PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Direct Numerical Simulation (DNS) and High-Fidelity Large-Eddy Simulation (LES) for Improved Prediction of In-Cylinder Flow and Combustion Processes

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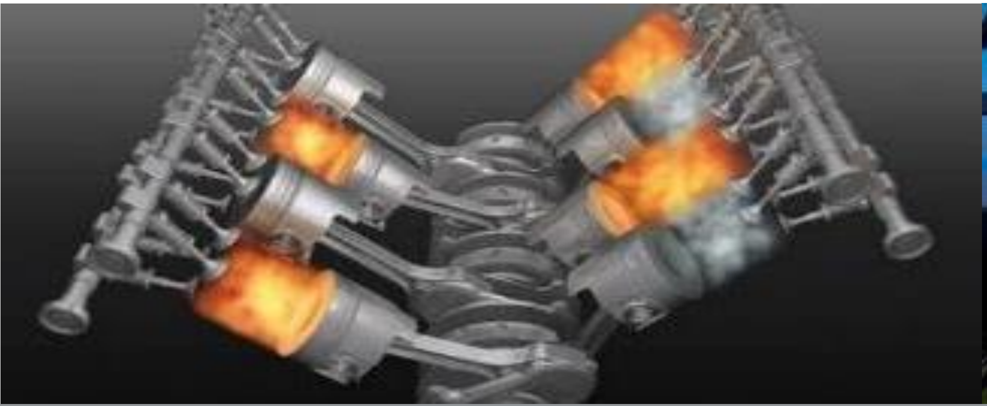
2021 DOE Vehicle Technologies Office Annual Merit Review
June 21-25, 2021
Project # ACE146



This work was performed as part of the PACE program. Special acknowledgments to the program managers Gurpreet Singh and Mike Weismiller

Overview

Timeline

- **PACE started in Q3, FY19**
- **PACE will end in FY23 (~25% complete)**
- **Focus and objectives of individual tasks will be continuously adjusted**
- **Overall PACE work plan discussed in ACE138**

US Fiscal years run from October 1 through September 30

Budget

Task	Description	FY20	FY21
A.M.05.01 Ameen, ANL	Spray and Combustion model implementation	$350k	$340k*
A.M.05.02 Ameen, ANL	Gridding, validation, and workflow development	$350k	$300k
S.M.02.01 Chen, SNL	DNS and modeling of turbulent flame propagation & end gas ignition	$50k	$50k
S.M.02.02 Chen, SNL	Flame wall interactions	$150k	$50k

*Listed funding also supported ANL research presented in ACE 143

Barriers

US DRIVE Advanced Combustion and Emission Control Roadmap

- Incomplete understanding of the dynamics of fuel-air mixture preparation
- Incomplete understanding of stochastic combustion problems (CCV, misfire, knock)

PACE Major Outcomes

- MO1: Current models do not accurately predict knock response to design changes
- MO5: Homogeneous and stratified lean/dilute engine efficiency and emissions are not accurately predicted
- MO8: Understand and improve dilute combustion strategies during cold start and cold operation to reduce emissions

Partners

- **PACE is a DOE-funded consortium of 6 National Laboratories working towards a common goal (ACE138)**
- **Specific partners on this work include:**
  - LLNL on surrogate development and kinetics
  - Nek5000 development team at ANL, UIUC
  - PELE development team at LBNL, NREL, ORNL, SNL
  - Additional details on later slides

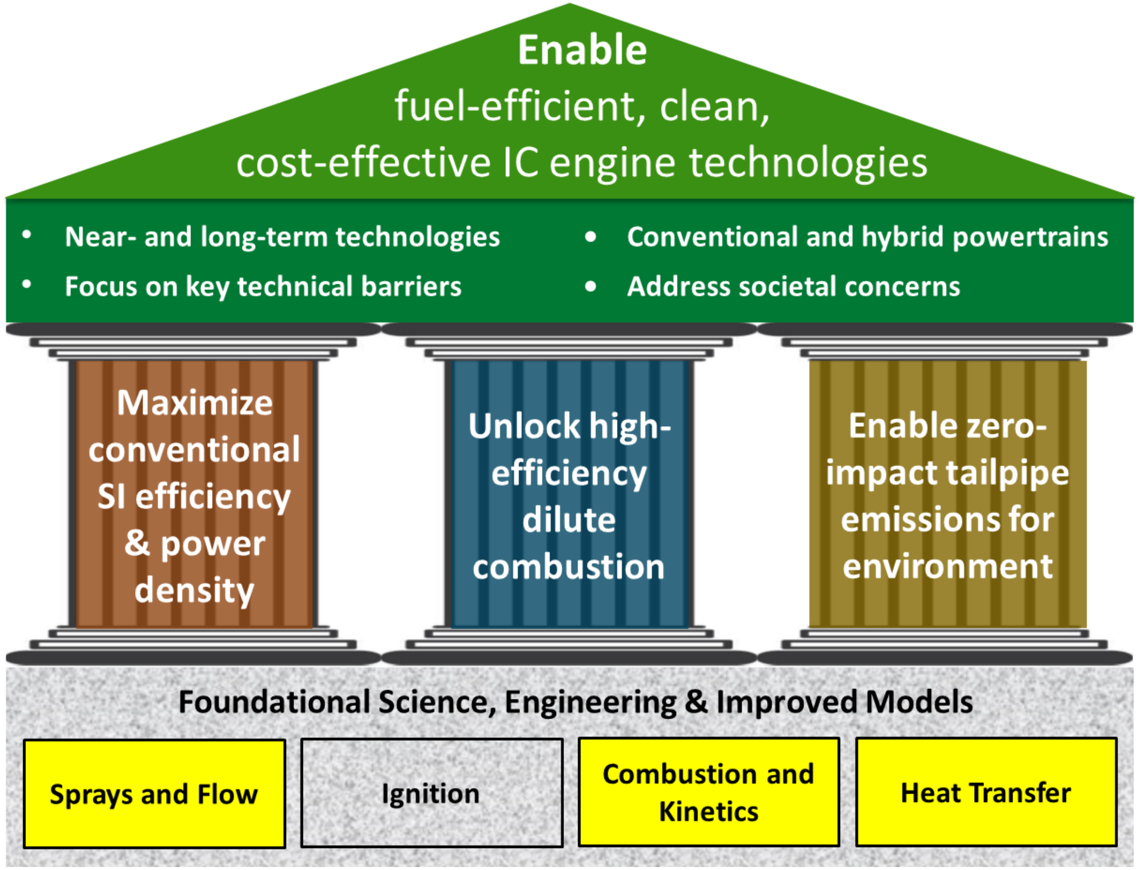
Relevance

Overall Relevance of PACE:

PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions

To achieve PACE objectives, we need:

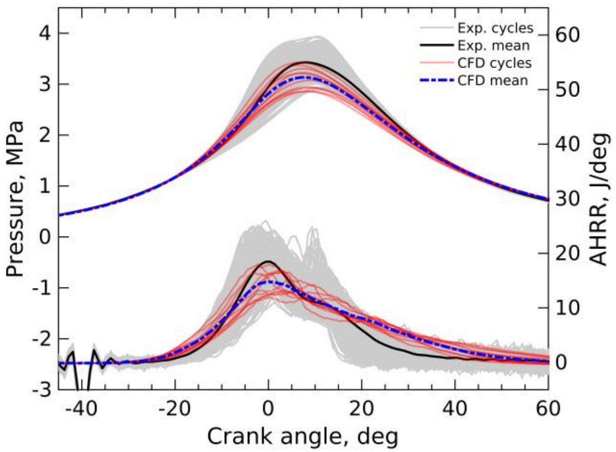
- Better understanding of CCV under lean/dilute operations to develop mitigation strategies
- Accurate knock models under high-load operation
- Accurate flame-wall interaction models under lean/dilute and cold-start conditions
- Accurate wall heat transfer models



Use high-fidelity simulation tools and DOE leadership-class machines to develop accurate submodels for combustion, heat transfer, and CCV.

Relevance: Need for more predictive models

PACE Major Outcome 5
Dilute Cyclic Variability (M Ameen, owner)

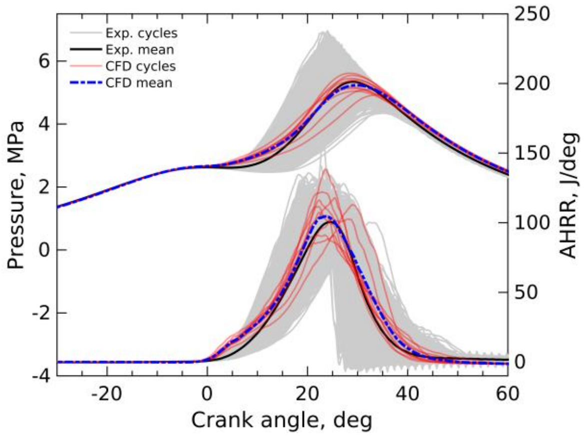


Target	Success	Baseline
COV	10%	100%
CA10-90	10%	36%

Simulations performed by Chao Xu (ANL)

- CCV is not well-captured.
- Need to tune combustion model parameters from one operating condition to the next.
- Late-stage combustion is not captured well – need for better flame-wall interaction models and wall heat transfer models.

PACE Major Outcome 1
High Load Knock (S Som, owner)



Target	Success	Baseline
KLSA	1 CAD	3 CAD
CPU cost	5x faster/5x more physics	---

- Current practice is to use Livengood-Wu integrals* to predict end-gas autoignition which are not sufficiently accurate.
- Need for faster and more accurate end-gas autoignition models.

*Yue, Z., Xu, C., Som, S. et al., “A Transported Livengood-Wu Integral Model for Knock Prediction in CFD Simulation” ASME ICEF 2020

Milestones

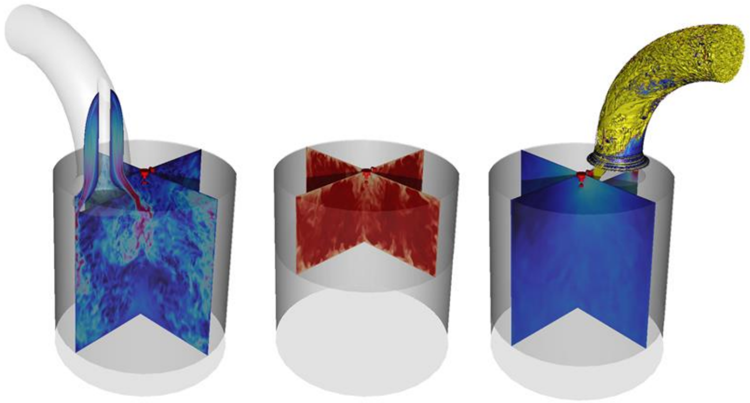
Month/Year	Description of Milestone	Status	Lab
Q2 FY21	Improved wall and heat transfer models using DISI DNS	Completed	ANL
Q4 FY21	Multi-cycle LES Dataset for the motored Sandia DISI engine with flow and spray	On Track	ANL
Q3 FY21	High-fidelity LES of evaporating ECN Spray G simulated using Nek5000	On Track	ANL
Q2 FY21	Improved flame propagation models coupled with PACE ignition model implemented into Nek5000 and validated using DNS dataset	Delayed to Q4 FY21	ANL
Q4/FY21	DNS of end gas ignition under boosted conditions, flame-wall interaction and soot	On Track	SNL

Approach: Leverage Exascale-ready DOE codes to accomplish PACE objectives

Nek5000 (ANL)

High-fidelity DNS/LES of ICE flows

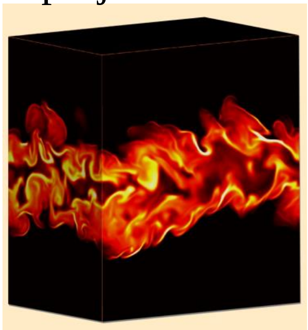
- Spectral element method (**SEM**)-based spatial discretization delivering minimal numerical dispersion and dissipation and **exponential grid convergence**
- Body-fitting capabilities for **complex geometries,** Arbitrary Lagrangian Eulerian (ALE) capabilities to handle **moving boundaries**
- Capability to model fuel sprays and combustion
- Mesh generation: supports major 3^{rd} party meshing tools
- Supported by DOE through ASCR and ECP (Exascale Computing Project) funding: **~$7.6M**



S3D (SNL)

DNS of turbulent reactive flows

- Solves compressible reacting Navier-Stokes, total energy and species continuity equations
- High-order finite-difference methods
- Detailed reaction kinetics and molecular transport models
- Lagrangian particle tracking (tracers, spray, soot)
- In situ analytics and visualization
- Geometry using immersed boundary method
- Refactored for heterogeneous architectures using dynamic task-based programming model (Legion)
- Sustained funding from ASCR through SciDAC partnerships, Exascale Computing Initiative combustion co-design (ExaCT), and through ASCR core CS projects



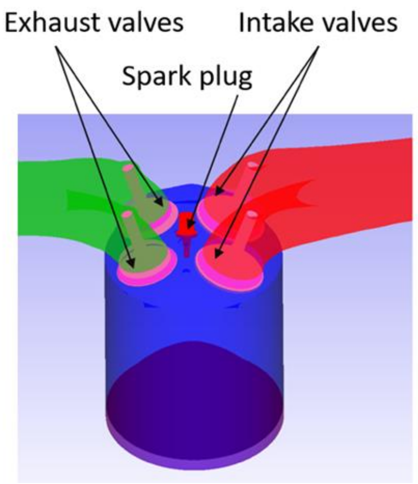
Approach: Leverage heavy DOE ASCR (Advanced Scientific Computing Research) investments in these codes to achieve **PACE objectives**

Approach – Multi-Cycle Simulations to Study CCV (ANL)

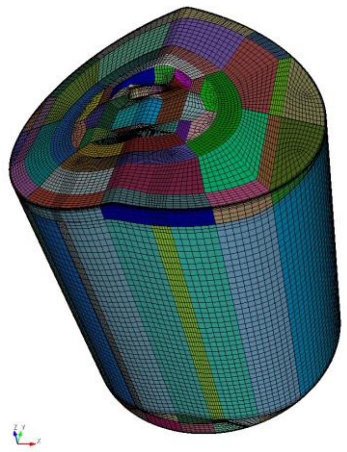
Objective: Understand relevant in-cylinder flow features that can affect CCV under lean/dilute conditions
Approach: Combination of open-cycle engineering and wall-resolved high-fidelity LES of the Sandia DISI engine

Open-cycle engineering LES simulations using Converge → Closed-cycle high-fidelity LES simulations using Nek5000

Simulation parameters	
Nek5000	
Element count	100K - 370K
Number of grid points	50M - 200M
Max. Δx	0.7 mm
Min. Δx	0.002 mm
Converge	
Number of grid points	1M – 1.5M
Max. Δx	1.0 mm
Min. Δx	0.25 mm

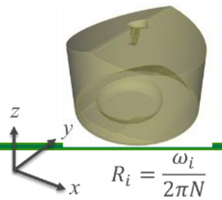


CFD Setup for open-cycle simulations using Converge.


