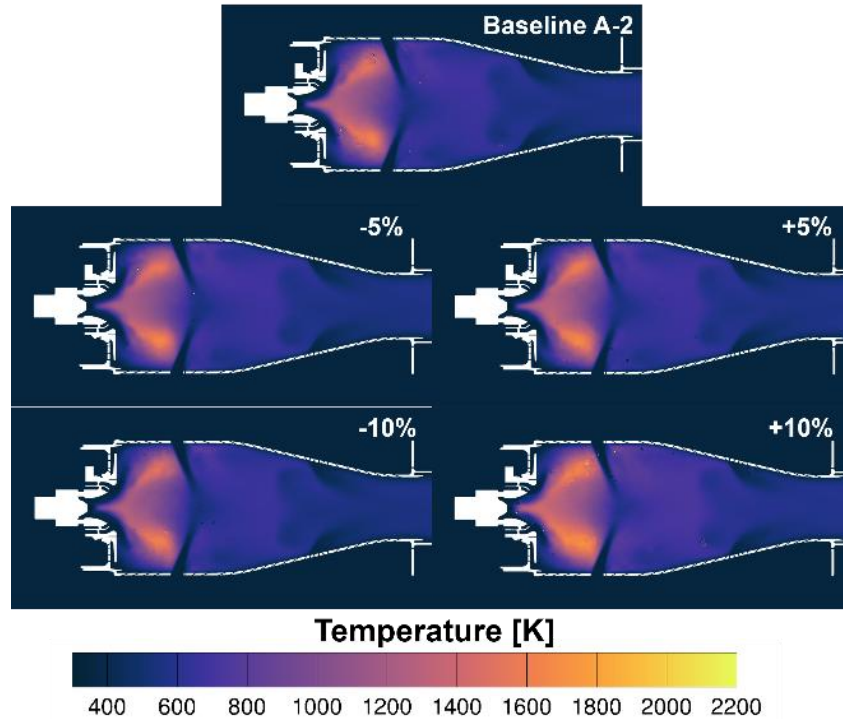
- Changing the mean of the droplet diameter by $\pm 5\%$ and $\pm 10\%$, retaining the same distribution
- No changes to:
 - Fuel physical properties
 - Spray velocity initialization
 - Chemical properties
 - Chemical mechanism
 - Fuel mass flow rate



