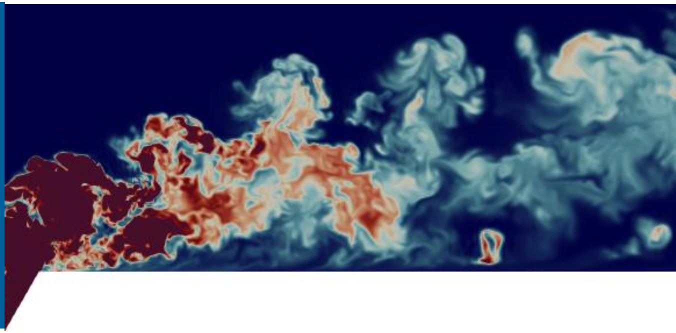
2025 DOE Vehicle Technologies Office Annual Merit Review, June 2-5, 2025

Project ID: ORMA 015

PREDICTIVE CFD TOOLS FOR OFF-ROAD IC ENGINES UTILIZING ALTERNATIVE FUELS



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OVERVIEW

ICE = Internal Combustion Engine

Timeline

- Project start: 08/29/2023
- Project end: 08/28/2027
- Percent complete: 40%*

** As of April 2025*

Budget

- DOE funding in FY25: $600k
- Industry cost-share in FY25: $450k
  - Caterpillar funds-in: $150k
  - Caterpillar in-kind: $100k
  - Convergent Science in-kind: $200k

Barriers

- Limited understanding of the impact of alternative fuel properties on off-road engine performance and emissions.
- Limited availability of predictive modeling tools to support the design of future internal combustion engines (ICEs) for off-road applications.

Main Partners

- Argonne National Laboratory (Lead)
- Caterpillar Inc.
- Convergent Science Inc.

RELEVANCE/OBJECTIVES

CFD = Computational Fluid Dynamics
H_2 = Hydrogen
MeOH = Methanol

Opportunity:

- **Use alternative fuels to mitigate emissions from the off-road sector:**
  - *With light-duty sector easier to electrify, off-road emissions share might increase.*
  - *Hydrogen (H_2) and Methanol (MeOH) align very well with off-road applications.*

Challenge:

- **Alternative fuels have unique properties that affect engine operation:**
  - *Some of these properties also affect specific engine components (e.g., injectors).*
- **Large engines require large computational resources and scalable codes:**
  - *It is vital to not only develop better models, but also to define best-practices to run those models.*

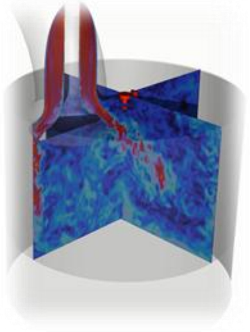
Objective:

- **Develop predictive modeling tools and model best practices to accelerate the design of ICEs for off-road applications using H_2 and MeOH:**
  - *Evaluate CFD model deficiencies and needs for specific fuels of interest.*
  - *Adapt/calibrate existing CFD models or develop brand new CFD models.*

APPROACH

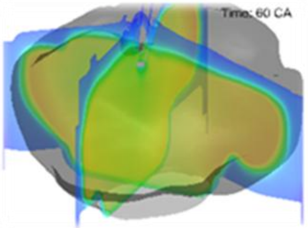
DNS = Direct Numerical Simulations

DNS to support model development



H_2 ICE research will focus on regular and abnormal combustion

CFD models and best practices

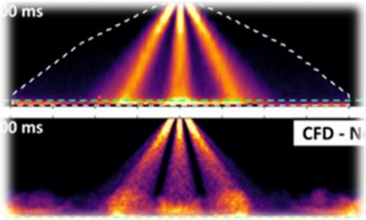


Task 1:
CFD modeling of Hydrogen ICEs*
Years 1 & 2

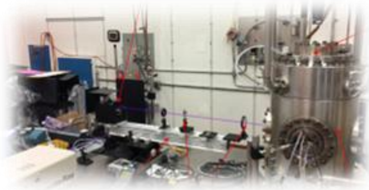
Engine data for model validation/calibration

* *Cat ® engine data being modeled in **Task 1** was produced by introducing hydrogen into a natural gas single-cylinder engine*

CFD models and best practices

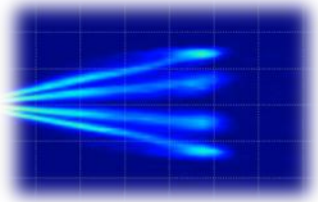


Task 2:
CFD modeling of Methanol ICEs
Years 3 & 4



Injector hardware, spray vessel data, engine data

X-ray diagnostics



MeOH ICE research will focus on injection systems and sprays

PROPOSED RESEARCH AND MILESTONES

Task List (Year)	Status FY24 (Last Year)	Status FY25 (Today)
H_2 ICEs (Year 1): mixture formation and combustion		
Task 1.1: H_2 port fuel injection (PFI) and mixture formation (Year 1)	50%	✓
Task 1.2: Ignition from the passive prechamber spark-plug (Year 1)	✓	✓
Task 1.3: Ignition jets development and mixing (Year 1)	✓	✓
Task 1.4: Flame propagation and combustion (Year 1)	25%	✓
Task 1.5: Conjugate heat transfer (CHT) calculations (Year 1)	0%	✓
H_2 ICEs (Year 2): abnormal combustion and heat transfer		
Task 1.6: Flame quenching and heat transfer (Year 2)	-	✓
Task 1.7: Pre-ignition (Year 2)	-	10%
Task 1.8: Knock (Year 2)	-	5%
Task 1.9: Emissions (Year 2)	-	50%

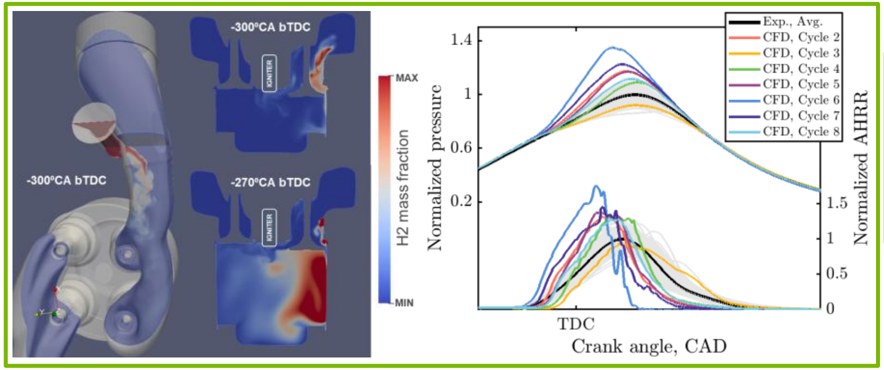
☺ We made progress with all H_2 ICE modeling tasks

☺ We successfully completed all Year 1 tasks and actively working on Year 2 tasks

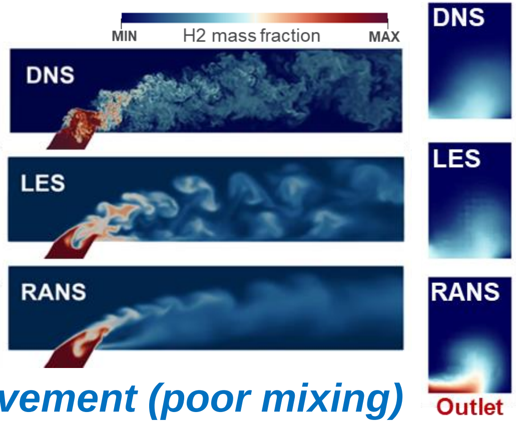
FY24 ACCOMPLISHMENTS RECAP

RANS = Reynolds-Average Navier-Stokes
LES = Large Eddy Simulations
MFB = Mass Fraction Burned
G-EQN = G-Equation; WSR = Well-Stirred Reactor