Mesh structure for closed-cycle Nek5000 simulations

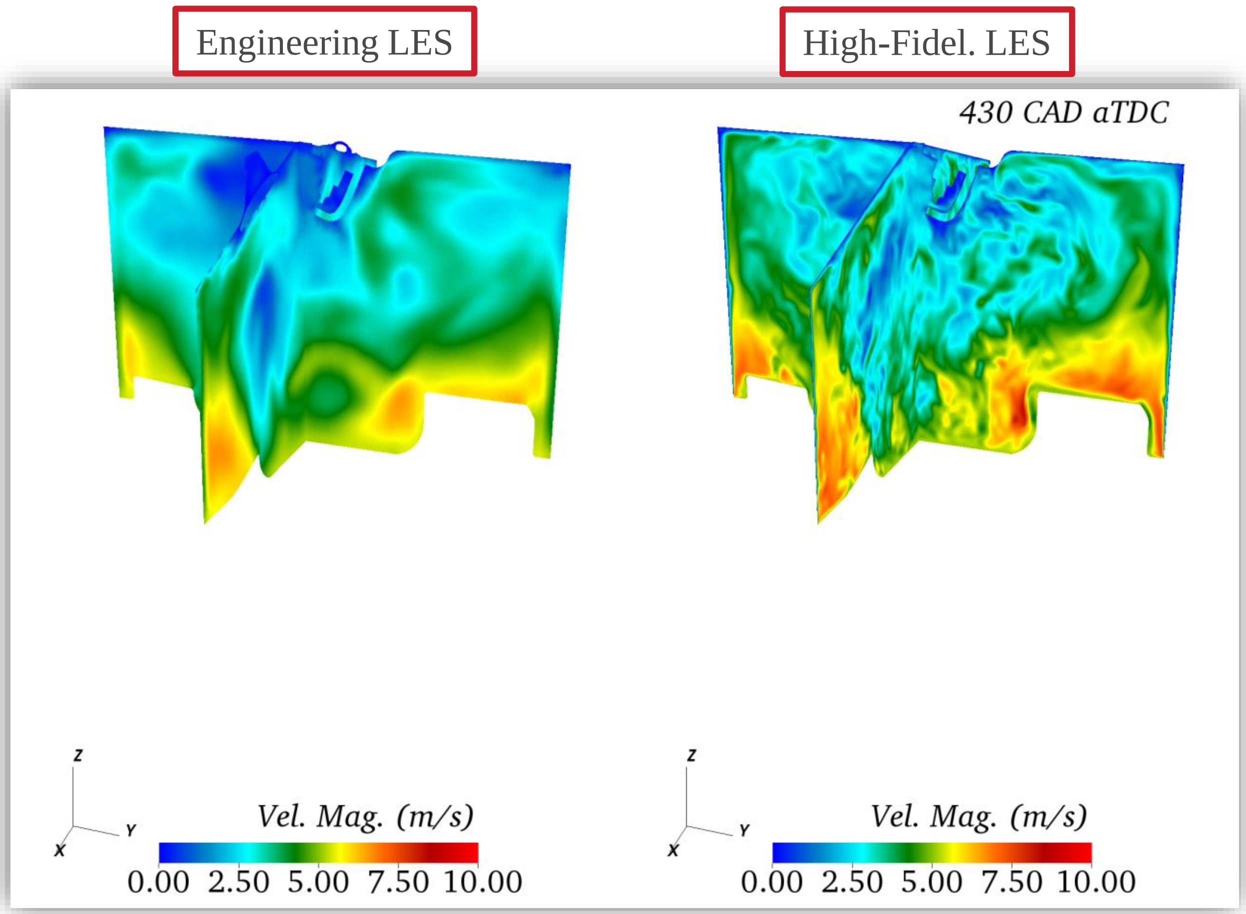
DISI Engine Specifications	
Bore	86 mm
Stroke	95.1 mm
Connecting Rod Length	166.7 mm
Compression Ratio	12:1
RPM	1000

Accomplishment: Demonstrated the need for high-fidelity simulations to capture CCV

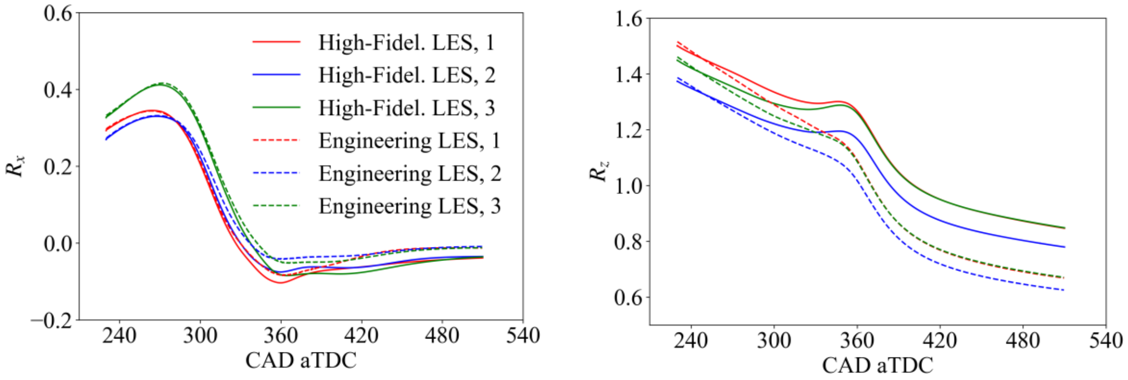


$$R_i = \frac{\omega_i}{2\pi N}$$

Flow Field Evolution



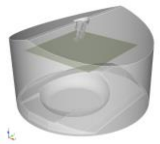
Tumble/Swirl Ratios



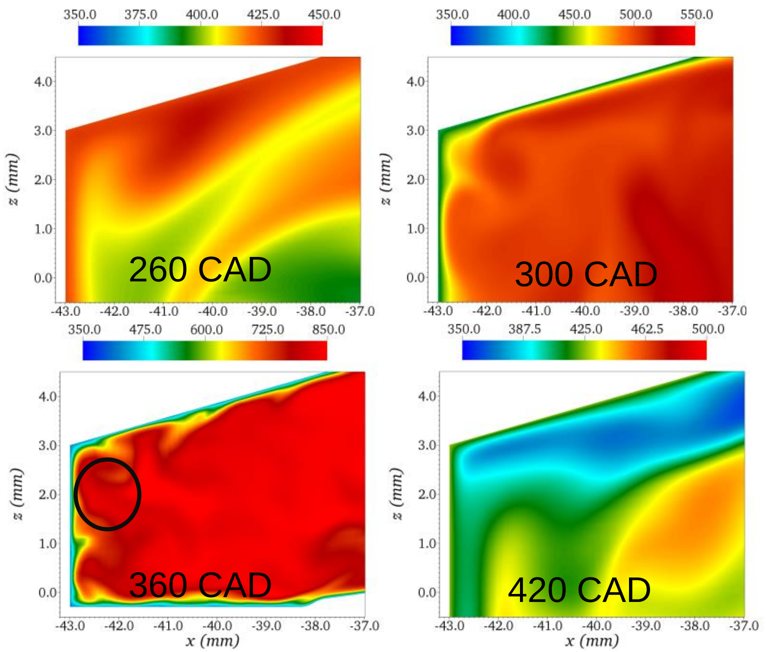
Evolution of X-tumble (left) and swirl (right) ratios during the compression/expansion strokes for 3 different cycles from engineering and high-fidelity LES simulations

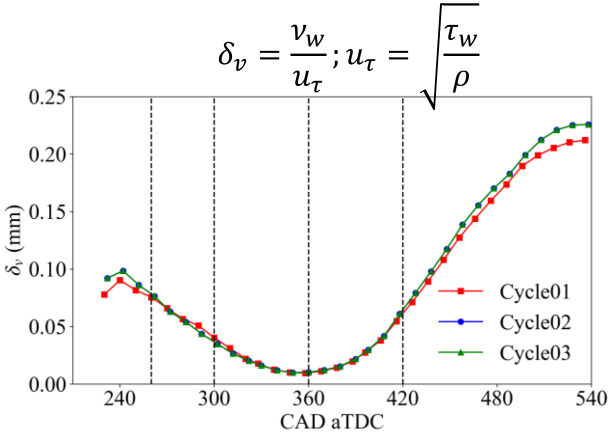
- High-fidelity LES shows a much larger range of flow features than engineering LES
- Large-scale structures are similar during early compression, but smaller scale features affect the large-scale feature evolution at later crank angles – can impact flame growth.
- Demonstrates the need for high-fidelity LES calculations to investigate CCV in flowfield
- Next step: Evaluate the effect of flowfield variability on CCV of combustion (FY22)

Accomplishment: High-fidelity simulations provide insights into wall boundary layers and turbulent kinetic energy distribution



Thermal boundary layer evolution

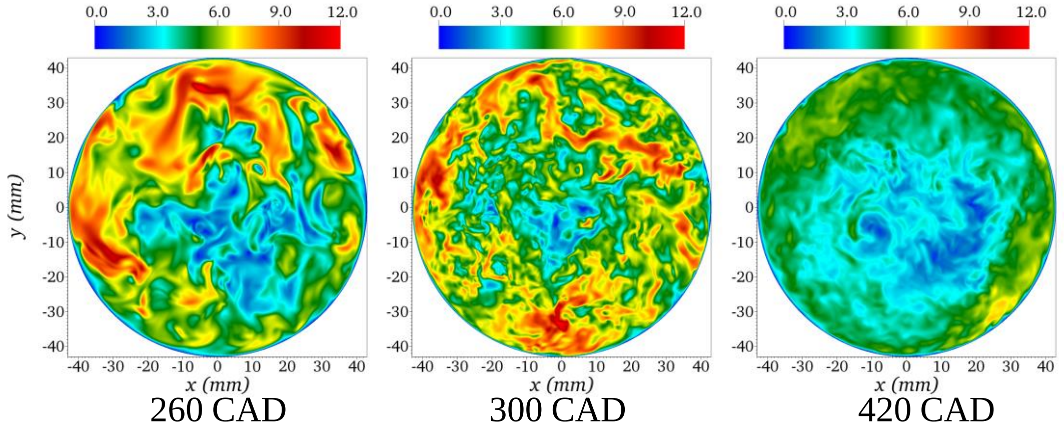




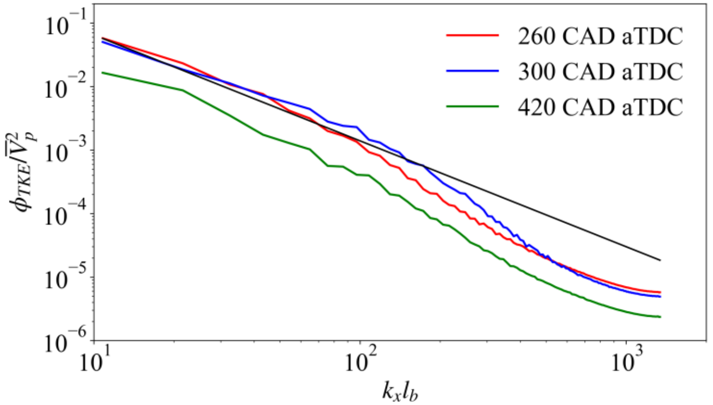
Left: Evolution of thermal boundary layer during a single cycle
Right: Evolution of viscous length scale near the liner during compression/expansion

- Thermal and momentum boundary layer thicknesses reduce with increasing compression.
- Near TDC, boundary layer thicknesses (<0.25 mm) are smaller than typical engineering LES simulation grid sizes – need for accurate wall models.

Turbulence distribution



Appearance of smaller scale structures with increasing compression. Need higher resolution at higher compression.