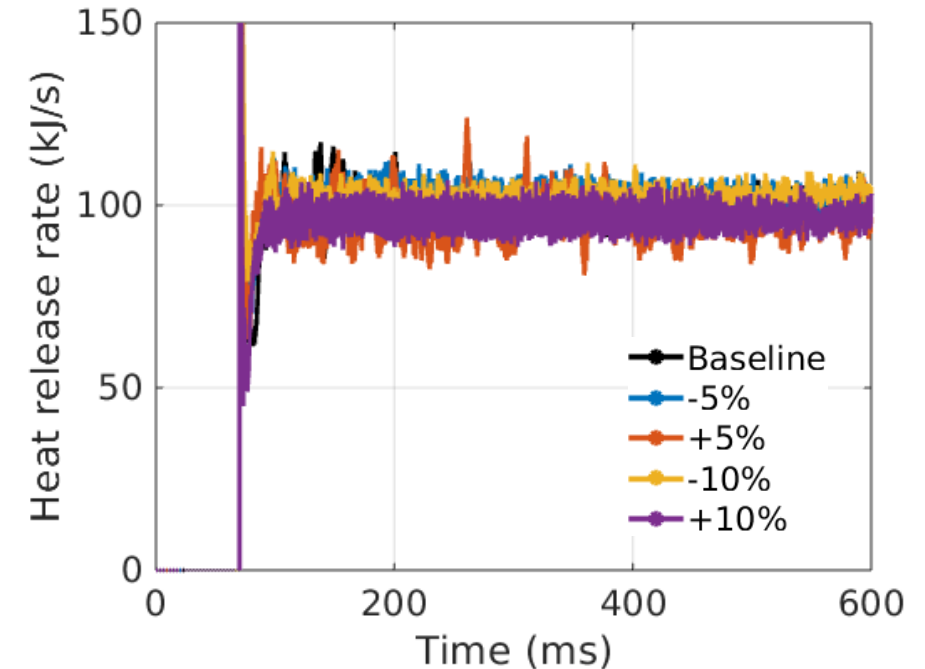
GLOBAL CHARACTERISTICS

Temperature distribution and heat release rate

Center plane
slice with
temperature
contours



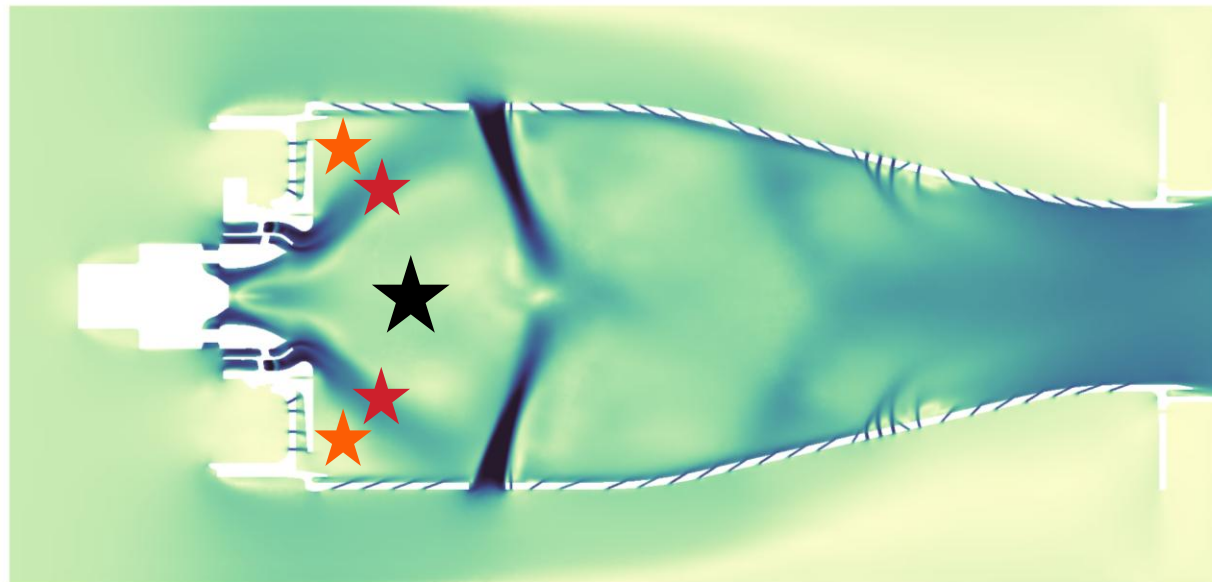
Heat release rate variation with time for all cases



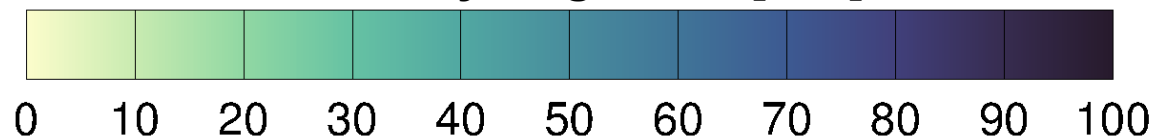
- Center plane temperature distributions qualitatively look similar for all cases.
- The asymmetric behavior is seen from all the temperature distributions.
- The heat release rate, which is a global metric, shows no significant differences
 - Global behavior may not be significantly impacted by the change in droplet sizes used in this study

BASELINE A-2 CASE

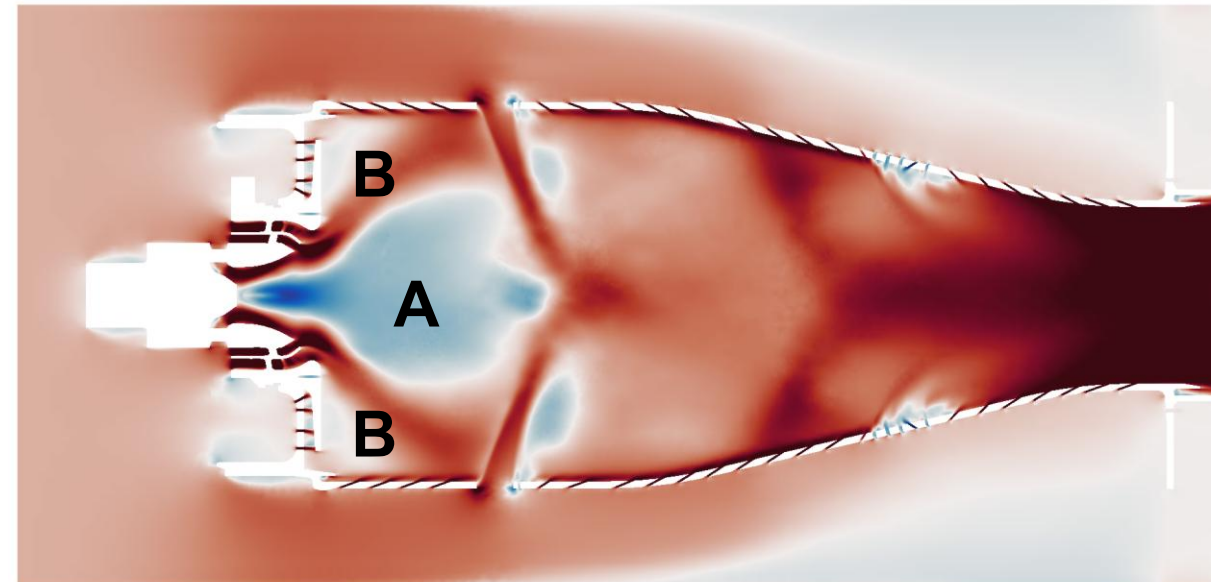
Flow-field and region identification



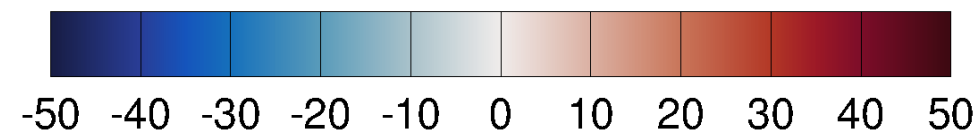
Velocity Magnitude [m/s]