1. PFI-induced stratified mixture led to large cyclic variability

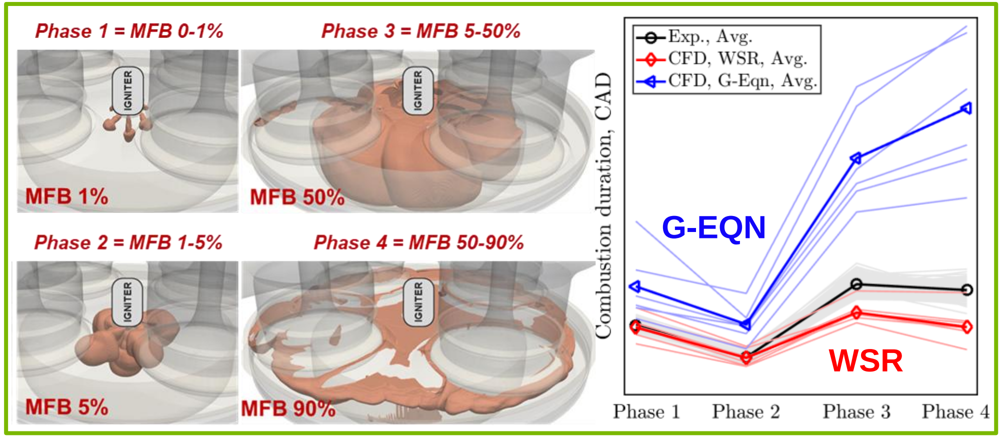


DNS to study PFI mixing process

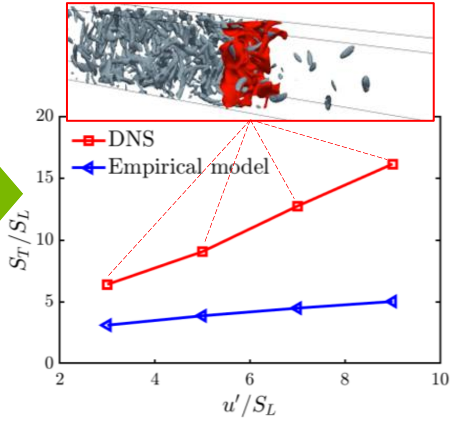


RANS needs improvement (poor mixing)

2. CFD analysis highlighted RANS combustion model performance



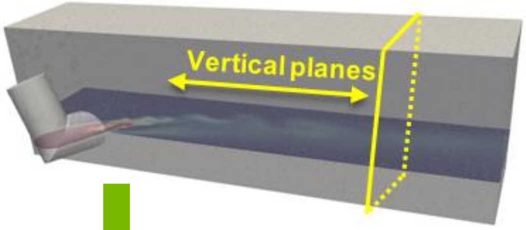
DNS to study combustion process



G-EQN needs improvement (slow burn)

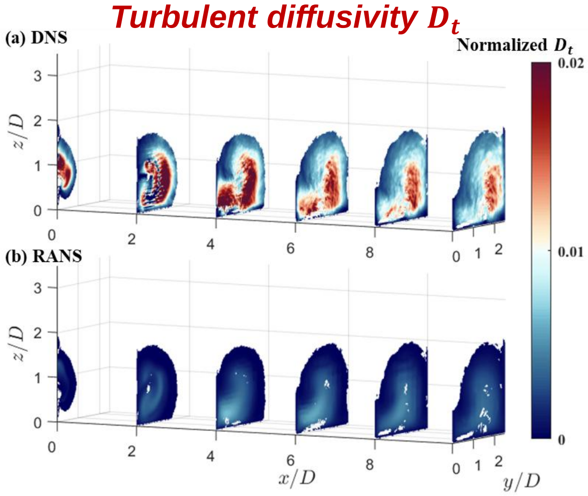
FY25 TECHNICAL ACCOMPLISHMENTS

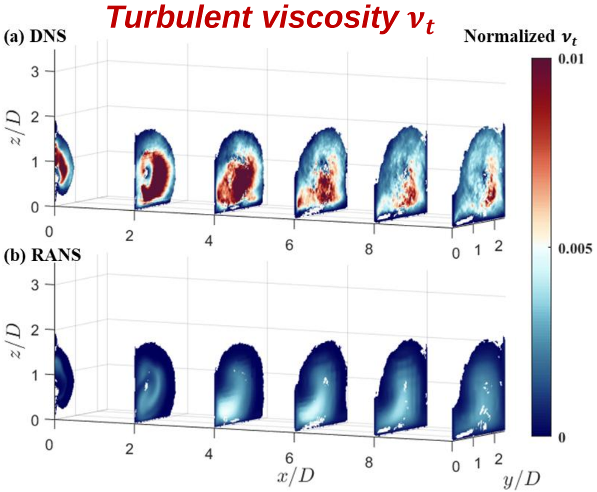
1. RANS mixing model performance assessed based on DNS data



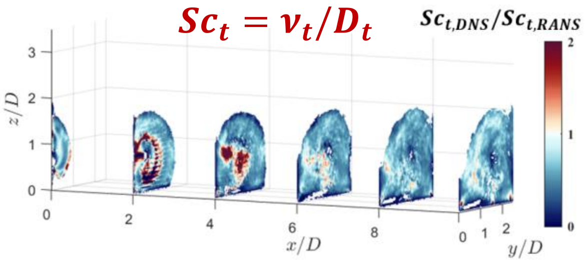
$$\widetilde{Y_k'' u_j''} = -\boldsymbol{D_t} \frac{\partial \widetilde{Y}_k}{\partial x_j}$$

$$\boldsymbol{D_t} = \frac{\boldsymbol{\nu_t}}{\boldsymbol{Sc_t}}$$





- D_t from RANS is significantly under-predicted throughout the domain, compared with DNS results.
- D_t (and therefore <u>mixing</u>) <u>under-prediction</u> attributed to:
  1. Under-prediction of ν_t compared to DNS.
  2. Over-prediction of Sc_t compared to DNS.



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FY25 TECHNICAL ACCOMPLISHMENTS

2. RANS mixing model improved based on DNS data

Turbulent species flux formulations

DNS data provide all quantities + optimized constants *

- Gradient-diffusion hypothesis (**GDH**)

$$\widetilde{Y_k''u_i''} = -D_t \frac{\partial \widetilde{Y}_k}{\partial x_i} = -\frac{\nu_t}{Sc_t}\frac{\partial \widetilde{Y}_k}{\partial x_i}$$

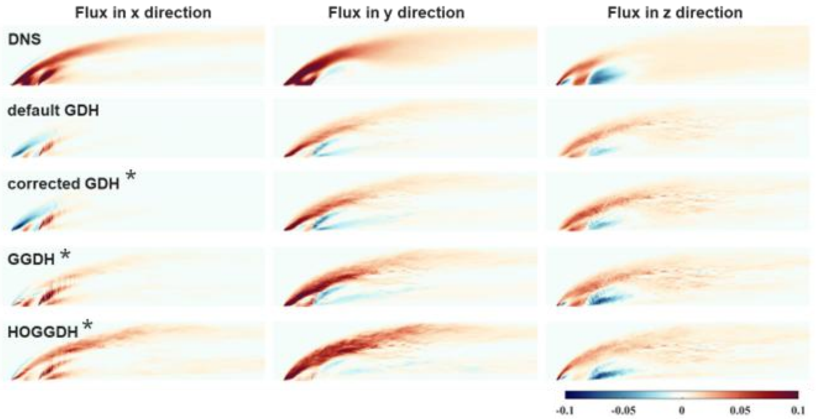
- Generalized GDH (**GGDH**)

$$\widetilde{Y_k''u_i''} = -C_\theta \frac{\nu_t}{k}\widetilde{u_i''u_j''}\frac{\partial \widetilde{Y}_k}{\partial x_j}$$

- Higher-order GGDH (**HOGGDH**)

$$\widetilde{Y_k''u_i''} = -C_\theta \frac{\nu_t}{k^2}\widetilde{u_i''u_k''}\widetilde{u_k''u_j''}\frac{\partial \widetilde{Y}_k}{\partial x_j}$$

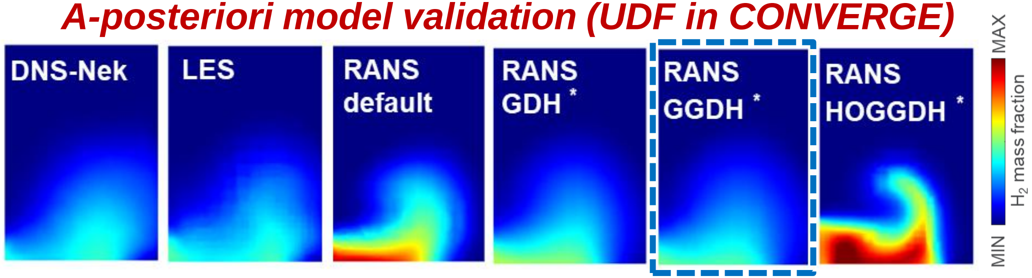
A-priori model validation



Final model configuration

1. **GGDH** formulation **with optimized model constants** (based on DNS);
2. **Improved C_μ** constant (based on DNS data) **that improves ν_t** $= C_\mu \frac{k^2}{\varepsilon}$.