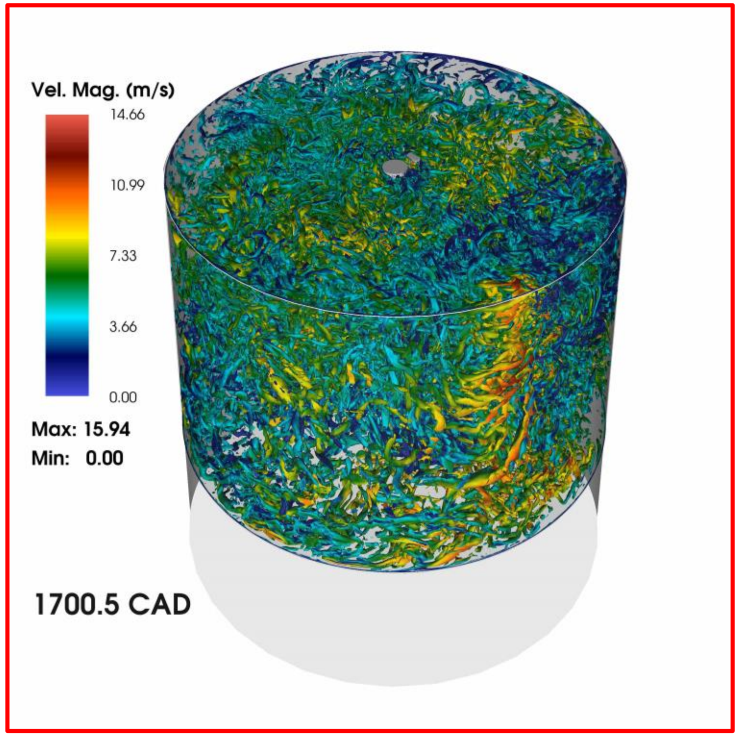


1D velocity spectra at a plane below the spark plug showing the shift in energy distribution. More energy content in all the scales at higher compression.

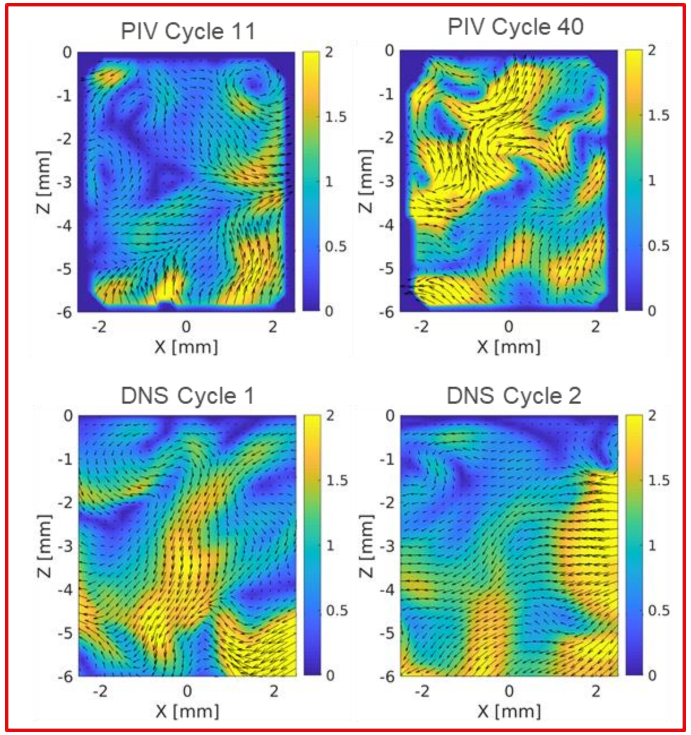
Accomplishment: DNS of Compression/Expansion Strokes of TCC-III Engine with Experimental Validation

Objective: Perform DNS of motored engine flows to develop improved wall models

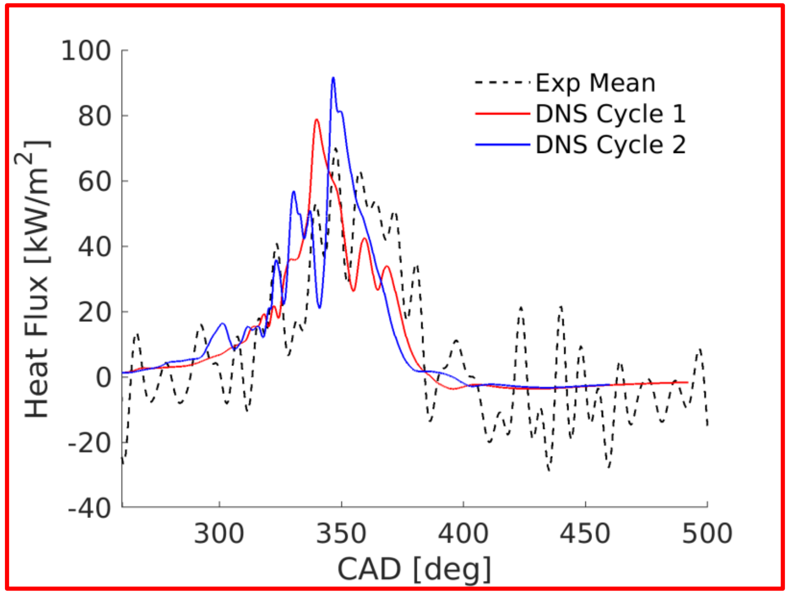
2020 U.S. DRIVE Highlight



Visualization of the λ_2 iso-surfaces during the compression stroke showing the appearance of smaller scale flow features



Flowfield near the head at CAD340



Evolution of heat flux at the probe location on the head

- Performed DNS of compression/expansion strokes of TCC-III motored operation at 800 (FY20) and 500 RPM (FY21)
- Validated the flowfield and heat transfer using experimental measurements to increase confidence in the accuracy of the DNS. Overall, excellent agreement between DNS and experiments.

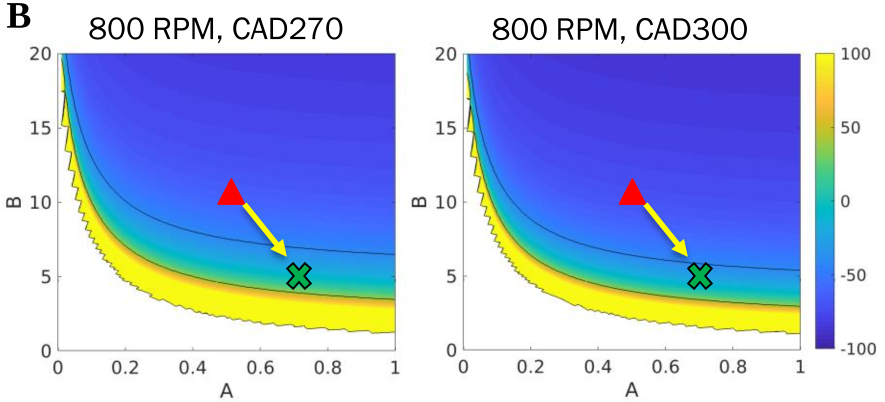
Accomplishment: Developed Improved Heat Transfer Models using DNS Dataset

Objective: Tune model parameters in the Rakopoulos model formulation to improve wall heat flux prediction by using DNS data at 500 and 800 RPM

$$T^+ = \frac{1}{A}\log\left(y^+ + \frac{1}{APr}\right) - \frac{1}{A}\log\left(40 + \frac{1}{APr}\right) + B$$

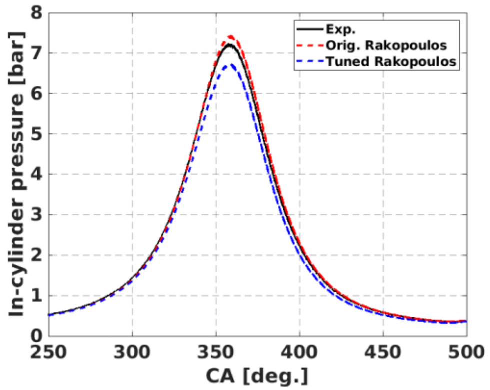
A-Priori Evaluation of DNS data to develop improved heat transfer models

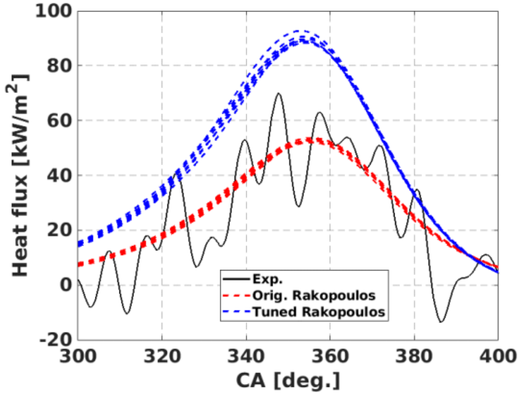
% Error in heat flux prediction as a function of A and B



- Performed tuning of the Rakopoulos heat transfer model using DNS dataset.
- Changing (A,B) from (**0.4747**,**10.2394**) to (**0.7**,**5.0**) increases the heat flux and reduces model error to **< 30%** for near-wall grid sizes < 1 mm across different RPMs and CADs

A-Posteriori Error Estimation of the tuned heat transfer model in Converge engineering LES Simulations

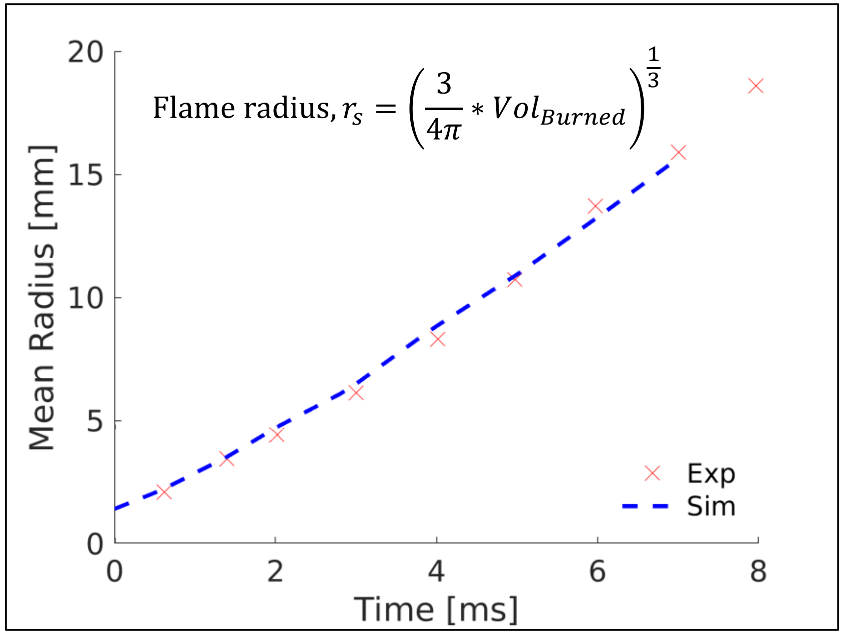




- Implemented the tuned heat transfer model in Converge and performed multi-cycle engineering LES (min grid size=0.25 mm).
- Tuned heat transfer model leads to larger wall heat transfer as compared to the original model. Trends as expected as the a-priori analysis results.
- Tuned model leads to larger error in heat flux as compared to the original model; needs further analysis. Shows importance of a-posteriori analysis.
- Next step: Repeat analysis under fired conditions (FY22).
- Improved models will be shared across PACE.

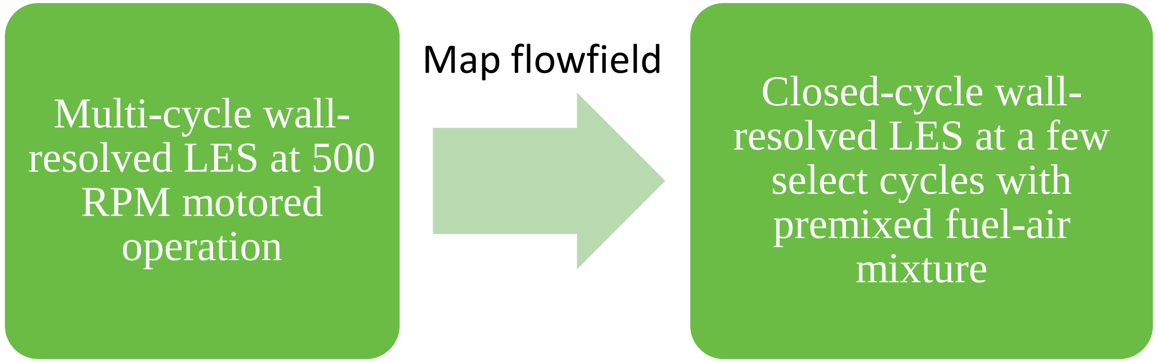
Accomplishment: Evaluated accuracy of baseline ECFM model using wall-resolved LES simulations in Nek5000

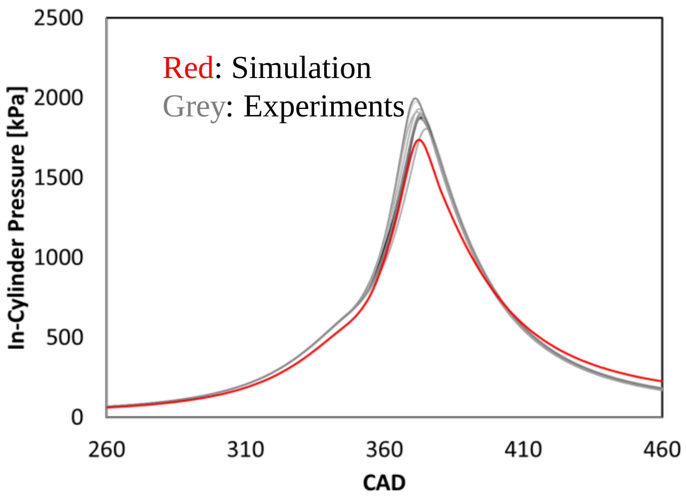
Objective: Implement ECFM combustion model in the Nek5000 engine simulation setup and validate against experimental dataset.



Validation of ECFM in a constant-volume turbulent premixed flame propagation from Renou and Boukhalfa (CST, 2001).