- ★ Central recirculation zone
- ★ Swirling flow shear layers
- ★ Corner recirculation zones



Axial Velocity [m/s]

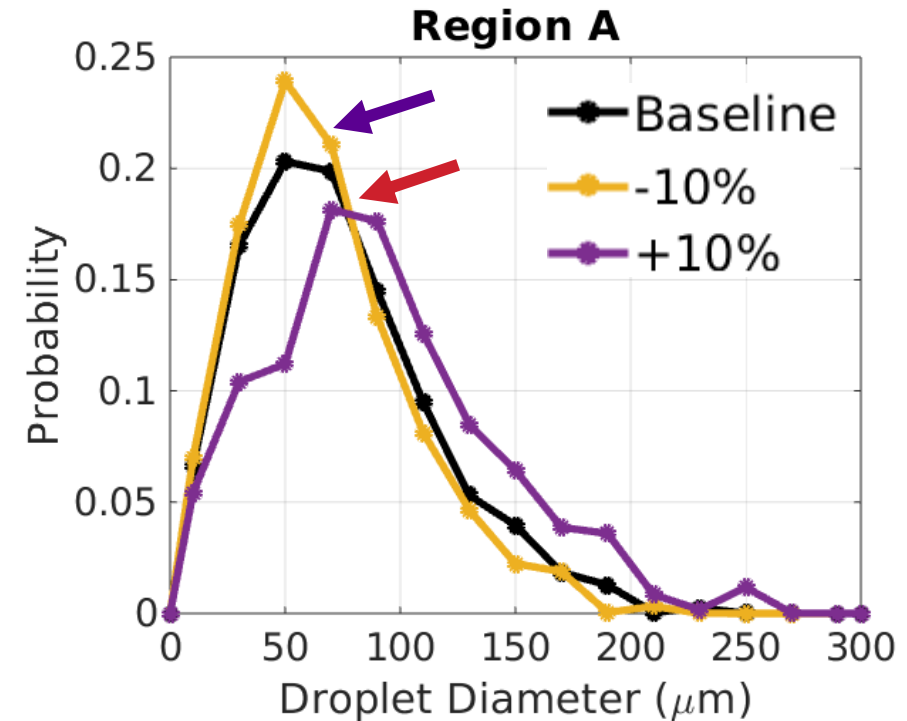
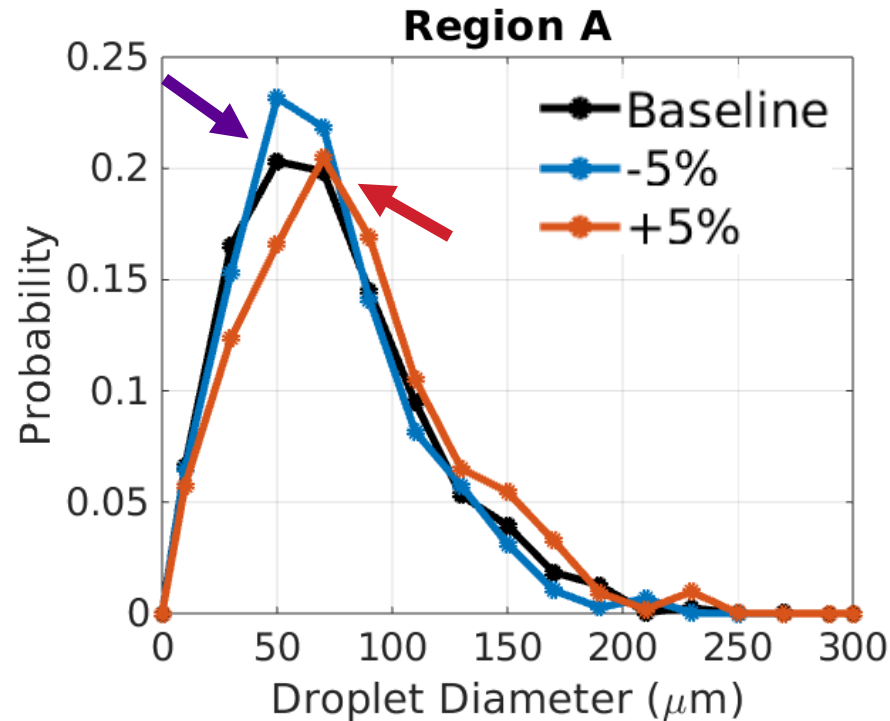


- Region A ★
- Region B ★ ★

DROPLET SIZES – REGION A (CRZ)