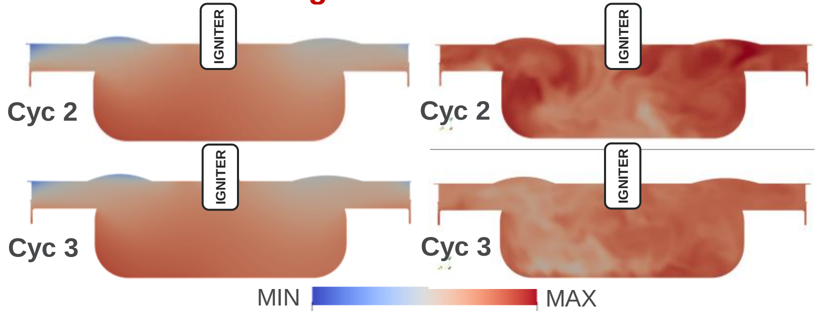
A-posteriori model validation (UDF in CONVERGE)



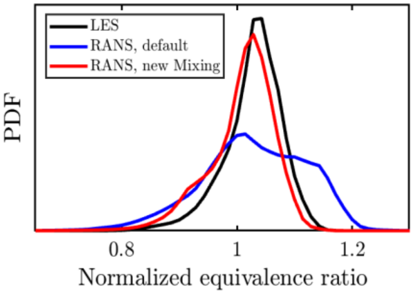
New RANS mixing model with similar accuracy to DNS/LES

FY25 TECHNICAL ACCOMPLISHMENTS

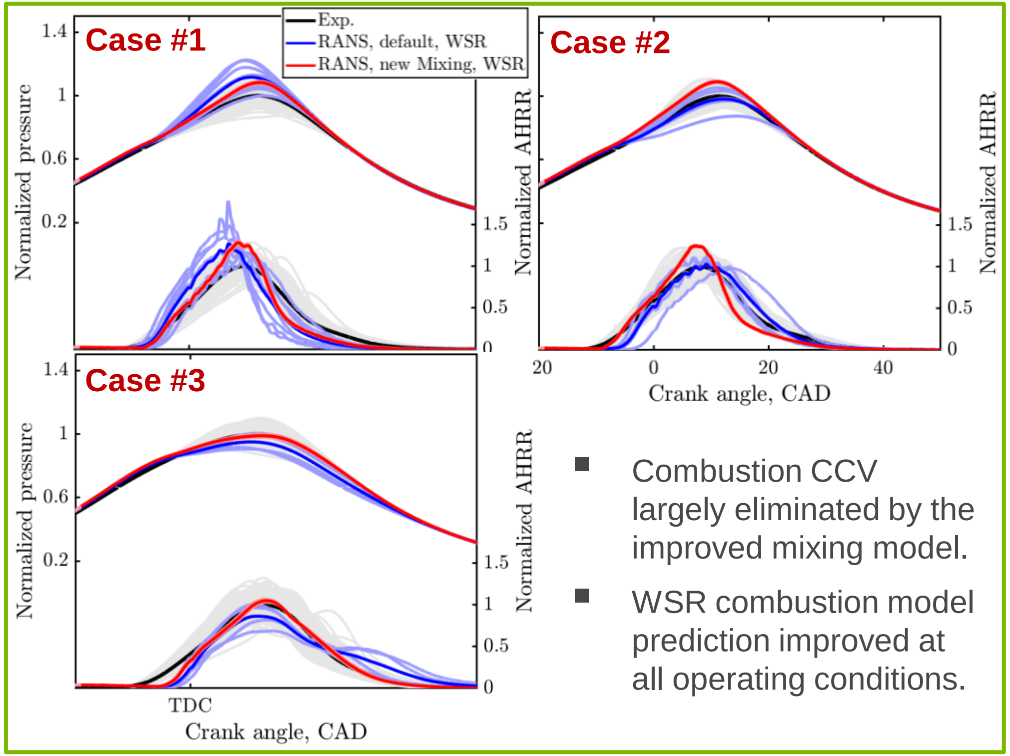
3. RANS new mixing model demonstrated in engine simulations



PDF of Equivalence Ratio



- RANS + new mixing model increased mixture homogeneity and eliminated cyclic mixture variability.
- Good agreement with LES (PDF of Eq. Ratio).



- Combustion CCV largely eliminated by the improved mixing model.
- WSR combustion model prediction improved at all operating conditions.

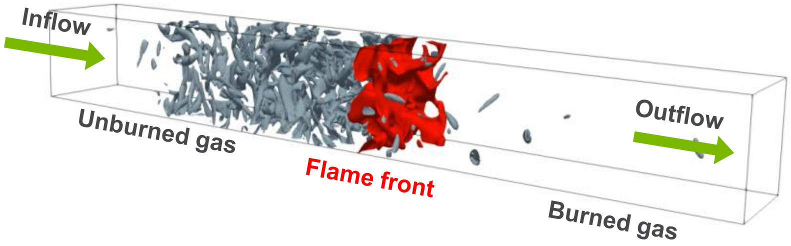
The new model improved RANS predictions of PFI mixing and combustion

Case #1 = High-load, nominal λ; Case #2 = Moderate-load, nominal λ; Case #3 = High-load, leaner

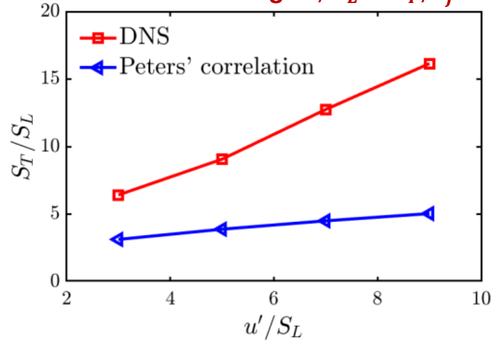
FY25 TECHNICAL ACCOMPLISHMENTS

4. G-Equation combustion model improved based on DNS

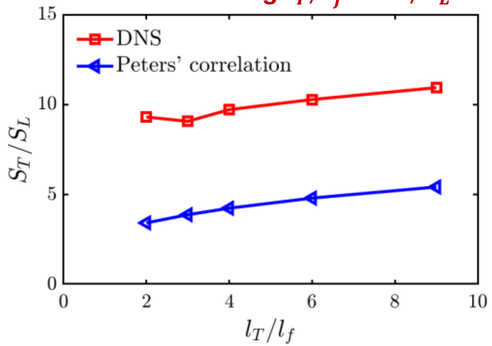
DNS of “Flame-in-Box” configuration



DNS 1: increasing u'/S_L at l_T/l_f=3



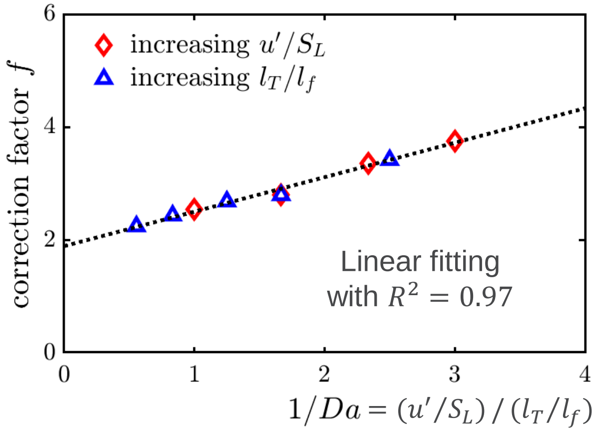
DNS 2: increasing l_T/l_f at u'/S_L=5



Improved Peters’ correlation:

$$\frac{S_T}{S_L} = 1 + \frac{u'}{S_L}\left[-\frac{a_4 b_3^2}{2b_1}Da + \left\{\left(\frac{a_4 b_3^2}{2b_1}Da\right)^2 + a_4 b_3^2 Da\right\}^{0.5}\right] * \boldsymbol{f}$$