Preliminary validation of ECFM for fired (stoichiometric propane) TCC-III at 500 RPM





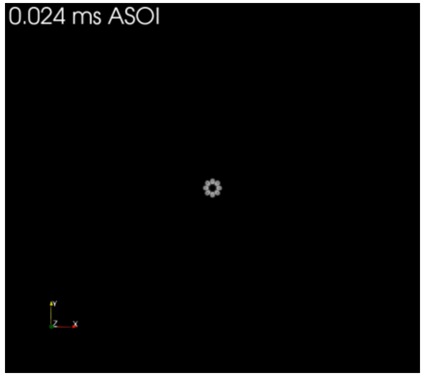
- Implemented the ECFM model in the Nek5000 engine simulation setup with a spherical ignition source.
- Performed preliminary closed-cycle simulations for the TCC-III fired operation.
- Baseline ECFM model fails to predict the peak pressure and late-stage combustion behavior.
- Motivates need for improving ECFM closure terms and ignition model

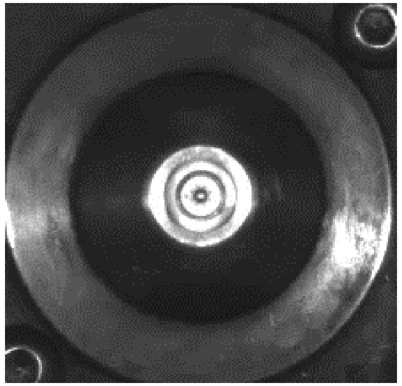
Accomplishment – GDI spray simulations with Nek5000 (1/2)

Objective: Implement spray modeling capabilities in Nek5000 to make the code ready to perform engine simulations in FY22

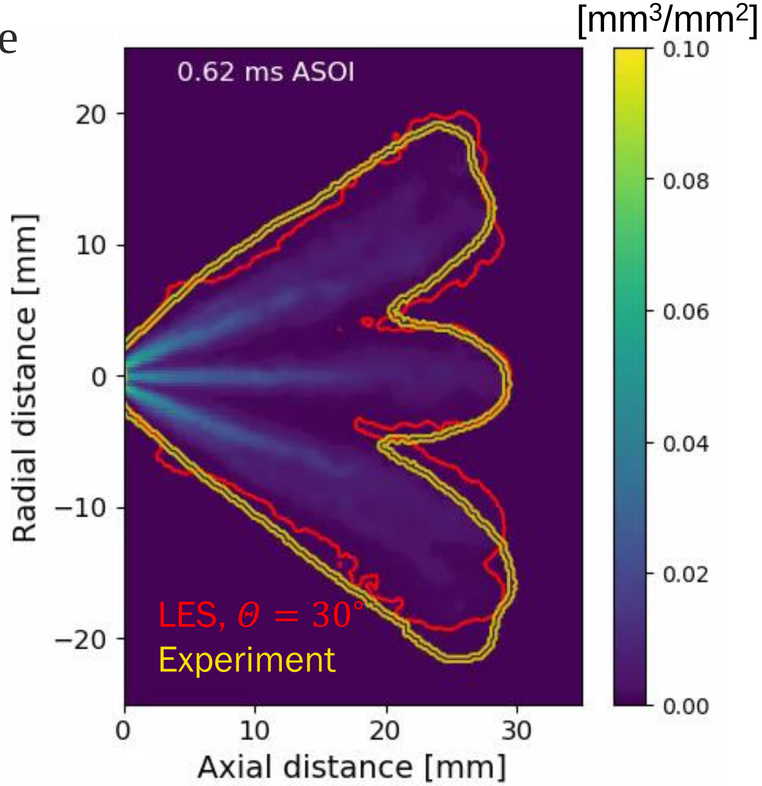
- Performed high-resolution LES of ECN Spray G 8-hole injector, standard conditions.
- Spray parameters were tuned to match experimental liquid penetration, based on the PLV=0.2e-3 threshold:
  - Cone angle degree, plume direction, area contraction coefficient and B_1 parameter were varied.

(Colmenares, J., Ameen, M., Patel, S. (2021) ASME ICEF)



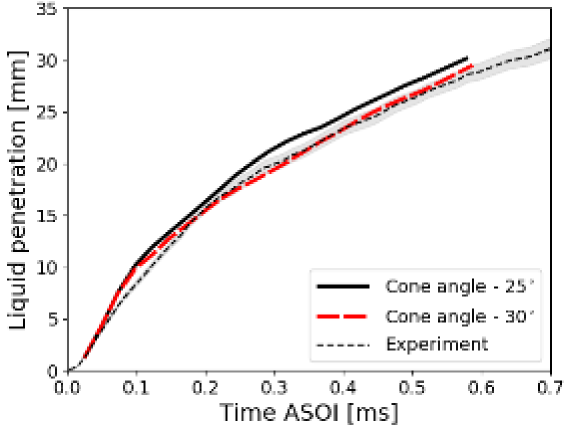


Volume render of LVF from LES vs. Mie scatter, front view.



PLV=0.2e-3 contours.

Nozzle Diameter	165 μm
Injection pressure	20 MPa
Ambient density	3.5 kg/m^3
Ambient gas	Nitrogen
Ambient temperature	573 K
Fuel	Iso-octane
Injection time	0.76 ms
Plume cone angle, Θ	**25°, 30°**
Plume direction	**33°**
Area contraction, C_a	**0.65**

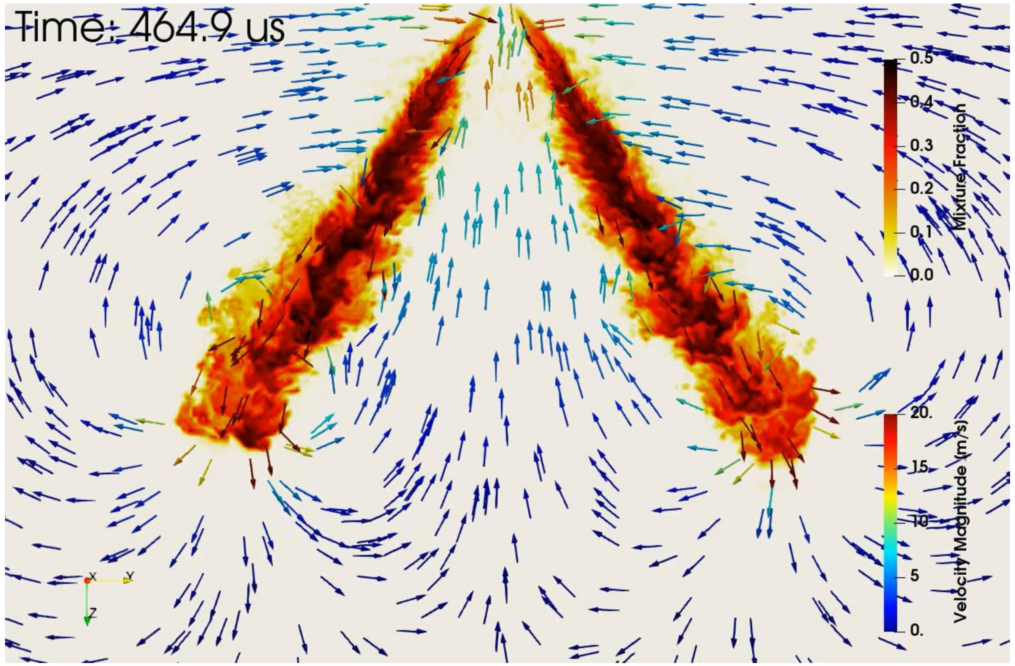


Physical models	
Evaporation model	Abramzon & Sirignano
Breakup model	KH-RT
Droplet distortion	TAB

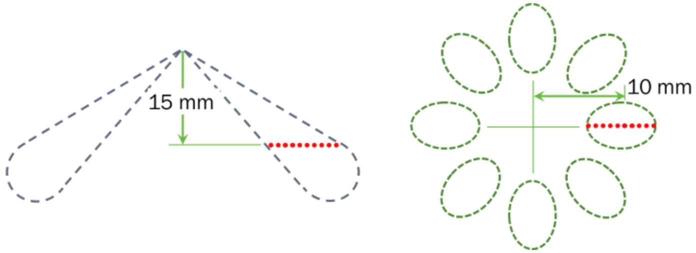
Breakup model parameters	Value
B_0	0.61
B_1	80
C_{RT}	0.4

Order	$N = 5$
Minimum Δx @ axis [mm]	0.033
# elements	270 k
# unique grid points	33.9 M

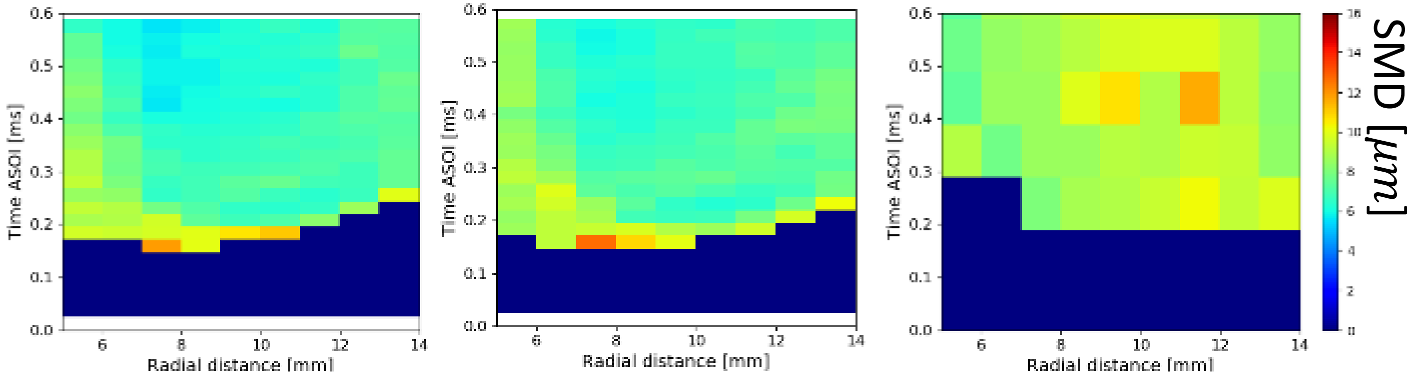
Accomplishment – GDI spray simulations with Nek5000 (2/2)



Gas mixture fraction, with vectors indicating velocity direction colored by velocity magnitude.

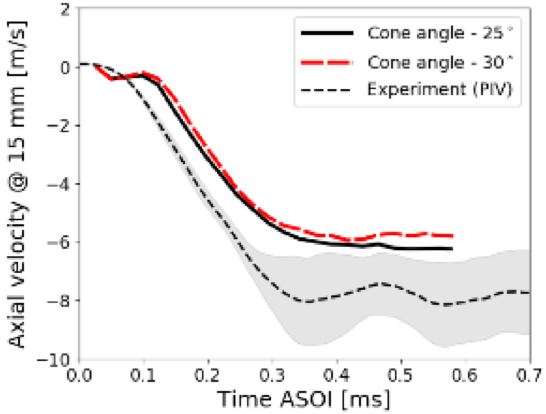


Schematic of sampling locations



Droplet Sauter mean diameters (SMD). a) LES with 25° cone angle, b) a) LES with 30° cone angle, c) PDI experiments (Parrish, 2015).

Axial velocity evolution at 15 mm below the injector tip – PIV vs simulations



- Inter-plume recirculation is well captured, though there is room for improvement.
- Droplet sizes are under predicted towards the plume center, but well captured towards the edge of the plume.
- Even with high fidelity simulations, there are inaccuracies in the gas phase flowfield - need for improved Lagrangian spray models.
- Demonstrated the readiness of Nek5000 to perform wall-resolved LES/DNS of fired engines (FY22)