Comparison between baseline and $\pm 5\%$, $\pm 10\%$

D. Dasgupta, S. Som, Journal of Engineering for Gas Turbines and Power 148 (1), 011007

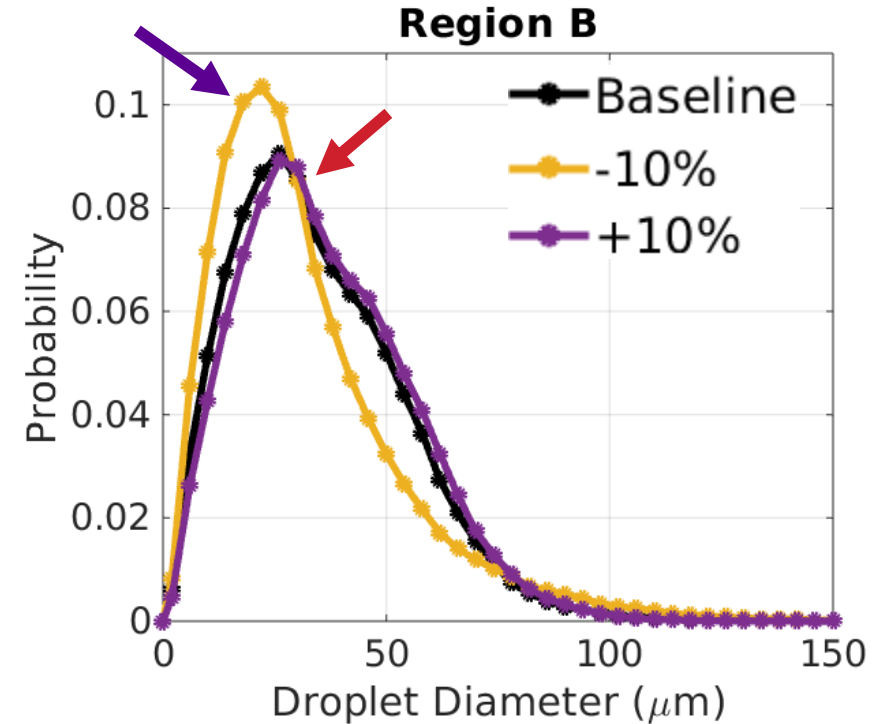
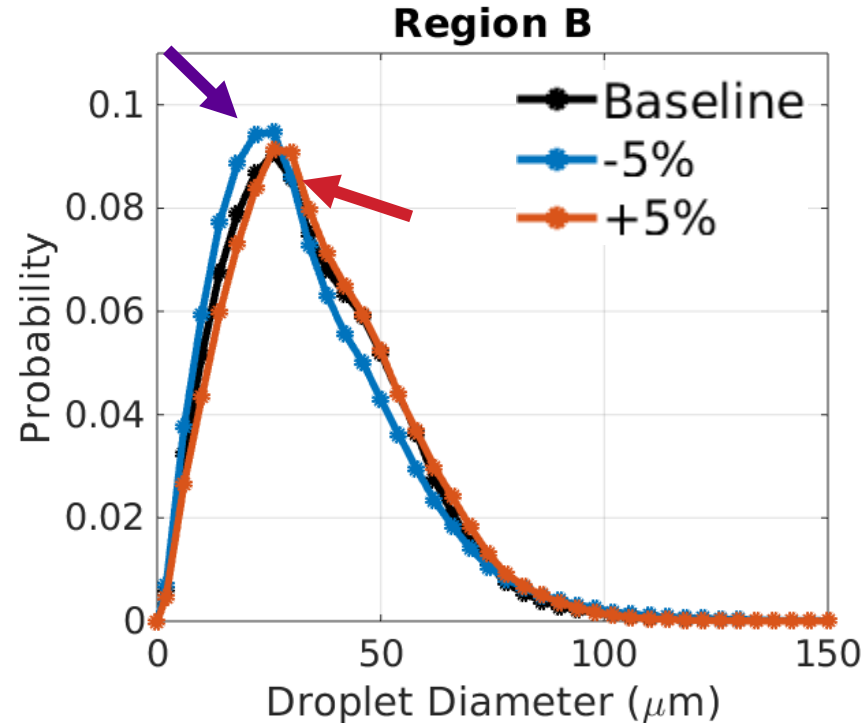


- The peak of the baseline, -5% and -10% occur at 50 μm .
- For the +5%, +10%, the distribution and peak move towards a higher value
 - The larger unevaporated droplets survive the flame
 - For the -5%, -10% and baseline, smaller droplets may not survive the flame.