Correction factor $\boldsymbol{f} = \frac{(S_T/S_L)_{DNS}-1}{(S_T/S_L)_{model}-1}$



- Peters’ correlation significantly underpredicts S_T, leading to poor G-Eqn. performance.
- A correction factor for Peters’ correlation was proposed based on DNS data:
  - *Additional correlations from literature used at very high values of (u', l_T).*

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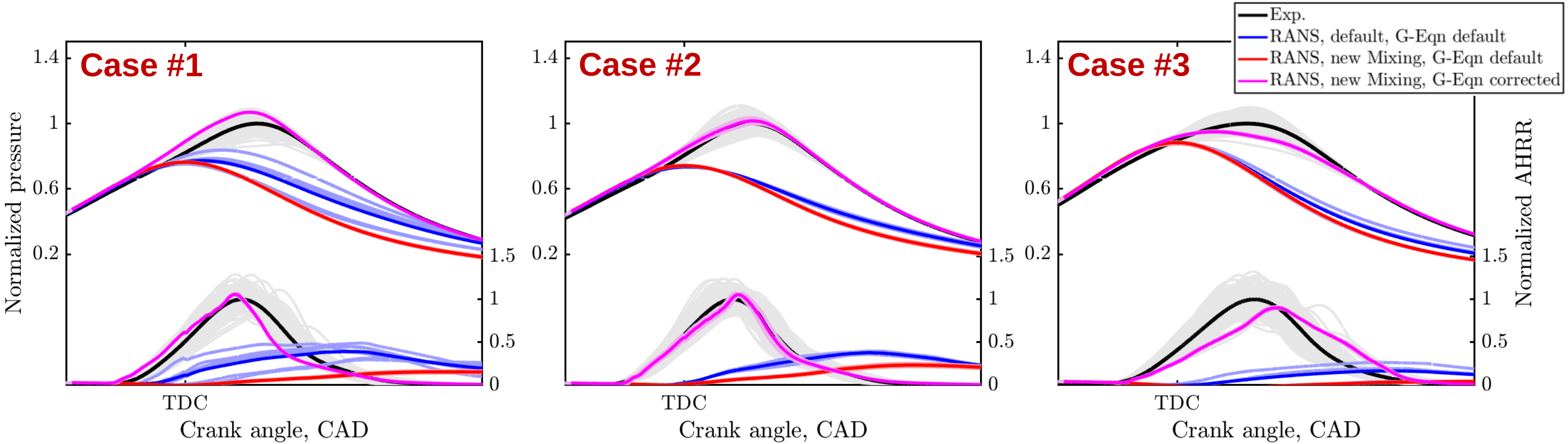
FY25 TECHNICAL ACCOMPLISHMENTS

5. Improved G-Equation model demonstrated in engine simulations



- Across all operating conditions, good agreement with experimental data is achieved when using the new mixing model and the improved G-Equation combustion model:
  - *The default G-EQN model significantly under-predicted the burning rate.*
  - *No model tuning was shown to be effective with the default G-EQN.*
  - *Further improvement possible for leaner condition (Case #3) with additional DNS data.*

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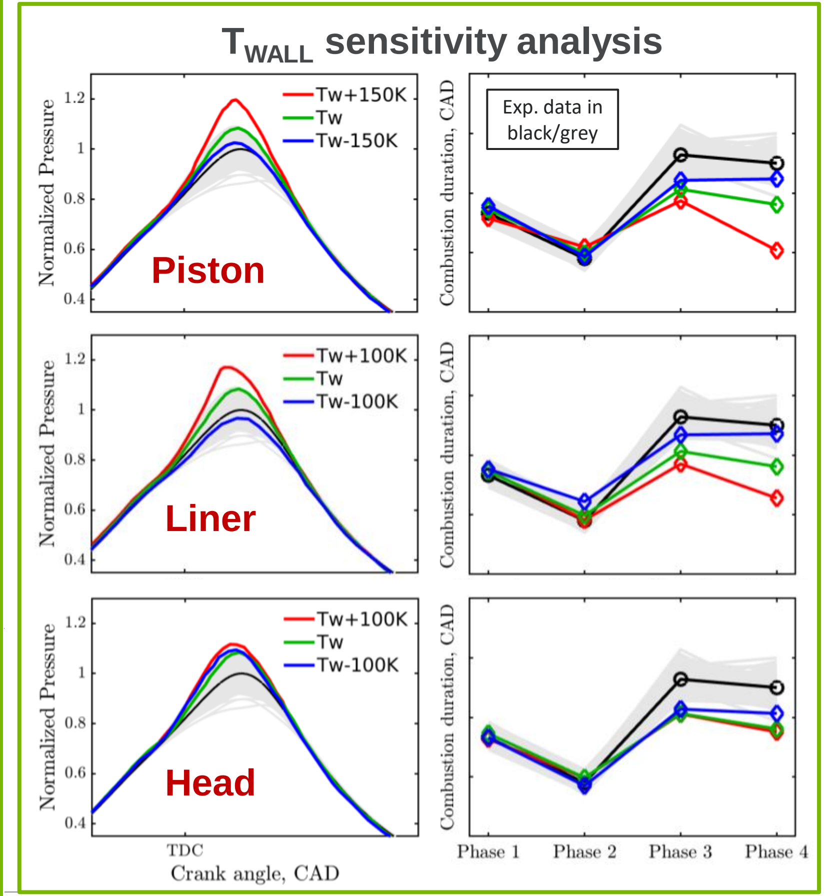
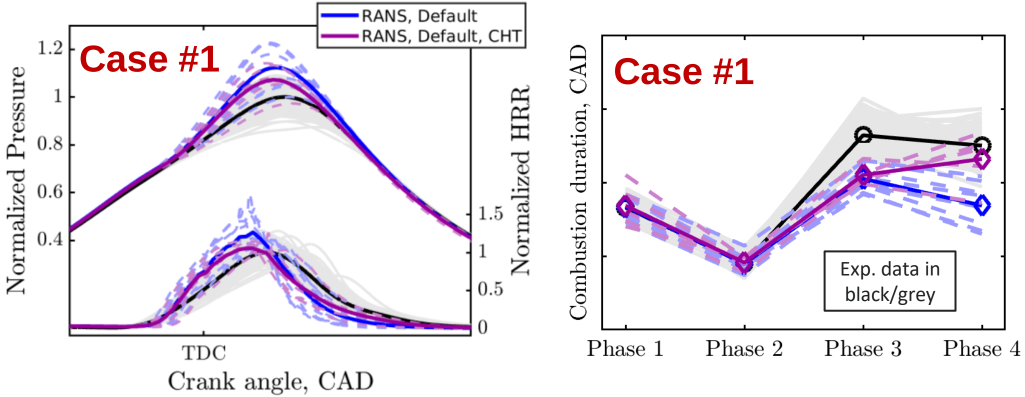
FY25 TECHNICAL ACCOMPLISHMENTS

6. Conjugate Heat Transfer (CHT) calculations completed



- **Sensitivity analysis** of T_{WALL} boundary conditions was performed for piston, liner, and head:
  - *CFD results very sensitive to piston/liner T_{WALL}.*
- **CHT model** was built for: **Piston**, **Liner**, and **Exhaust valves** (to evaluate pre-ignition from Exhaust valves).