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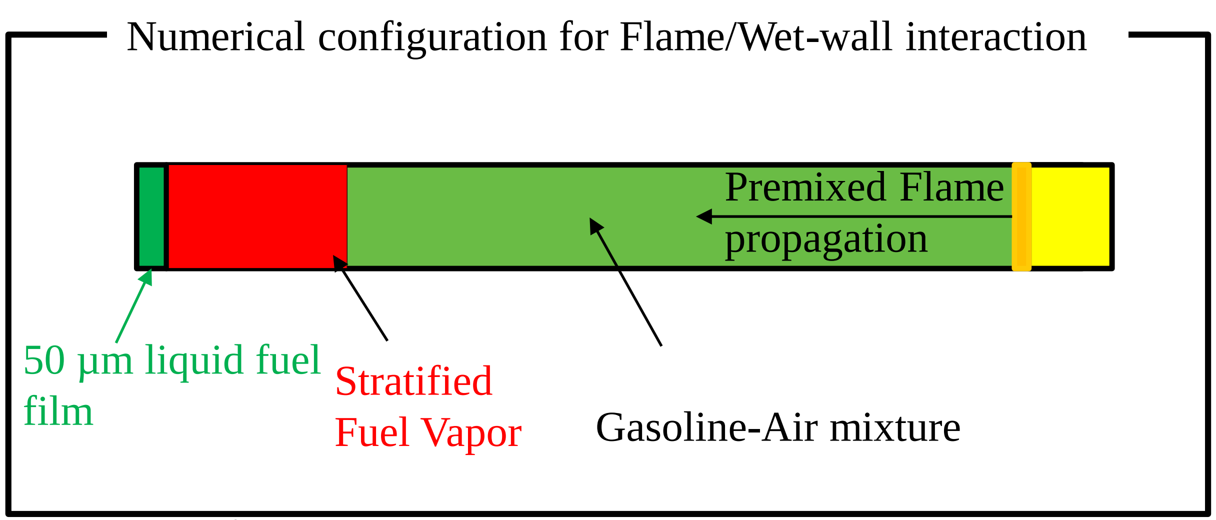
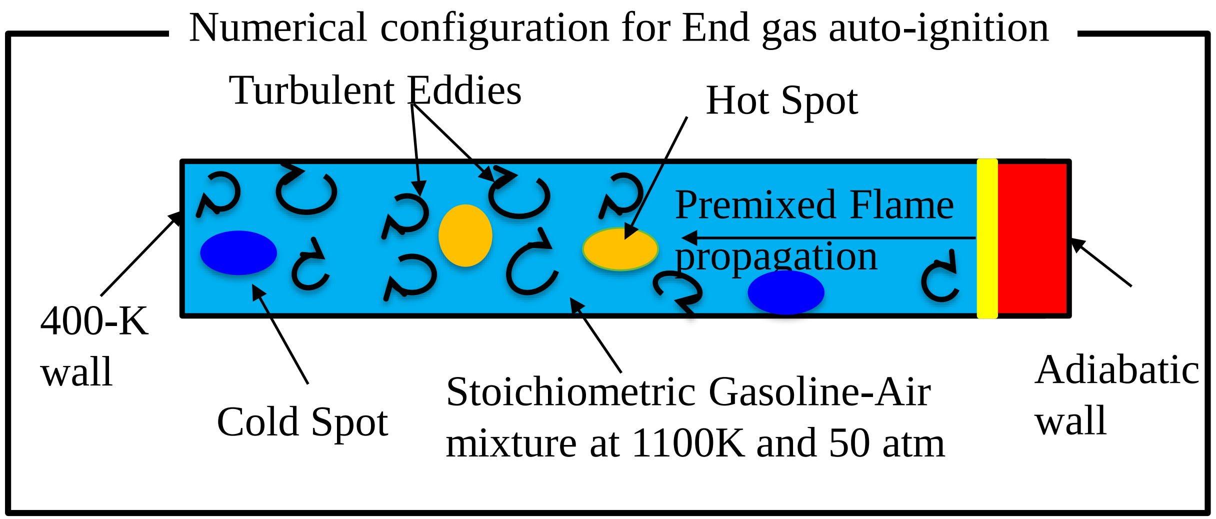
Approach – Fully resolved simulations of flame/wet wall interactions, end-gas auto-ignition and detonation (SNL)

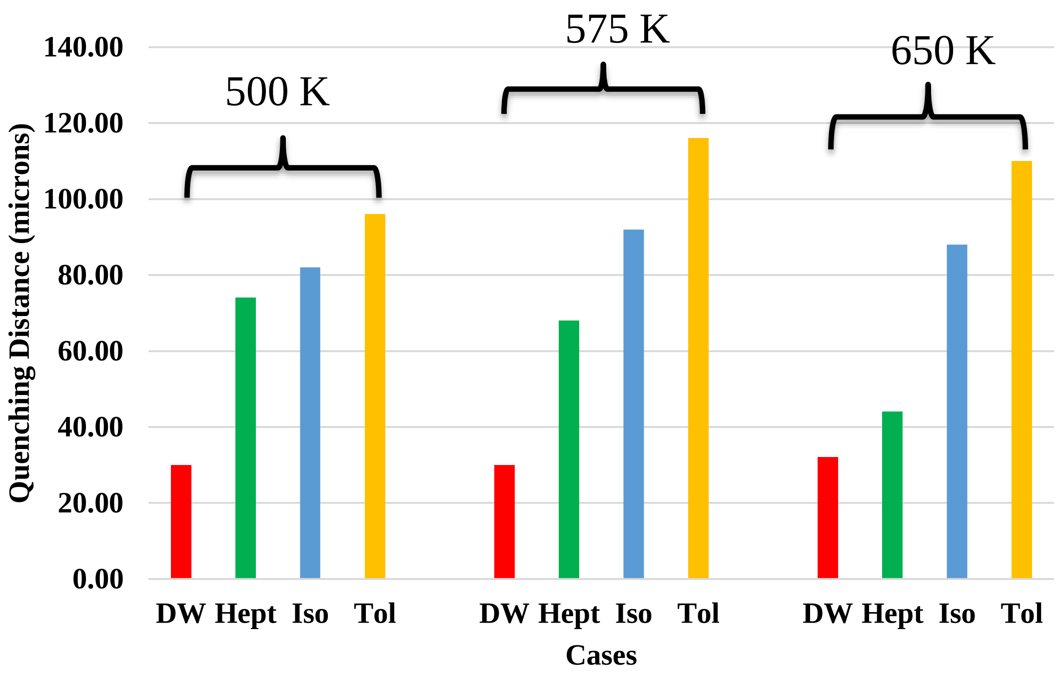
- Gaps in existing models of flame/wet wall interactions and knock
  - Flame wall interactions mainly focused on wall heat flux with little effort to model processes impacting emissions while utilizing quenching Peclet numbers for identifying the quenching zone that are only valid for dry walls
  - Most knock models rely on presumed pdfs of local mixture fraction/enthalpy and there is a lack of high-fidelity DNS datasets, especially those valid for multi-component gasoline surrogates to verify the underlying assumptions
- Low dimensional (1D/2D) fully resolved simulations allow exploration of wide thermochemical parametric space which is not possible with computationally expensive 3D DNS
  - Identify the effects of various parameters on the overall trend of relevant physics
  - Provide datasets for wide range of relevant conditions to aid model validation/development

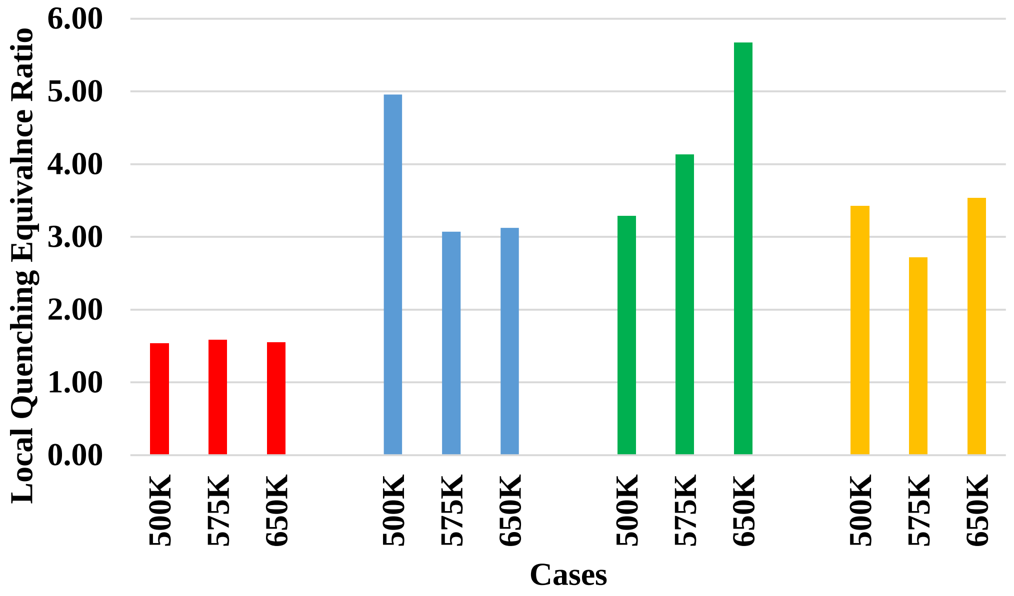




1: Pal et al. JERT, 140(10) 102205 (2018)

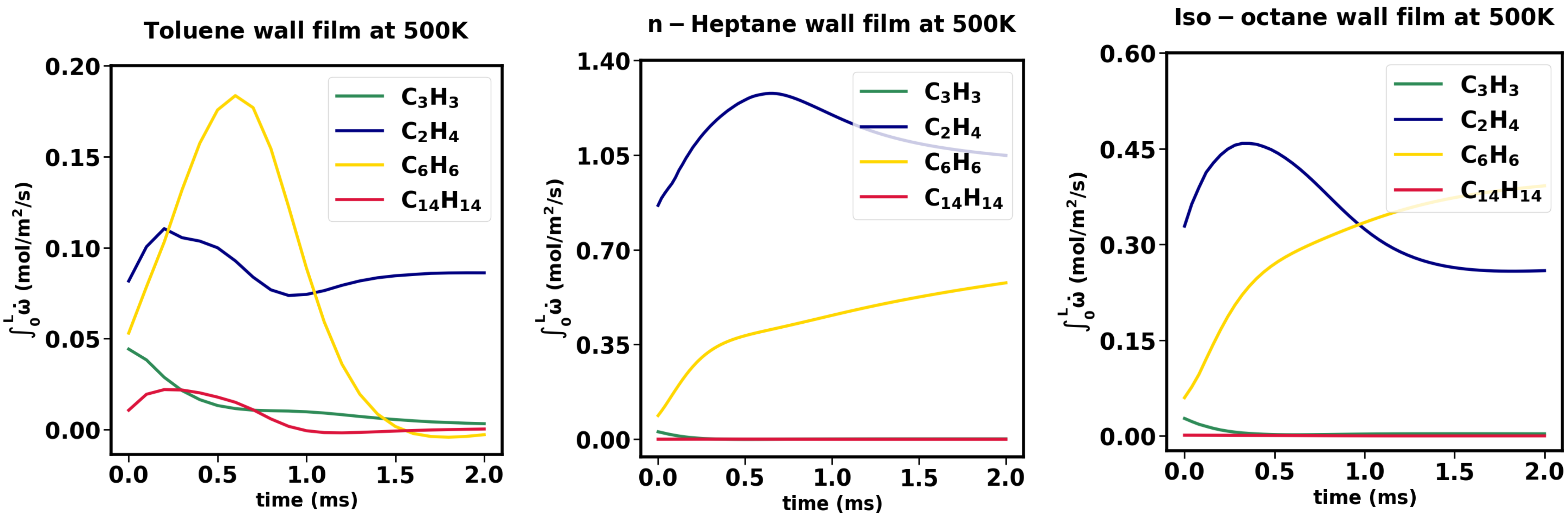
Accomplishments: Quantified quenching distances during flame-wet wall interaction through fully resolved 1D simulations





- Wet walls, in general, lead to larger quenching distances with higher emissions than dry walls as previously observed by Tao et al. (IJER 2018)
- Rich flammability limit is the dominant quenching mechanism in the presence of wet walls, in agreement with the observations of Tao et al. (IJER 2018)
- The magnitudes of quenching distance (and hence quenching Peclet numbers) as well as quenching equivalence ratio are highly dependent upon the fuel wall film composition

Accomplishments: Quantified emissions of soot precursors upon flame quenching in the presence of wet walls



- While the bulk gas composes of stoichiometric mixture, quenched layer consists of rich stratified mixture
- Upon quenching, C_6H_6 production in the toluene case is accompanied by noticeable production of $C_{14}H_{14}$ unlike the iso-octane or n-heptane case
- New PACE developed mechanism with more detailed PAH chemistry will be tested in FY 22

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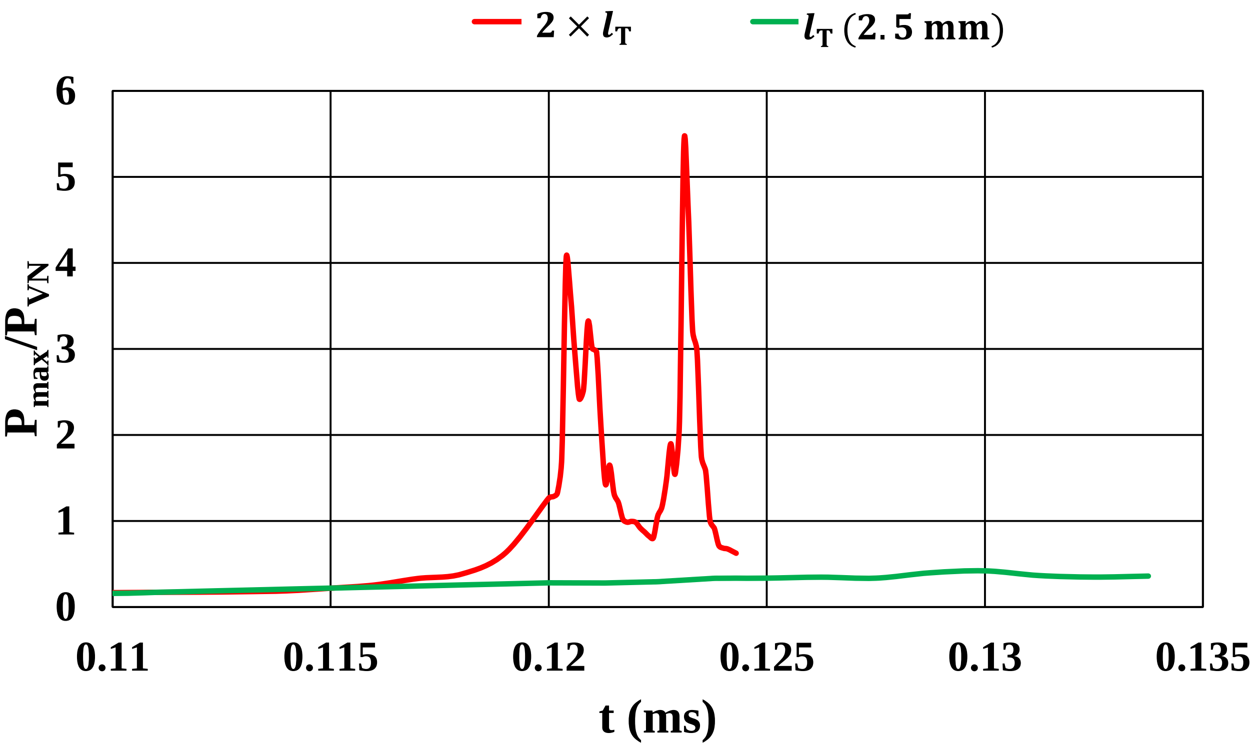
Accomplishments: Identified transition point from mild-knock to detonation through 2D DNS of end-gas auto-ignition