DROPLET SIZES – REGION B

Comparison between baseline and $\pm 5\%$, $\pm 10\%$

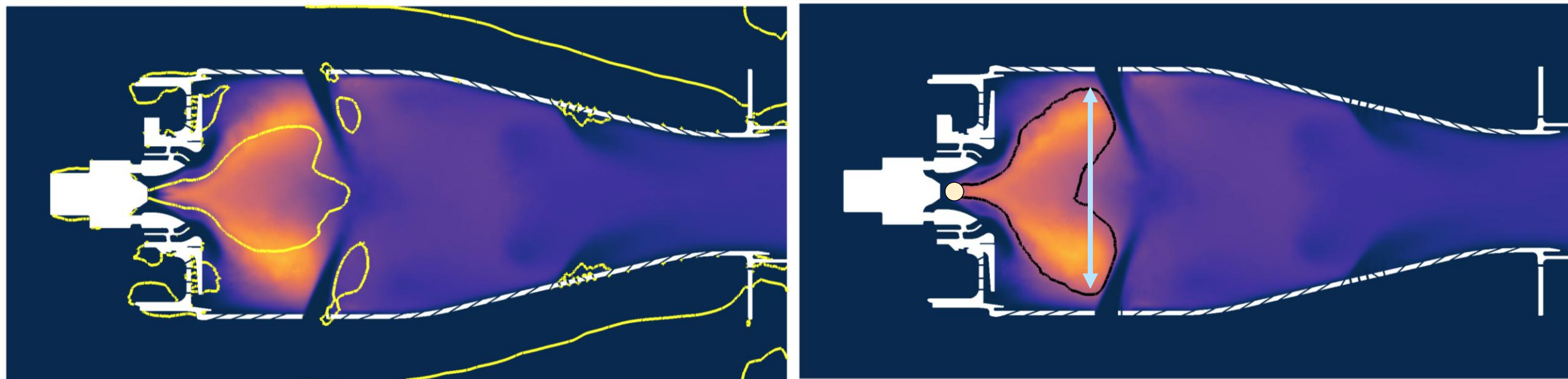
D. Dasgupta, S. Som, Journal of Engineering for Gas Turbines and Power 148 (1), 011007



- +5% and +10% distributions are similar to the baseline
- The distribution of the -5% and -10% can be seen to move towards smaller sizes, the deviation is low.
 - The smaller droplets vaporize and reach an equilibrium between new droplets entering this region and vaporization of the droplets.

BASELINE A-2 CASE

Temperature, flame anchoring, flame spread



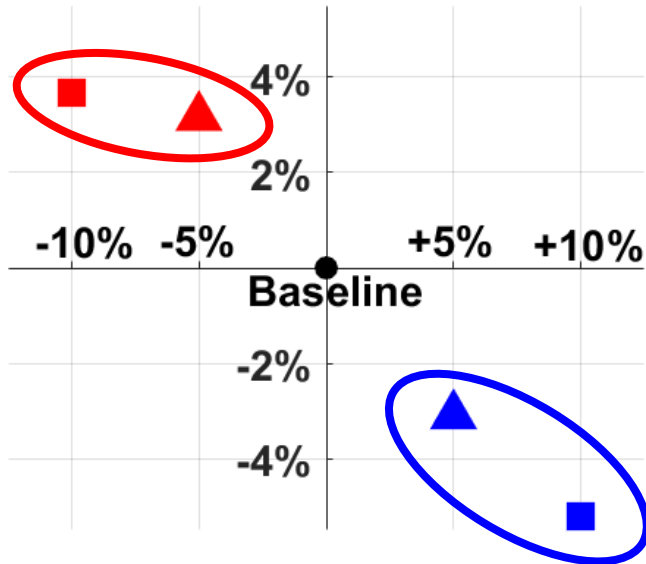
- Zero axial velocity iso-contour
- 1200 K iso-contour – defining the flame shape
- Flame anchoring location – axial location of the 1200 K iso-contour closest to the nozzle
- ↔ Flame spread – maximum distance in the radial direction of the 1200 K iso-surface

FLAME BEHAVIOR

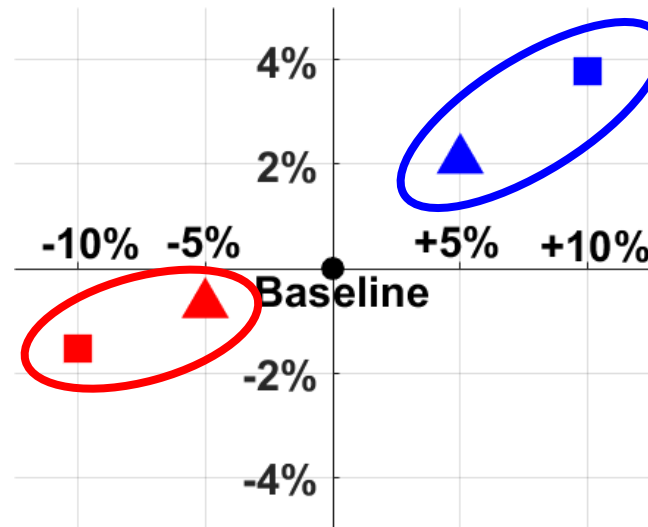
Comparison between baseline and $\pm 5\%$, $\pm 10\%$

D. Dasgupta, S. Som, Journal of Engineering for Gas Turbines and Power 148 (1), 011007

Flame Anchoring Distance:
% change w.r.t. Baseline



Flame Width:
% change w.r.t. Baseline



- **For flame anchoring:**

- Decrease in droplet sizes -> the location moves slightly downstream
- Increase in droplet sizes -> the location moves slightly upstream.