- CHT model predicts lower surface temperature than initially imposed and calculates longer combustion duration in Phase 4 → **CHT improves the agreement with experiments.**

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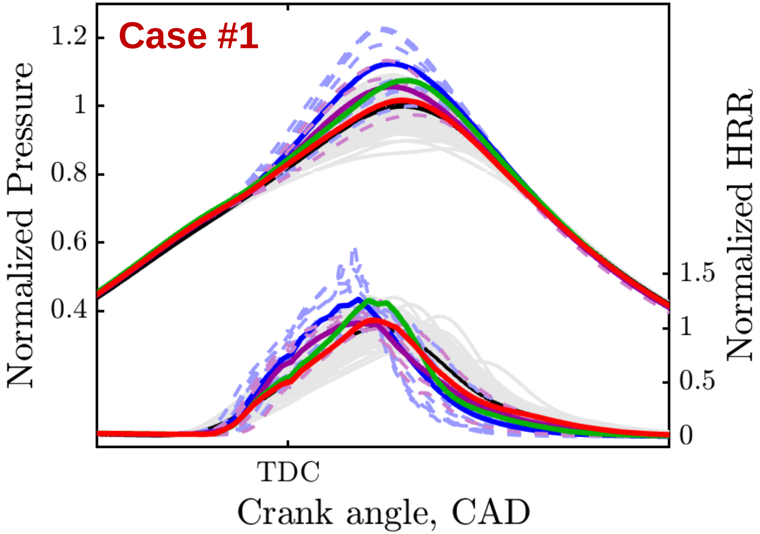
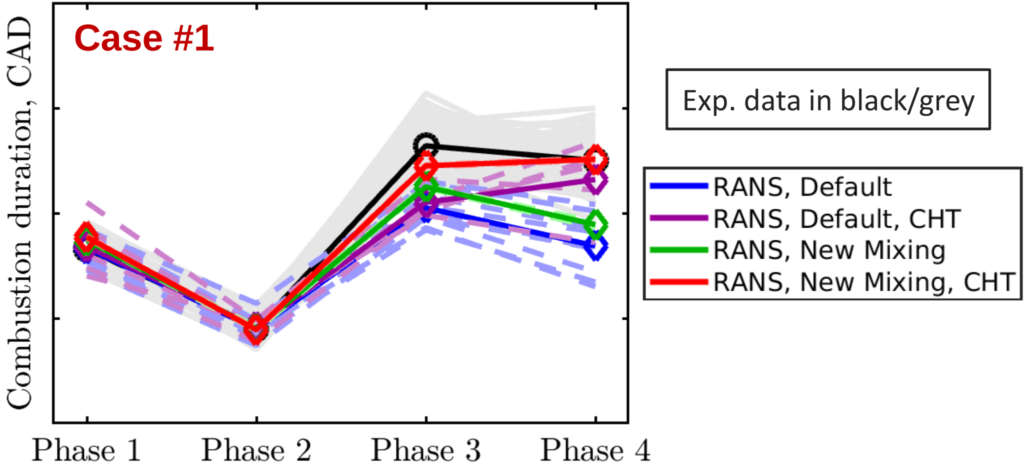
FY25 TECHNICAL ACCOMPLISHMENTS

7. CHT and Mixing model combined to improve performance of the finite rate chemistry combustion model (WSR) – Part I



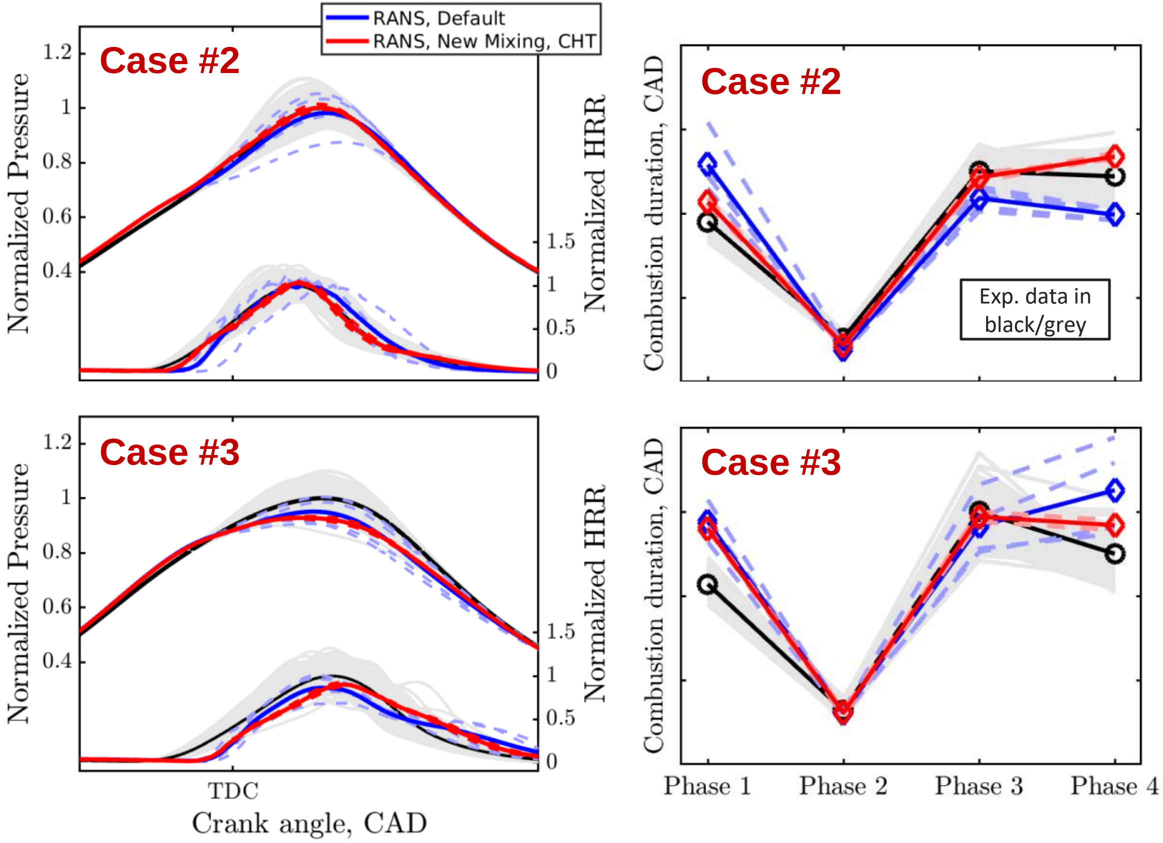


- CHT contributes to slowing down combustion rate at late stages.
- New Mixing model enhances homogeneity and eliminates cycle to cycle variation.
- CFD prediction for MFB10-50% (Phase 3) is **further improved by combining the Mixing model with CHT → excellent agreement with experiments.**

FY25 TECHNICAL ACCOMPLISHMENTS

8. CHT and Mixing model combined to improve performance of the finite rate chemistry combustion model (WSR) – Part II

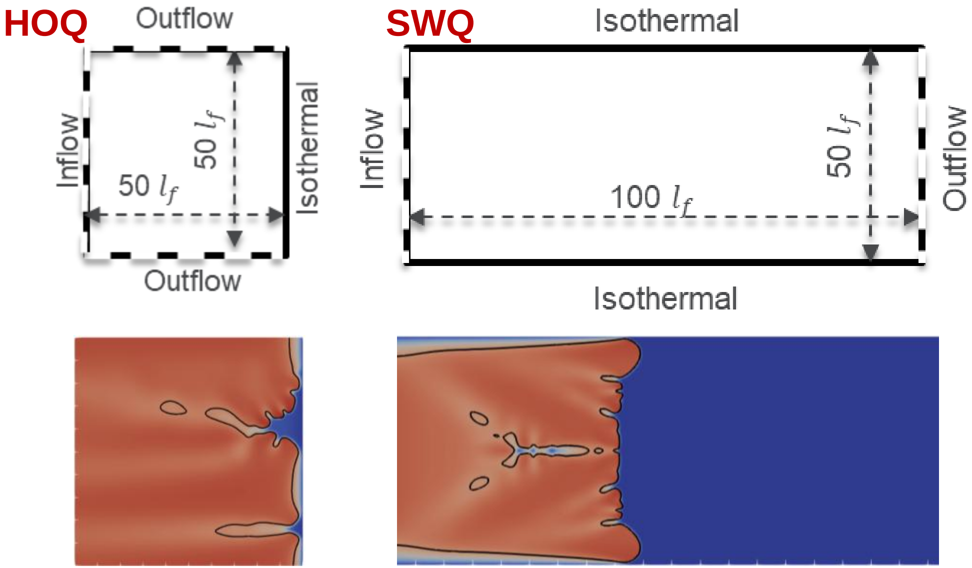
- CFD predictions of combustion duration for Phases 3 and 4, (MFB 10-90%), are repeatedly improved by using both CHT and the new Mixing model.
- Over multiple operating conditions, combining the mixing and CHT models led to better CFD predictions.
- Case #3 (leaner condition) will need additional investigations of the pre-chamber conditions to improve Phase 1 predictions.