- Parametric variations in temperature length scales ($l_T \sim 50 - 100 \times l_F$ where l_F = primary flame thickness) carried out at a fixed turbulence intensity ($u' = 3.72$ m/s), turbulence length scale ($l_{11} = 0.8$ mm) and RMS temperature fluctuation ($T_{RMS} = 15$ K)
- Detonation observed for $l_T \geq 5$ mm with maximum pressure (P_{max}) exceeding the Von-Neumann pressure (P_{VN})

- Mild knock observed for $l_T < 5$ mm with maximum pressure (P_{max}) seldom exceeding the equilibrium pressure (P_{eq})
- Results agree with previous studies using simpler fuels/configurations [1]
    - Recent DNS of knock phenomenon have revealed similar trends in 2D and 3D cases, with 3D cases leading to higher maximum pressures due to higher interactions between originating detonation fronts [1]
- Datasets will enable a-priori and a-posteriori evaluation of the widely used transported Livengood-Wu model

$$\frac{\partial \rho I}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} I - \rho D \nabla I) = \rho \dot{\omega}_{PDF,avg}$$

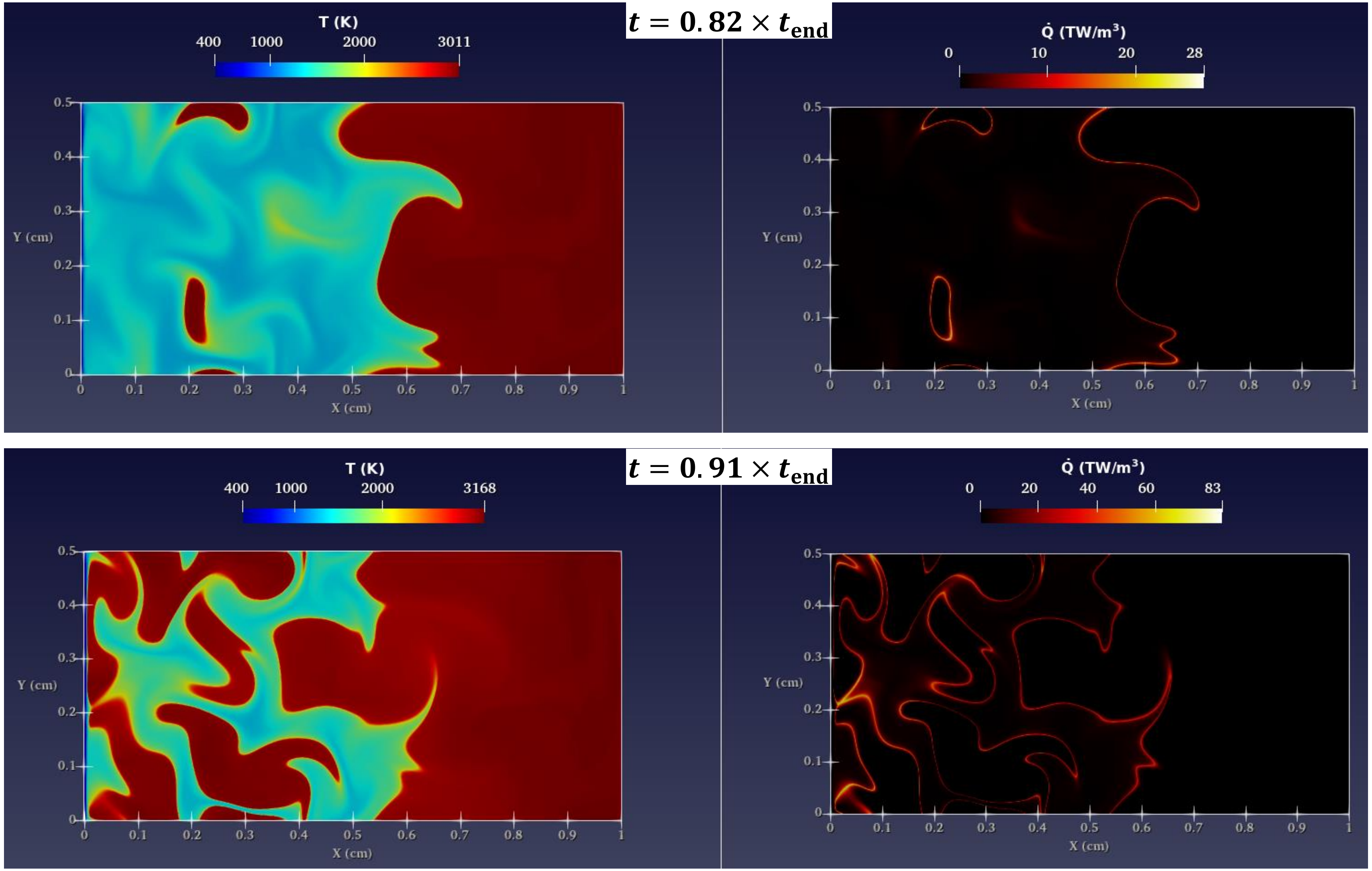
$$\dot{\omega}_{\mathrm{PDF,avg}} = \sum_{i=1}^{\Phi_{tot}} \sum_{j=1}^{T_{tot}} P(\Phi_i, T_j) \frac{1}{\tau(\Phi_i, T_j)} d\Phi dT$$

$\dot{\omega}_{\mathrm{PDF,avg}}$ usually evaluated using presumed PDF of local mixture fraction and enthalpy depicted below: [2]

$$P(Z, h_u) = \frac{1}{2\pi \cdot \sqrt{\widetilde{Z''^2}} \sqrt{\widetilde{h''^2_u}} \cdot \sqrt{1 - \rho_{Zh}^2}} \cdot \exp\left\{ -\frac{1}{2(1-\rho_{Zh}^2)} \cdot \left[\frac{(\tilde{Z} - \langle \tilde{Z} \rangle)^2}{\widetilde{Z''^2}} + \frac{(\tilde{h} - \langle \tilde{h} \rangle)^2}{\widetilde{h''^2_u}} - \frac{2\rho_{Zh}(\tilde{Z} - \langle \tilde{Z} \rangle)(\tilde{h} - \langle \tilde{h} \rangle)}{\sqrt{\widetilde{Z''^2}} \cdot \sqrt{\widetilde{h''^2_u}}} \right] \right\}$$

1: Luong et al., (FTaC, 2020, PROCI 2020)
2: D'Adamo et al., Applied Energy, 2017

Accomplishments: 2D DNS of mild-knock under boosted GDI engine conditions

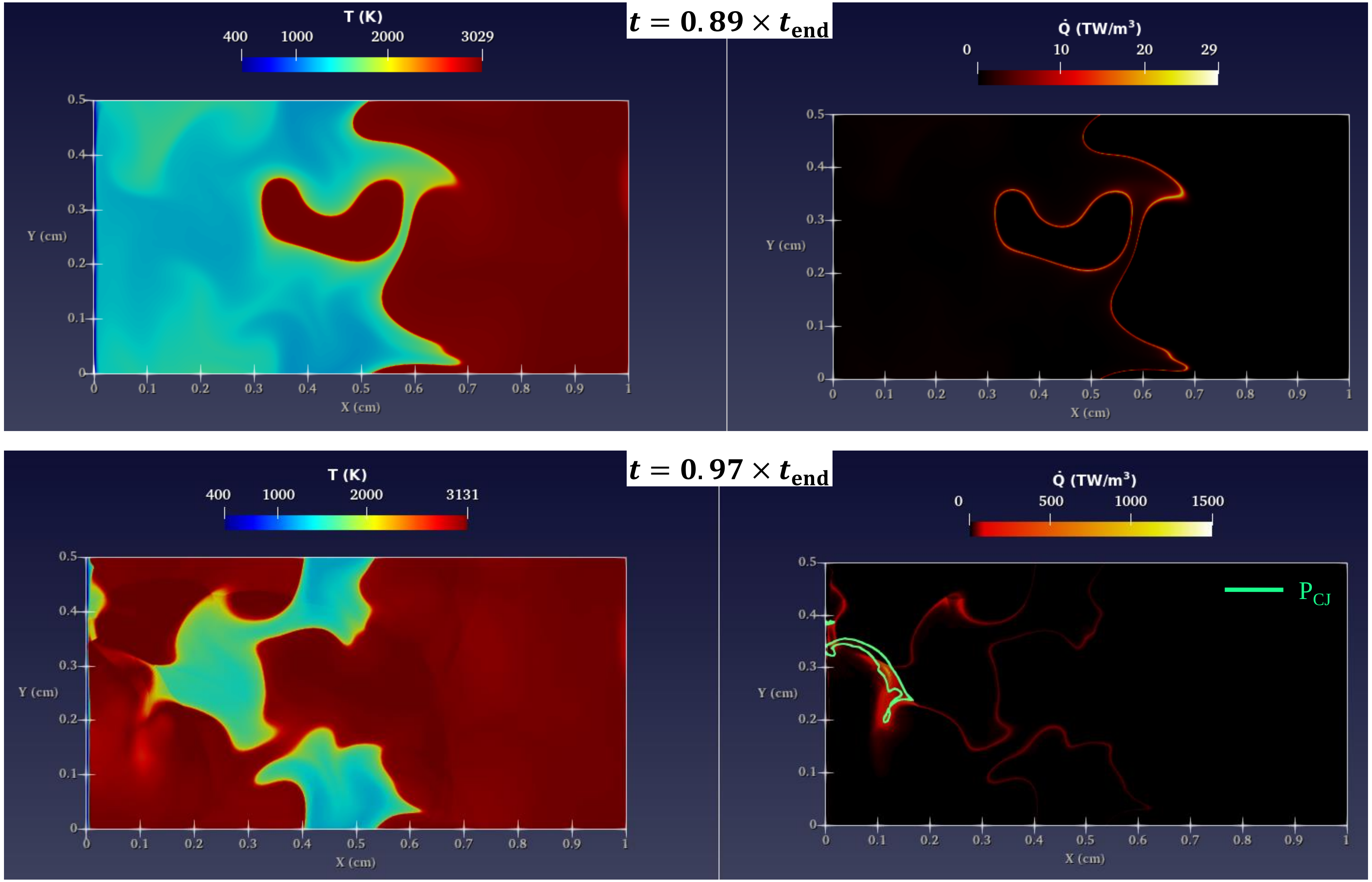


$l_T = 2.5$ mm

- Smaller length scales of temperature stratification tend to result in smaller, isolated hot-spots igniting in conjunction
- Eventually, volumetric ignition of the unburned end-gas occurs
- Not enough unburned mixture available for detonation to develop, $P_{max} \approx P_{eq}$

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

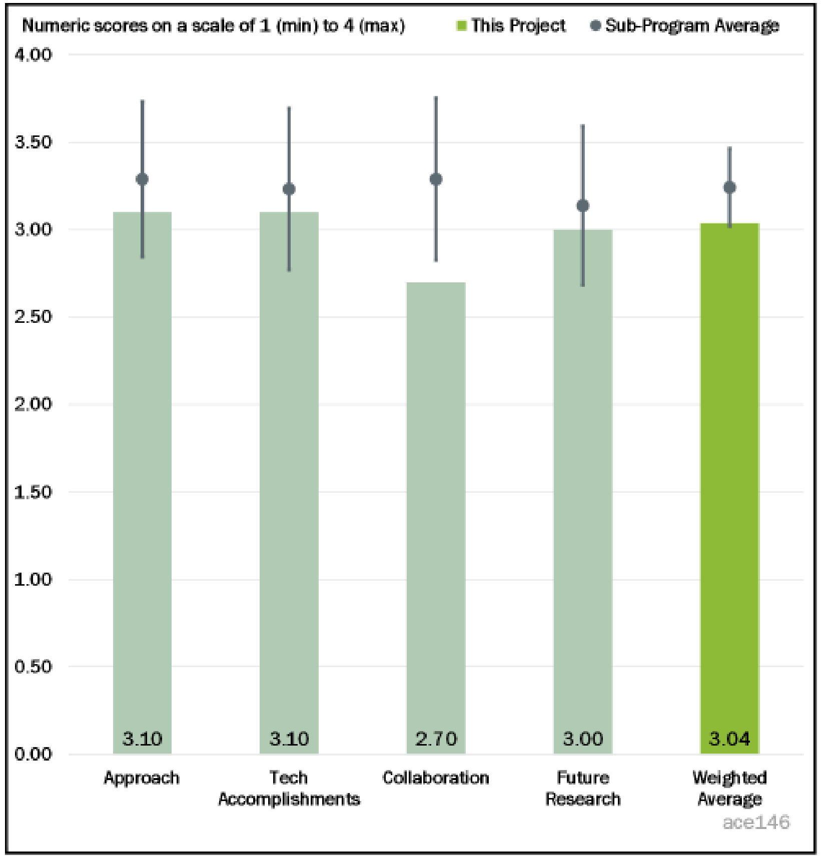
Accomplishments: 2D DNS of detonation under boosted GDI engine conditions



$l_T = 5$ mm

- Larger length scales of temperature stratification result in larger, isolated hot-spots igniting independently
- Pressure waves emanating from the igniting hot-spots get reflected off of the wall and couple with the reaction front
- As a result, there is an abrupt 20X increase in the heat release rate
- Eventually a developing detonation emerges due to the availability of sufficient amount of unburned mixture, $P_{max} > P_{CJ}$

Response to Previous Year Reviewer's Comments



- While the reviewer appreciated the importance of super high-fidelity simulations to provide benchmarks against which to compare more affordable simulations, it is still not clear how results from this work will be used to develop sub -to improve engineering level simulations.