- **For flame width:**

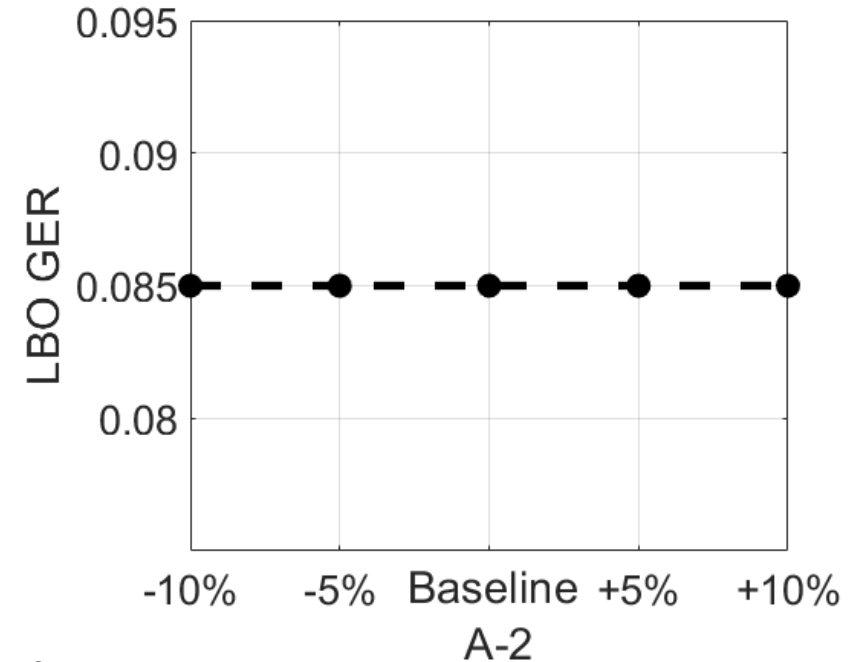
- Decrease in droplet sizes -> the spread is lower -> slightly more compact flames
- Increase in droplet sizes -> the spread is higher

LEAN BLOW OUT SIMULATIONS

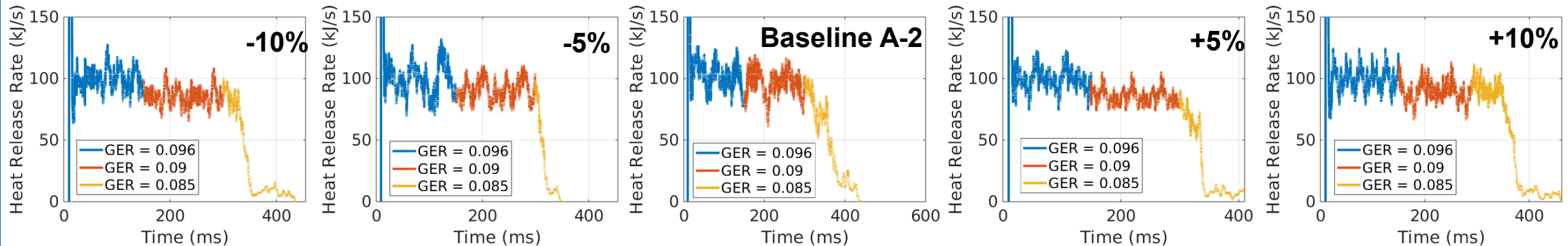
LBO prediction for all cases

- To ascertain the LBO GER, the GER is systematically reduced as 0.096 → 0.09 → 0.085.
- All five cases experience LBO at the same GER step of 0.085.
 - The LBO range for these cases is $0.085 \leq \text{GER} < 0.09$
- Localized variations noted for spray droplets and flame shape; the global behavior is not impacted by the change in the droplet sizes studied here.