FY25 TECHNICAL ACCOMPLISHMENTS

9. Near-wall flame quenching characteristics evaluated using DNS

- DNS simulations were conducted under conditions representative of a flame front approaching the piston surface.
- Two scenarios for quenching evaluated:
  - *Head on quench (HOQ)*
  - *Side wall quench (SWQ)*
- For both HOQ and SWQ cases, the **quench distance (l_q) was very small compared to typical RANS mesh size** ($\mathrm{dx_{min}} = 250\ \mu\mathrm{m}$).
- A wall quenching model would be irrelevant for H_2/air flames in RANS engine simulations, at current mesh resolutions.



	$l_{q,min}$	$l_{q,mean}$	$Pe_{q,min}$	$Pe_{q,mean}$
HOQ	$66\ \mu m$	$102\ \mu m$	0.9	1.4
SWQ	$96\ \mu m$	$96\ \mu m$	1.3	1.3

$$Pe_q = \frac{l_q}{l_f}$$

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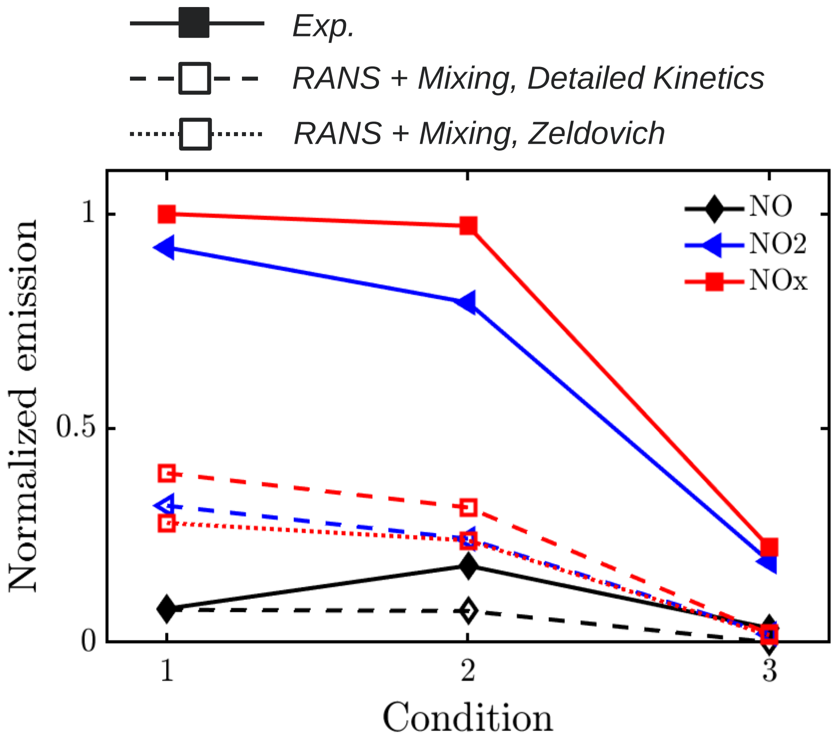
FY25 TECHNICAL ACCOMPLISHMENTS

10. NO_X emission model performance evaluated in engine simulations

- Chemical kinetics mechanism (UCSD) expanded to include NO_X formation chemistry:
  - *UCSD: 11 species + 23 reactions*
  - *Added NO_X sub-chemistry**
  - *UCSD + NO_X: 32 species + 207 reactions*
- Different methods to extract NO_X emissions from CFD evaluated to ensure fair comparison.
- Comparisons with experimental data were made for both NO_X magnitude and NO_X trend at varying operating conditions (cases #1-3) :
  - ***NO_X magnitude is under-predicted.***
  - ***NO_X trend is captured well.***



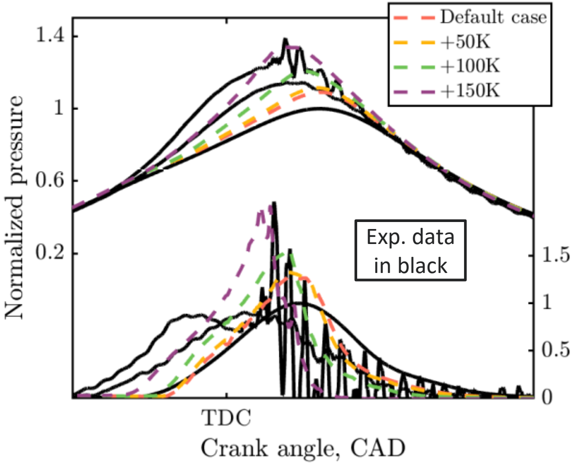
* P. Glarborg, et al. Progress in Energy and Combustion Science, 2018.

FY25 TECHNICAL ACCOMPLISHMENTS

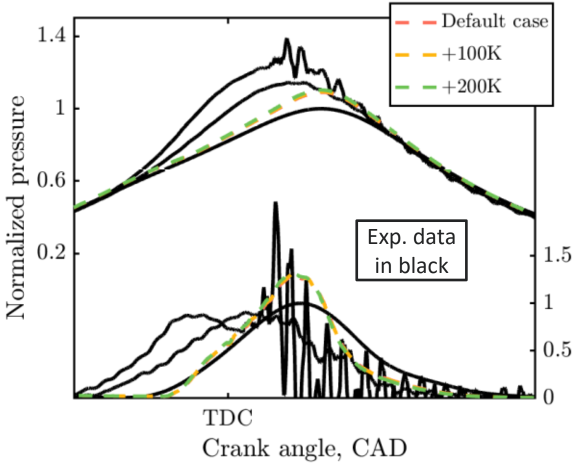
11. Preliminary evaluation of pre-igniting/knocking conditions

- Case #1 showed pre-ignition (sometimes followed by knock) propensity in engine experiments.
- Different strategies to reproduce the pre-ignition observed in experiments were evaluated:
  - Strategy 1: increase pre-chamber wall temperature → Pre-ignition triggered. Timing not captured.
  - Strategy 2: increase exhaust valve wall temperature → Pre-ignition not triggered.
  - Strategy 3: induce hot spot in the main-chamber → Pre-ignition triggered. Early-stage combustion captured.

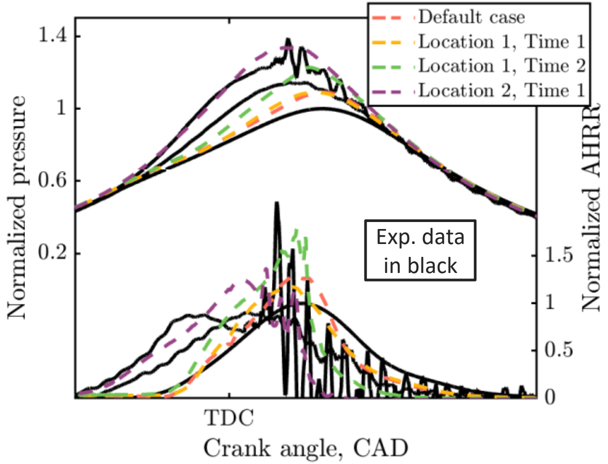
Strategy 1: hot spot in pre-chamber



Strategy 2: hot spot near exhaust valve



Strategy 3: hot spot in main chamber



Pre-ignition spot has significant impact on the combustion rate & end-gas auto-ignition

RESPONSES TO PREVIOUS REVIEW COMMENTS

"…the simplified intake port seems too simple…asked if there is any way to improve the model to have a more accurate geometry with both the intake valves and injector. This may have a significant impact on the cycle-to-cycle differences being seen in simulation..." **A simplified geometry is better for DNS cases and does not affect the physics (turbulent diffusivity of the injected gas) that we are trying to capture.**

"…the experimental data used for comparing cycle-to-cycle variation appears to be an average. This reviewer asked if there is a way to show best/worst experimental cycles for a comparison with the CFD data…." **We have been showing all (200) experimental cycles in our plots.**

"It is, however, useful to understand the degree to which differences between DNS, with very high fidelity, and RANS, with low processor cost, are impactful for the overall utility of the results" **This year we show the impact of improving RANS (based on DNS) on engine calculations.**

"…this report did not adequately describe boundary conditions such as bore, stroke, revolutions per minute, torque (%), intake manifold pressure and temperature, compression ratio, in-cylinder swirl ratio, etc. A summary table is recommended.." **Engine specs and operating conditions are now provided (see technical backup slides).**