In the current year, we demonstrated the use of DNS simulations to develop improved heat transfer and knock models. Plans are in place to implement these improved model into engineering level simulations

- The team would benefit by engaging an OEM partner.

We have held conversations with engine OEMs and plan to have them in the advisory board in FY22

- This appears to be a collection of unconnected efforts with no coherent plan for integrating them or collaborating among them. The three efforts are aligned with the overall PACE effort, but they are not clearly coordinated with each other.

We have improved coordination among the projects. The plan is to leverage the ASCR investments to provide high quality simulation datasets which will be used to develop improved submodels for spray, combustion, and heat transfer.

Partnerships/Collaborations

PACE Collaboration

- Bill Pitz, Scott Wagnon (LLNL) – Skeletal/reduced mechanisms for PACE surrogates
- Russell Whitesides (LLNL) – Implement fast chemistry and transport solvers
- Lyle Pickett, Julien Manin (SNL) – Spray vessel experiments
- Magnus Sjoberg (SNL) – Optical engine experiments

External Collaborators

- Pointwise Inc. – Fast and efficient mesh generation for Nek5000
- Paul Fischer (UIUC) – Solver development for compressible version of Nek5000
- Joe Insley, Silvio Rizzi (ANL-LCF) – Integrate in-situ visualization capabilities into Nek5000
- Kris Rowe (ANL-LCF) – GPU version of Nek5000
- Matthias Ihme (Stanford) – Implement non-equilibrium wall models in Nek5000
- Chao Xu, Pinaki Pal (ANL) – Submodel implementation in Nek5000
- PELE Team (LBNL, NREL, ORNL, SNL) – Submodel implementation and scalability in PELE

Remaining Challenges and Barriers

- **PACE-wide barriers discussed in ACE138**
- **Coupling with commercial CFD codes:**
  - Need to develop workflows to perform hybrid DNS/LES or LES/RANS simulations by coupling with commercial or open-source low-order CFD codes
  - Use data generated from DNS and wall-resolved LES simulations to improve submodels in commercial codes
- **Size and accuracy of skeletal/reduced mechanisms for PACE fuel surrogates:**
  - Collaborations with the PACE combustion/kinetics team to develop compact mechanisms (~100 species) with sufficient accuracy for the high-fidelity DNS simulations
- **Computational resources may be limited:**
  - ALCC and INCITE proposals to be submitted for access to DOE leadership class machines
  - Long queue times on leadership-class machines
- **Proper archiving of data:**
  - High fidelity simulations will generate >100 TB of data. There is a need to develop efficient data analytics and ML tools, and workflow to share this data across the PACE program

Proposed Future Work- ANL

- **Spray Model Development in Nek5000**
  - Implement improved spray/wall interaction models (FY22 Q1)
  - Corrected Distortion, multi-component evaporation models from Sandia (FY22 Q2)
  - One-way coupling injection method using maps from internal-nozzle flow simulations from ANL (FY22 Q4).
  - Couple spray modeling with engine framework to simulate Sandia DISI engine to study CCV (FY22-FY23).
- **Combustion Model Development in Nek5000**
  - Improve submodels for flame propagation and flame-wall quenching using Chen's DNS dataset (FY21-FY22)
- **Multi-cycle LES/DNS of the Sandia optical DISI engine under fired conditions [FY21-FY23]:**
  - Improve understanding on causes of cyclic variability in flow, mixing, spray and combustion
  - Improve flame-wall interaction and wall heat transfer models
  - Archive numerical setup, flow and thermal data

Any proposed future work is subject to change based on funding levels

Proposed Future Work- SNL

- **Flame wall interaction**
  - Liquid film evaporation model implementation
  - 2D simulations with side wall quenching
  - Hybrid Method of Moments implementation
  - New gasoline surrogate (TPRF-Ethanol/PACE20) chemical mechanism to accurately capture PAH and subsequently soot formation
- **End gas autoignition**
  - Implement a scalar transport equation in S3D resembling the widely used transported Livengood-Wu integral model to assess its accuracy to predict knock in the presence of turbulence and temperature/mixture stratification
  - Parametrize laminar flame speeds at auto-ignitive conditions under the effect of time evolving pressure towards predictive turbulent flame speed models

Any proposed future work is subject to change based on funding levels

Summary

Relevance

- Cyclic variability mitigation and reducing cold start emissions are barriers to attaining higher efficiency for dilute SI combustion

Approach

- Leverage ASCR funded codes Nek5000 and S3D to perform high-fidelity simulations of the flow, spray and combustion processes in SI engines
- Adapt Nek5000 code into a simulation platform tailored for ICE simulations
- Multi-fidelity approach for improved wall heat transfer, combustion and emission models

Accomplishments

- Performed multi-cycle LES of the Sandia DISI and demonstrated potential causes of CCV
- DNS of the compression/expansion stroke performed on >400M grid points on >51,000 processors - Largest ever engine simulation
- Implemented spray submodels in Nek5000 and demonstrated the accuracy in modeling multi-hole evaporating sprays
- Implemented ECFM combustion model in Nek5000 and modeled fired engine simulations
- Demonstrated that one-way coupled soot models cannot capture soot onset or growth under pyrolysis conditions
- Simulated the chamber pre-burn for soot wall film experiment

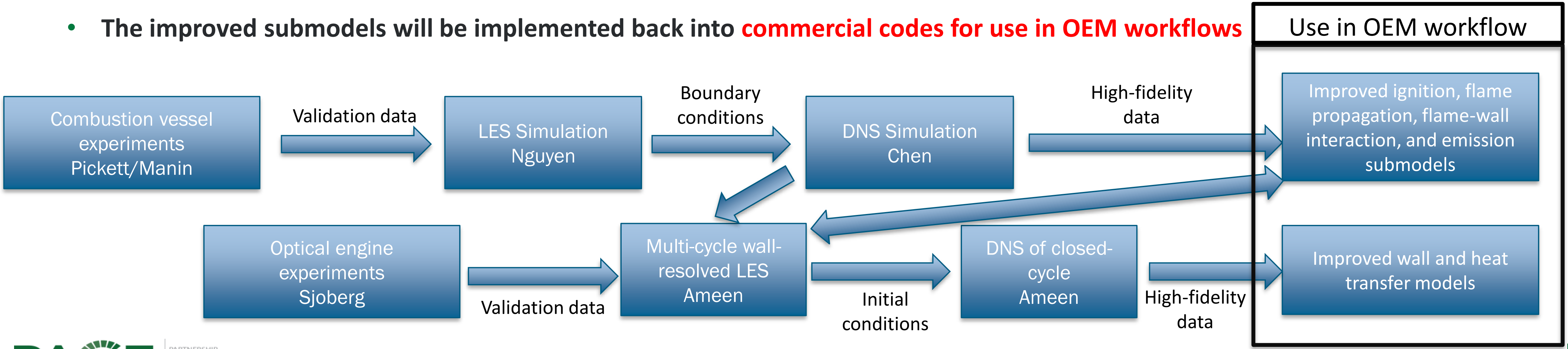
Future Work

- Multi-cycle LES of the Sandia optical DISI engine with spray and combustion
- Improve combustion submodels in Nek5000 using Chen's DNS dataset
- 2D DNS with S3D of flame wall interaction for a range of gasoline fuel surrogate: TPRF-Ethanol and PACE20
- 3D DNS with S3D of end gas ignition and flame wall interaction for selective conditions.

TECHNICAL BACKUP SLIDES

Approach: DNS/LES to Develop Submodels

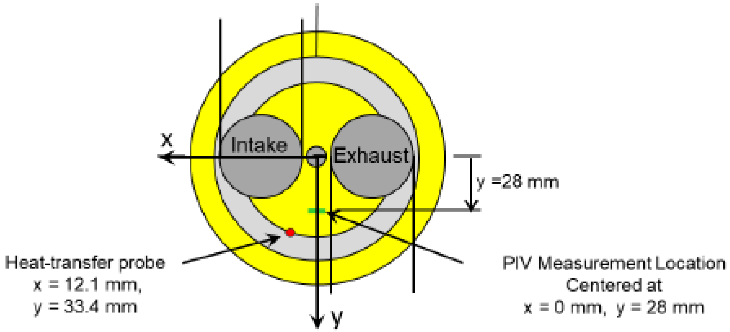
- **Adapt Nek5000 code into a simulation platform tailored for ICE simulations (ANL)**
  - Provide an accurate platform for testing and developing ICE-specific turbulence, spray and combustion submodels
  - Perform multi-cycle, high-fidelity wall-resolved LES to identify the root causes of cyclic variability and provide the understanding needed to design for their minimization
  - DNS of compression and expansion strokes to evaluate and improve wall and heat transfer models
- **Multi-fidelity approach for improved combustion and emission models (SNL)**
  - 1D and 2D DNS with large parametric variations to gain physical insight
  - Full 3D DNS simulations to provide high-fidelity and high quality data for developing submodels for flame propagation, flame-wall interaction, and emissions
  - Physics-based and data-driven sub-model development for both RANS/LES
- **The improved submodels will be implemented back into commercial codes for use in OEM workflows**



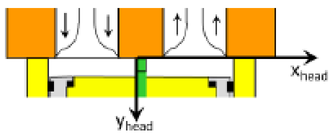
TCC-III Experimental Setup

Heat Flux Probe and PIV Measurement Planes

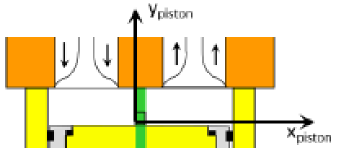
TCC-III Near-wall Coordinate Systems



View from top looking down,
and global coordinates x, y

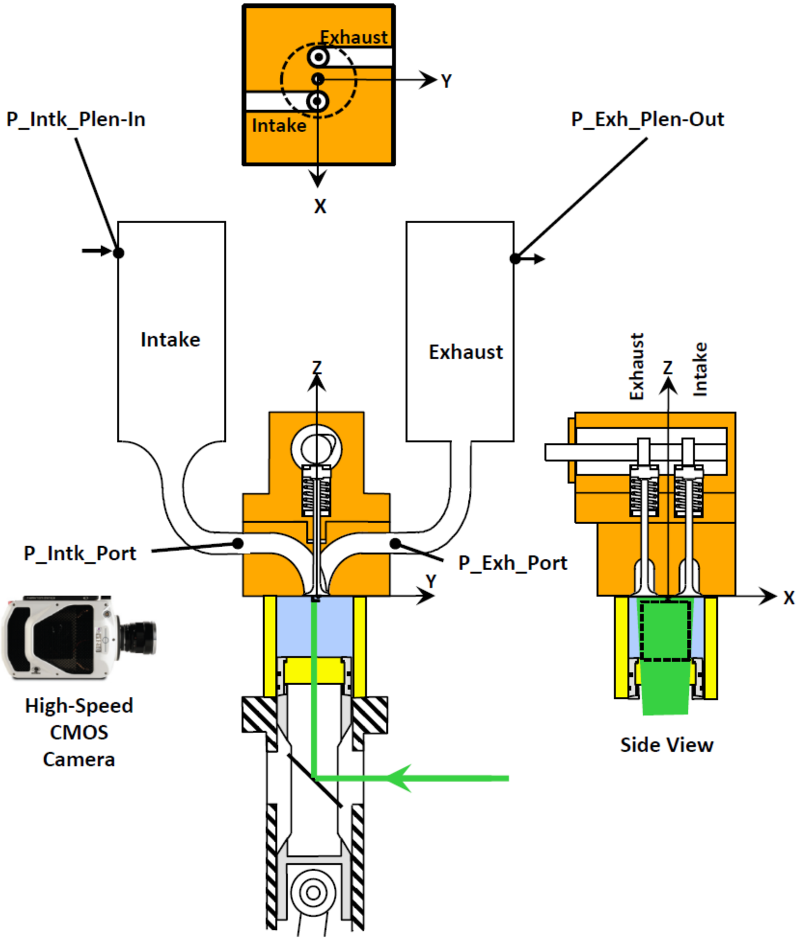


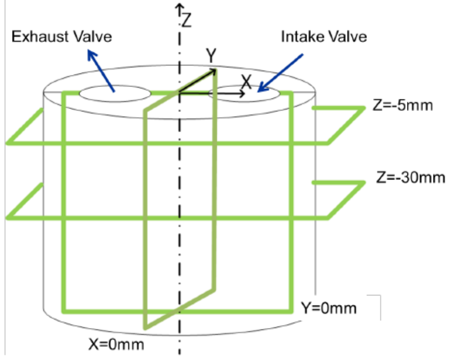
Head Field of View, 5x6 mm (nominal)
and head coordinates, x_{head}, y_{head}.



Piston Field of View, 4.5 x <5 mm (nominal)
and piston coordinates, x_{piston}, y_{piston}.
Camera-image was flipped vertically.