LBO GER for all cases



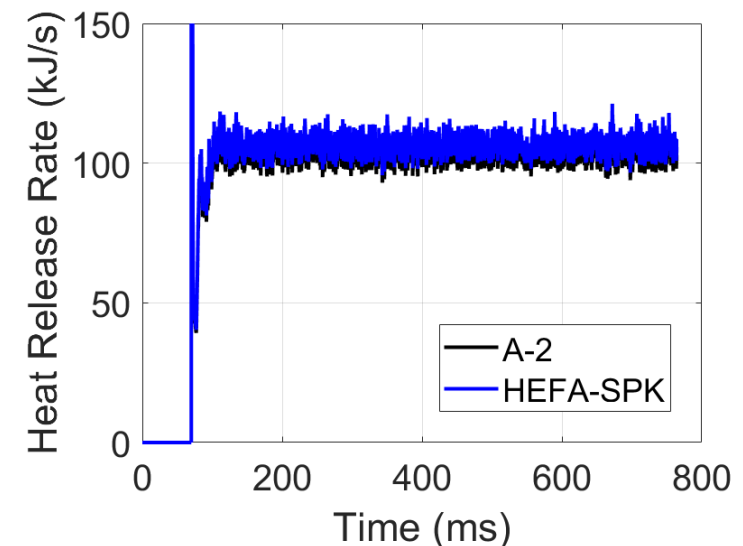
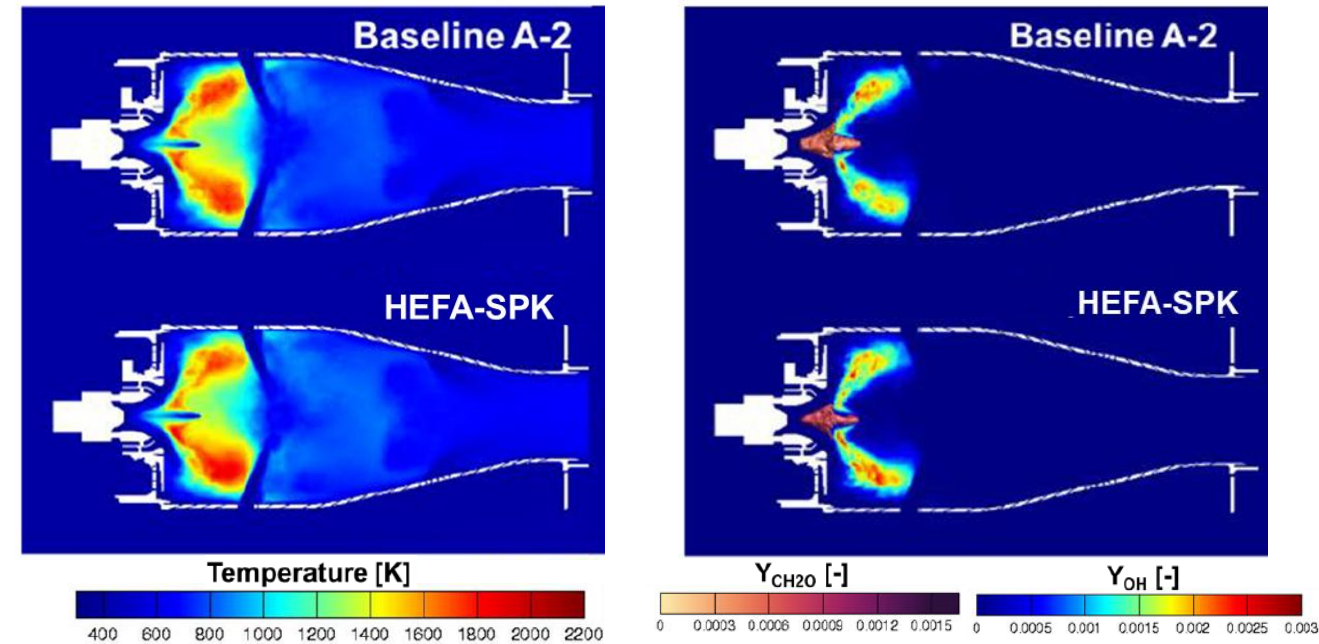
Heat release rate variation with time for all cases



COMPARISON BETWEEN FUELS

Similar flow-fields and global behavior between HEFA and Jet-A

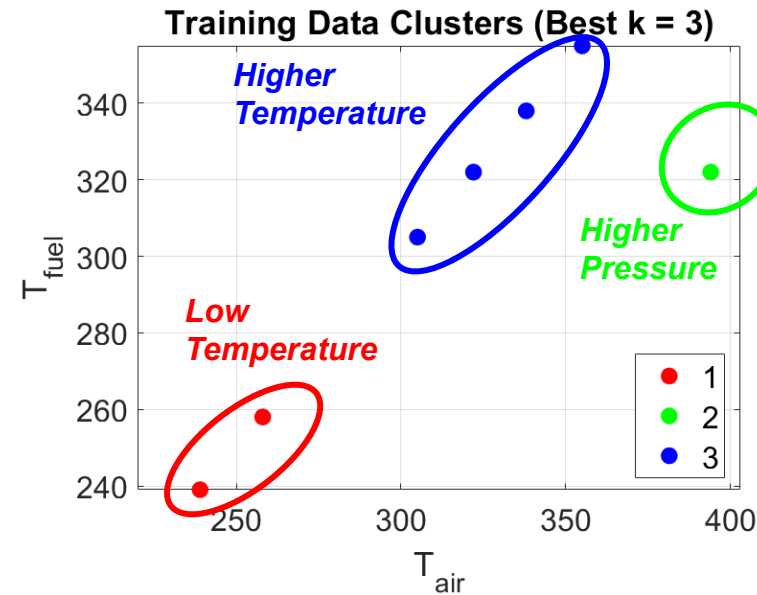
- Operating condition: $T_{\text{air}} = 394 \text{ K}$, $P = 2 \text{ atm}$
- Two fuels compared: Jet-A, HEFA-SPK
- Center plane temperature distributions qualitatively look similar.
- The heat release rate, which is a global metric, shows no significant differences
 - The mean heat release rate for HEFA-SPK is 3.6% higher than Jet-A
- The species' distribution (OH , CH_2O) is similar for both fuels.