"the collaboration on this project is relatively narrow, including ANL as the lead with one OEM and a CFD code supplier…It will be important to see further signs of collaboration as the project moves forward" **This being a CRADA between DOE/industry, it is not trivial to add more participants.**

"The reviewer encouraged the team to predict H2 combustion efficiency and H2 emissions as future goals" **This being a short task, we need to prioritize key topics. H_2 combustion efficiency is high at the conditions evaluated. H_2 emissions are important but less critical than NO_X.**

"This reviewer also posed a question to the project team, asking how to validate the conjugate heat transfer results from CFD" **It is challenging to comprehensively validate CHT calculations, but this year we clearly show the strong and beneficial impact on engine CFD calculations.**

"…it was identified that the key aspect, especially for hydrogen combustion, was the mixing model…this reviewer encouraged the team to consider reshaping the work to ensure this was fully addressed and would prefer to see a focus here rather than covering all topics…" **The mixing model development work is now complete, and we are also making good progress on all other topics.**

"The reviewer offered the following suggestion: a smaller PFI spark-ignited engine has been studied to run H2 with combustion data measurement, and this reviewer wondered if it would be valuable to validate the models to such existing data then re-apply them to a large bore and lower speed engine with prechamber" **The main concern is that most of the work done here would not be consistent with a smaller PFI engine (e.g., the operating conditions of pressure and temperature for DNS and G-EQN model improvement will be very different in a smaller engine).**

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COLLABORATION AND COORDINATION

Argonne National Laboratory

- High-fidelity engine modeling
- High-performance computing (HPC) resources
- CFD model development and implementation
- *X-ray diagnostics (MeOH task)*

Caterpillar

- Technical expertise in modeling and experiments
- Engine experimental data
- *Injection hardware and spray vessel data (MeOH task)*

Convergent Science

- CFD software licensing
- Technical expertise in engine modeling
- Technical support with CFD model implementation

While this is a CRADA between DOE and Industry, with a limited number of industry participants, we have been sharing and will continue to share the major findings of this work through several publications and presentations

REMAINING CHALLENGES AND BARRIERS

- **CHT calculations contributed to significantly improve CFD predictions of combustion rates for finite-rate chemistry approach (WSR model) but are roughly 2.5 times more expensive than imposing T_{WALL} boundaries:**
  - Develop best-practices to run CHT effectively (faster) as well as alternative approaches (e.g., imposing varying T_{WALL} boundaries based on CHT).
  - Confirm findings for alternative combustion model formulations (G-EQN).
  - Couple with heat transfer models available in CONVERGE.
- **With the fuel/air mixing problem being solved, the CFD model is ready to face the pre-ignition challenge (and the knock challenge as well):**
  - CHT will help with characterizing hot-spot formation.
  - Focus will be shifted over lube oil induced pre-ignition.
- **NO_X predictions shows that trends are captured but magnitudes are not:**
  - Evaluate alternative fuel/NO_X kinetics.

PROPOSED FUTURE RESEARCH

Task List (Year)	% Completion	Next Steps
H_2 ICEs (Year 1): mixture formation and combustion		
Task 1.1: H_2 PFI and mixture formation (Year 1)	✓	
Task 1.2: Ignition from the passive prechamber spark-plug (Year 1)	✓	
Task 1.3: Ignition jets development and mixing (Year 1)	✓	
Task 1.4: Flame propagation and combustion (Year 1)	✓	
Task 1.5: Conjugate heat transfer (CHT) calculations (Year 1)	✓	Define CHT best practices
H_2 ICEs (Year 2): abnormal combustion and heat transfer		
Task 1.6: Flame quenching and heat transfer (Year 2)	✓	
Task 1.7: Pre-ignition (Year 2)	10%	Complete by end of FY25
Task 1.8: Knock (Year 2)	5%	Complete by end of FY25
Task 1.9: Emissions (Year 2)	50%	Complete by end of FY25
MeOH ICEs (Years 3 & 4)		Start in FY26

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

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SUMMARY

Objectives

- Develop predictive CFD modeling tools and simulation best practices for the design of future ICEs for off-road applications utilizing alternative fuels like Hydrogen (H_2) and Methanol (MeOH).

Approach

- Task 1 on H_2 ICE modeling (Year 1 & 2) followed by Task 2 on MeOH ICE modeling (Year 3 & 4).
- For Task 1, we use DNS calculations (Nek5000) to improve RANS CFD models (CONVERGE).

FY25 Technical accomplishments

- New RANS mixing model developed based on DNS and demonstrated in engine simulations.
- G-Equation combustion model improved based on DNS and demonstrated in engine simulations.
- Conjugate Heat Transfer (CHT) calculations completed (significantly improved engine simulations).
- Near-wall flame quenching characteristics evaluated using DNS.
- NO_X emission model performance evaluated in engine simulations.
- Focus shifted over abnormal combustion (pre-ignition leading to knock).

Future work *

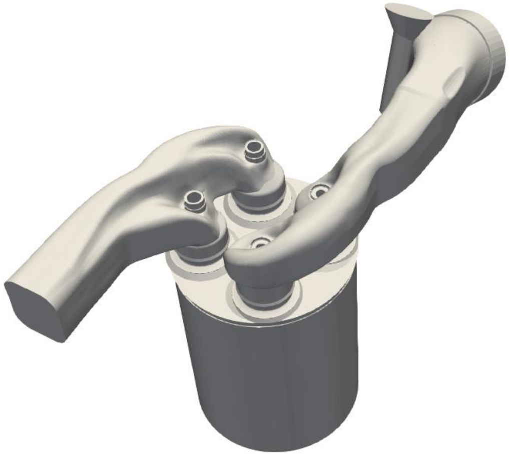
- Complete best-practices for CHT calculations to achieve faster turnaround time.
- Complete abnormal combustion studies (pre-ignition, knock) and NO_X chemistry evaluation.
- Wind Task 1 (H_2 ICEs) down and start Task 2 (MeOH ICEs)

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

TECHNICAL BACKUP SLIDES

TECHNICAL BACKUP SLIDES

Engine specs and operating conditions evaluated in this project



Engine Parameter	Specifications
Bore	170 mm
Stroke	250 mm
Compression Ratio	13:1
Engine speed	1500 rpm
Air/Fuel Ratio	2.5 < λ < 3.5

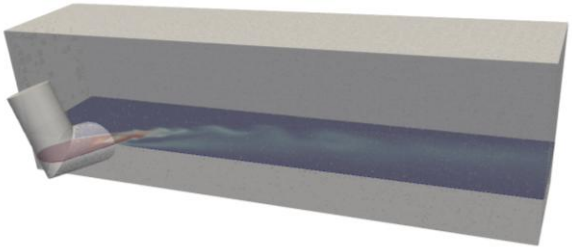
Test case #	Description
1	High-load, nominal λ (lean)
2	Moderate-load, nominal λ (lean)
3	High-load, increased λ (ultra-lean)

TECHNICAL BACKUP SLIDES

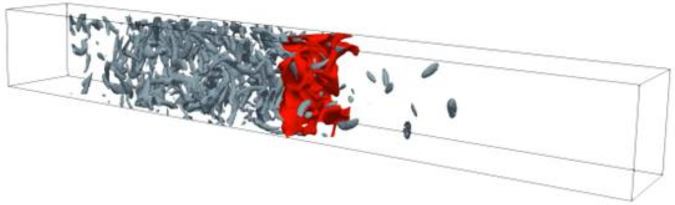
Summary of Numerical Configurations, CFD tools, and Methods