Coordinate system and image-plane labels used in file structure

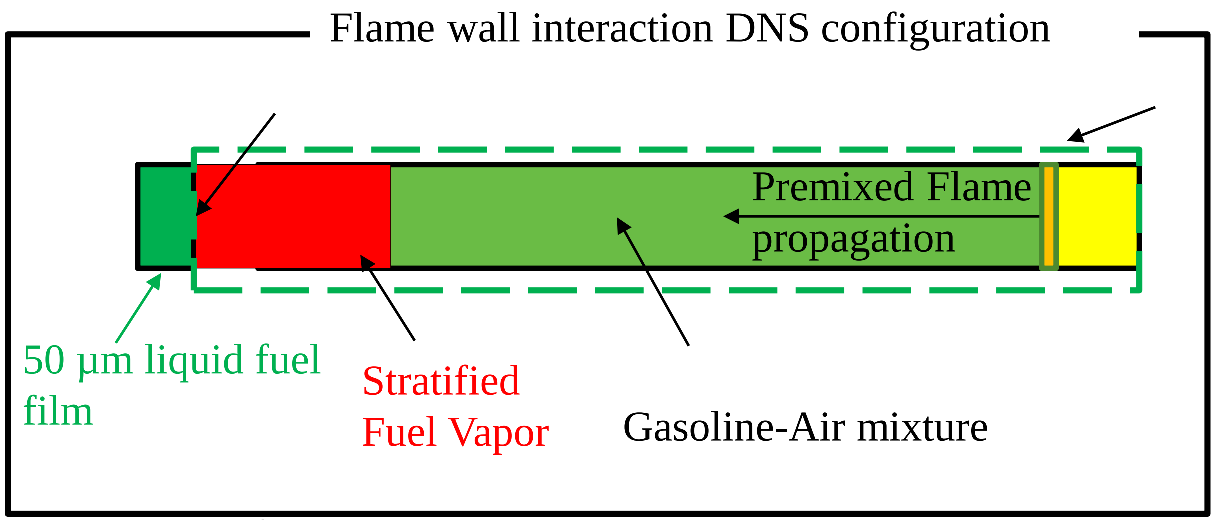


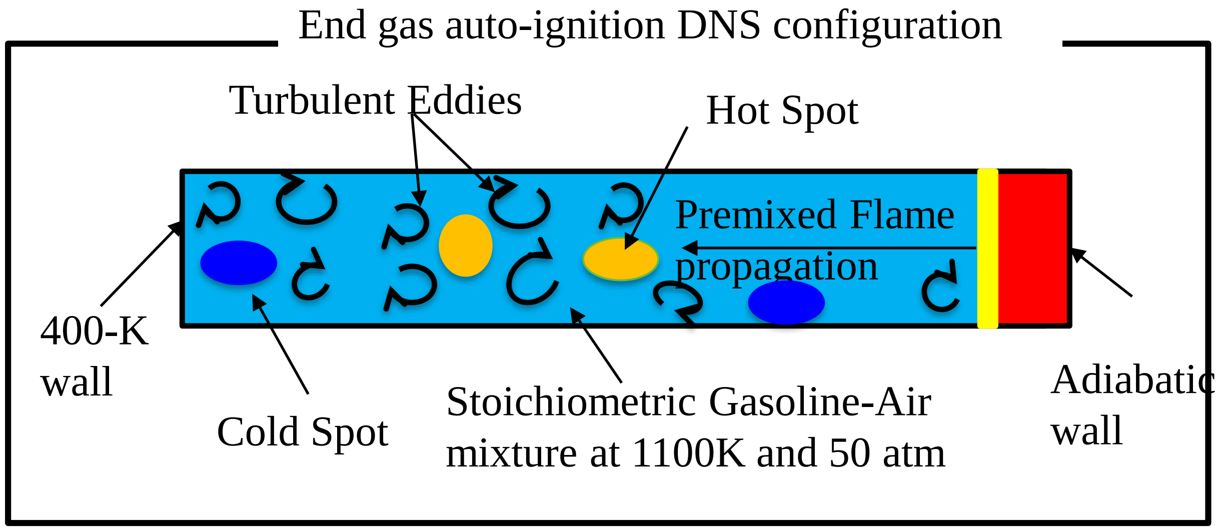


PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Approach – DNS simulation of flame wall quenching, end-gas autoignition, flame deflagration and detonation

- **3D DNS simulations using gasoline surrogate are extremely expensive**
  - Chemical mechanism consists of 100s of species
  - End gas auto-ignition simulations require high temporal and spatial resolution due to fast propagating reaction fronts coupled with pressure waves
  - Flame wall interaction requires large parametric variations because of thermochemical mixture sensitivity
- **Computationally efficient 1D-2D DNS is utilized for large parametric variations**
  - Reduced TPRF-Ethanol gasoline mechanism with 165 or 118 species[1]
  - Variations in temperature, pressure, mixture stratification
  - Detailed analysis of flame quenching, auto-ignition, flame detonation and deflagration behavior
  - Identify relevant cases for 3D DNS simulations



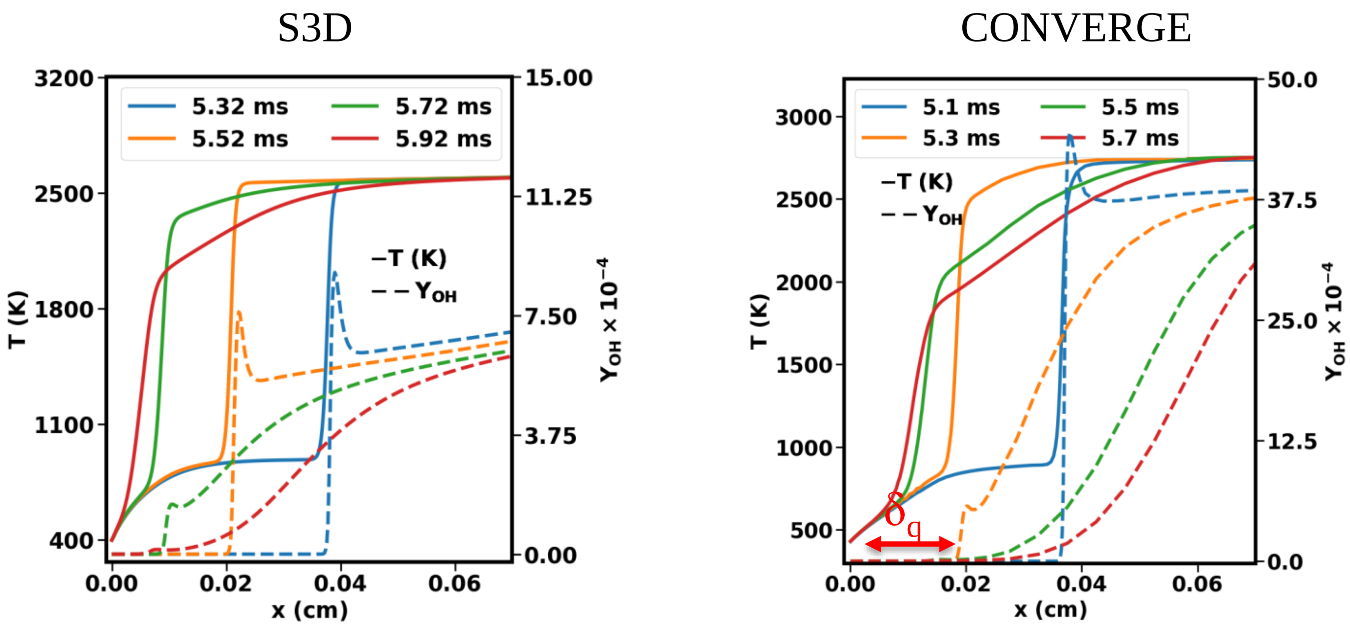


PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

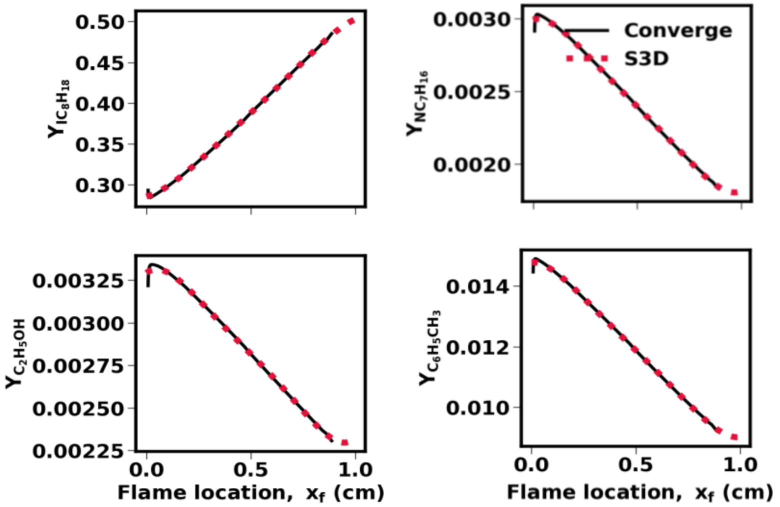
1: Pal et al. JERT, 140(10) 102205 (2018)

Accomplishments: 1D DNS flame-wall interaction simulations S3D/CONVERGE setup validation

- **To validate the permeable wall boundary condition in S3D, numerical results from S3D and CONVERGE for the dry wall case were compared.**
- **Wet wall boundary conditions implemented as permeable wall condition based on fuel evaporation rate calculated by CONVERGE.**
- **High order S3D DNS code**
  - 8th order central differencing scheme
  - 4th order explicit Runge-Kutta time integrator
- **CONVERGE**
  - PISO algorithm with fully conserved formulation
  - 1st order implicit Euler time integration scheme
  - 2nd order flux blending scheme
  - Variable time step sizes



Dry wall quenching characteristics		
Code	Quenching distance (δ_q) [μm]	Peclet number (Pe_q)
S3D	32	3.04
CONVERGE	29	2.77



Despite the difference in the numerical implementation, both codes are in good agreement

PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

KNOCK PREDICTION

- Transported Livengood-Wu integral I,

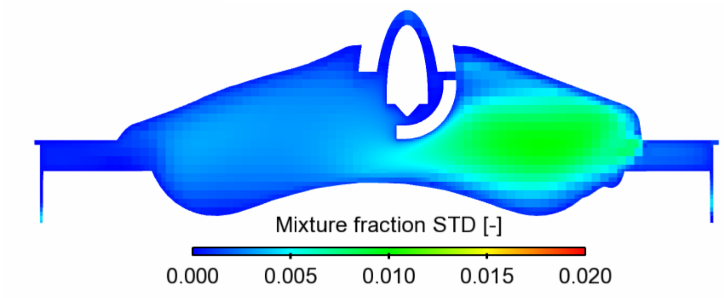
$$\frac{\partial \rho I}{\partial t} + \nabla \cdot (\rho \boldsymbol{U} I - \rho D \nabla I) = \rho \dot{\omega}$$

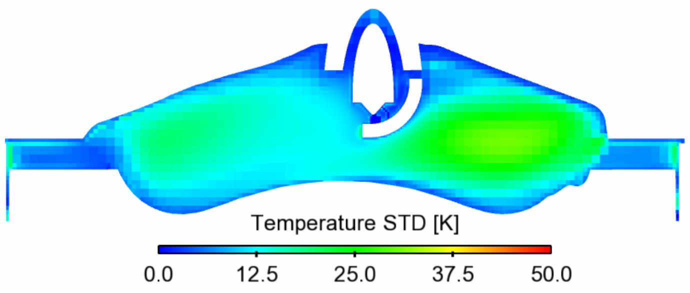
- Solving the reaction rate $\dot{\omega}$ with sub-grid fluctuation,

$$\dot{\omega}_{PDF,avg} = \sum_{i=1}^{\Phi_{tot}} \sum_{j=1}^{T_{tot}} P(\Phi_i, T_j) \frac{1}{\tau(\Phi_i, T_j)} d\Phi dT$$

- Local PDF of mixture fraction and enthalpy,

$$P(Z, h_u) = \frac{1}{2\pi \cdot \sqrt{\widetilde{Z''^2}} \sqrt{\widetilde{h''^2_u}} \cdot \sqrt{1-\rho_{Zh}^2}} \cdot \exp\left\{ -\frac{1}{2(1-\rho_{Zh}^2)} \cdot \left[\frac{(\tilde{Z} - \langle \tilde{Z} \rangle)^2}{\widetilde{Z''^2}} + \frac{(\tilde{h} - \langle \tilde{h} \rangle)^2}{\widetilde{h''^2_u}} - \frac{2\rho_{Zh}(\tilde{Z} - \langle \tilde{Z} \rangle)(\tilde{h} - \langle \tilde{h} \rangle)}{\sqrt{\widetilde{Z''^2}} \cdot \sqrt{\widetilde{h''^2_u}}} \right] \right\}$$

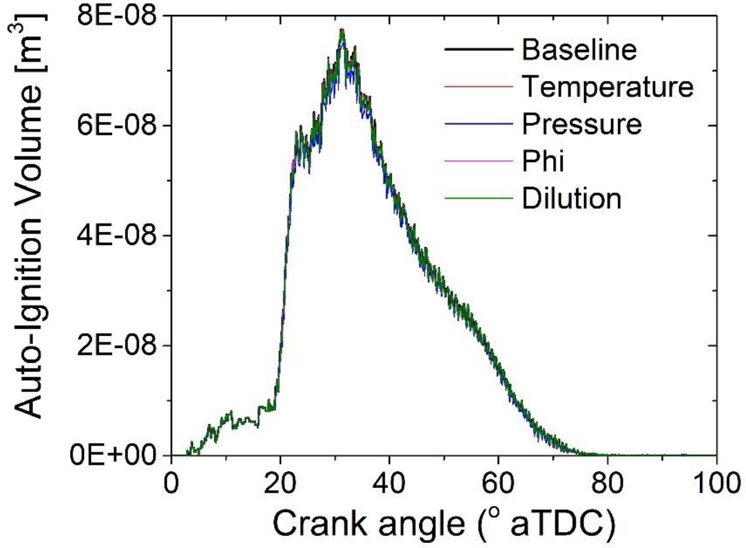




- τ is tabulated a priori.

	Min.	Max.	Step
Temperature	500 K	1500 K	10 K
Pressure	10 bar	70 bar	5 bar
Phi	0.4	2	0.1
Dilution	0	0.2	0.05

- Auto-Ignition volume: total in-cylinder volume where I reaches 1.



D'Adamo et al., Applied Energy, 2017