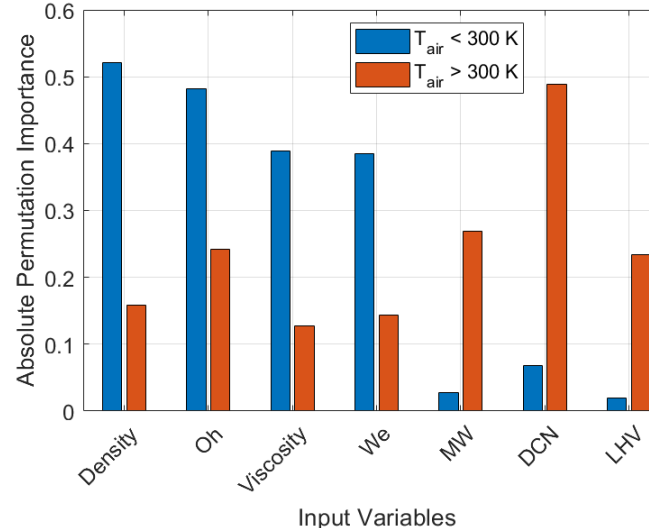
UNRAVELING UNDERLYING PHYSICS

Model development for LBO behavior at varying operating conditions

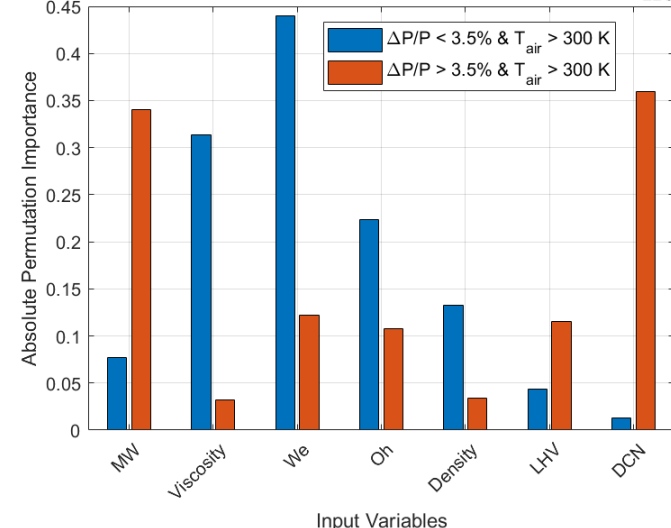
- Model for assessing the importance of different parameters on LBO
 - Cluster the input space (k-means) to train one regression model (random forest) for each cluster
 - Compute permutation importance to assess which parameters have a stronger influence on each cluster
- Identified clusters separate the operating space based on air temperature and pressure drop within the combustor.
- Comparing clusters 1 and 2+3
 - At lower air temperature, fuel physical properties and atomization influence LBO.
 - At higher temperature, chemical properties influence LBO
- Comparing clusters 2 and 3
 - At lower pressure drop, fuel physical properties and atomization influence LBO.
 - At higher pressure drop, chemical properties influence LBO



Absolute Variable Importance Comparison for Predicting ϕ_{LBO}



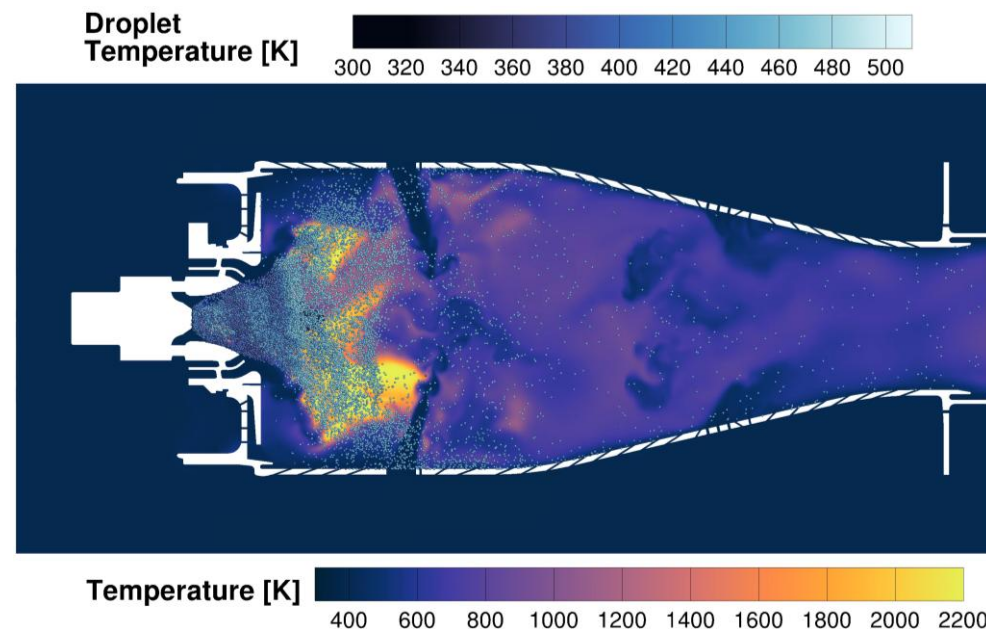
Absolute Variable Importance Comparison for Predicting ϕ_{LBO}



KEY TAKE-AWAY AND FUTURE WORK

How does change in fuel properties impact the flame behavior at stable and off-normal conditions?

- Fuel property impact flame behavior
- Changes in droplet sizes may or may not lead to significant changes
- Global behavior such as heat release rate and lean blow out behavior along with local behavior shed light into dynamics
- Future Work:
 - Expand the analyses to operating conditions where pronounced impact of atomization is observed
 - Create an operability map relating fuel properties to lean blow out global equivalence ratio





THANK YOU!
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