- Real engine

- Simplified intake port



- Turbulent premixed flame in a box



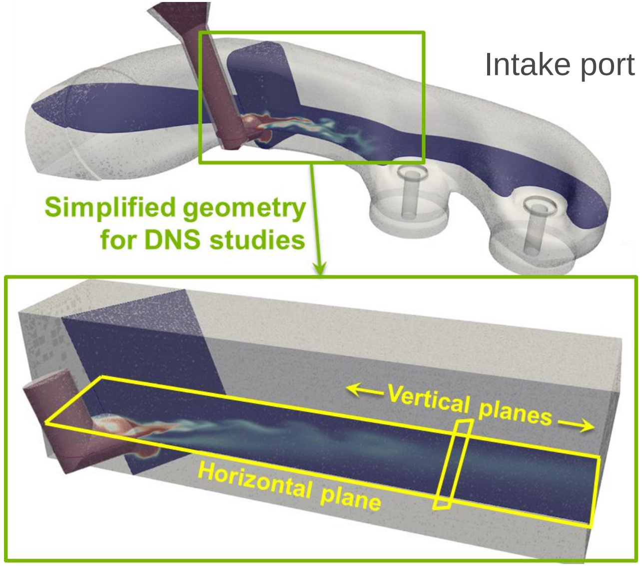
Numerical approach	RANS	LES	DNS
CFD solver	**CONVERGE 4.0**		**Nek5000**
Turbulence model	RNG *k-ε*	Dynamic Structure	None
Combustion model	Well-stirred reactor (WSR) and G-Equation (G-EQN)		Finite rate chemistry
Transport model	Mixture-averaged model to account for differential diffusion		
Chemical kinetics model	UCSD mechanism (11 species, 23 reactions)		
Grid control	Fixed embedding + Adaptive Mesh Refinement (AMR)		Non-uniform mesh

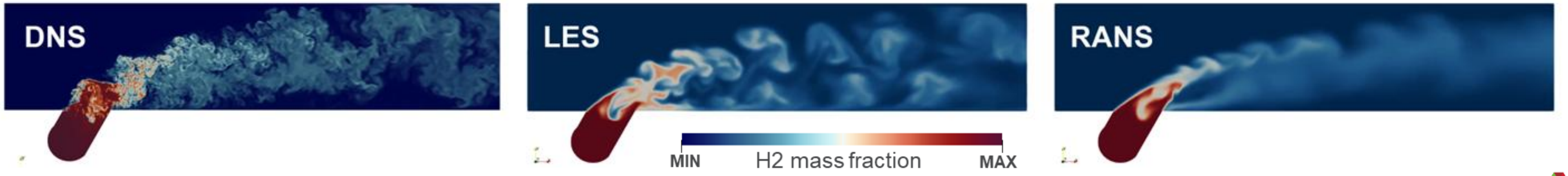
Re = Reynolds Number
CPU = Central Processing Unit

High-fidelity DNS-Nek5000 based on simplified intake port geometry

- Designed a simplified geometry that maintains same flow characteristics as in real engine intake port.
  - Reduced Re number: Re_{jet}=4600, $Re_{crossflow}$=22,000
- DNS performed using Nek5000.
  - Min cell size: 50 um, $y^+ \approx 1$, 93 M grid points
  - 60 hours per flow through time (FTT) using 2560 CPUs
  - 10 FTT needed to collect statistical quantities
- LES and RANS performed both using CONVERGE.

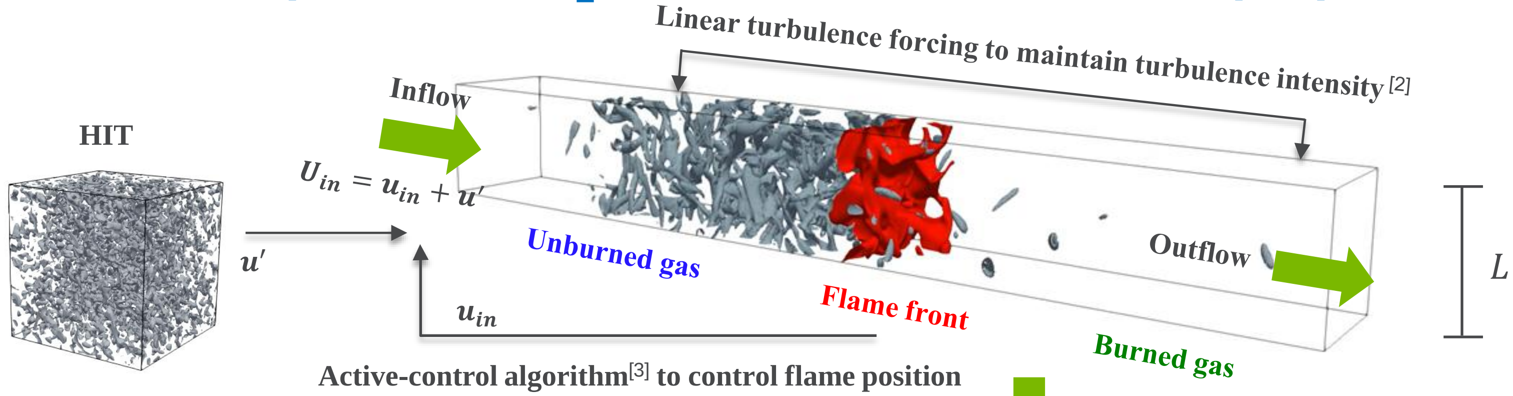
	Min cell size (um)	Grid points (M)	Wall time per FFT (h)	CPU numbers
LES	125	8.9	131	432
RANS	250	1.3	16	216





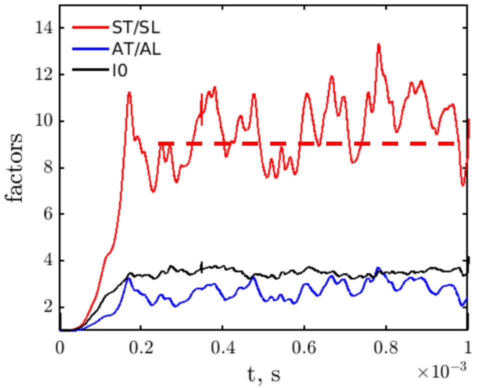
TECHNICAL BACKUP SLIDES

DNS of turbulent premixed H_2/air flames with Nek5000 (1/2)



$$S_T = \frac{1}{\rho_u Y_{H_2,u} A_L} \int_V \dot{\omega}_{H_2} dV$$

- Statistically-planar turbulent premixed flames propagate in a 3D box with L×8L×L
- Detailed chemical mechanism (11 species) and transport model (mixture-averaged transport)
- 56 M cells, 50 hrs simulation time (2560 CPUs) each case
- T_0, P_0 and ϕ are based on engine simulations



[1] Y. Wang, et al., CSSCI, Cleveland, 2024
[2] B. Bobbitt, et al., Phys. Fluids, 2016
[3] J. Bell, et al., Comm. App. Math. Com. Sc., 2007

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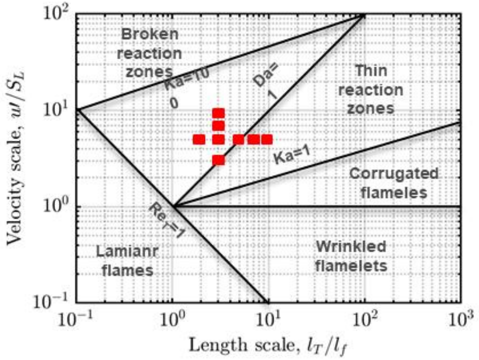
TECHNICAL BACKUP SLIDES

DNS of turbulent premixed H_2/air flames with Nek5000 (2/2)

- Lean premixed H_2/air mixture at high temperature and pressure
- UCSD mechanism with 11 species and 23 reactions
- Uniformly distributed spectral elements with a polynomial order of five, ensuring at least 12 grid points per laminar flame thickness

Borghi-Peters regime diagram



Case	u'/S_L	l_T/l_f	Ka	Da	Re_T	η [μm]	$k_{max}\eta$
L2	5	2	7.91	0.4	39.5	2.15	4.81
L3	5	3	6.46	0.6	59.3	2.37	5.33
L4	5	4	5.59	0.8	79.0	2.55	5.72
L6	5	6	4.56	1.2	118.5	2.82	6.34
L9	5	9	3.73	1.8	177.8	3.13	9.35
U3	3	3	3.00	1.0	75.1	3.48	7.81
U5	5	3	6.46	0.60	59.3	2.37	5.33
U7	7	3	10.69	0.43	83.0	1.84	4.14
U9	9	3	15.59	0.33	106.7	1.52	3.43

Grid convergence study

number of grids per l_f	15	12	9
S_T/S_L	9.89	9.95	9.43
A_T/A_L	2.79	2.84	2.71
I_0	3.54	3.51	3.48

Ka: the Karlovitz number

η: the Kolmogorov length scale

Da: the Damkhöler number

k_{max}: the maximum wavenumber magnitude

$Re_T = u' l_T/\nu$: the turbulent Reynolds number

$k_{max}\eta$ > 2 means we are adequately resolved