PURDUE UNIVERSITY | School of Aeronautics and Astronautics

Argonne NATIONAL LABORATORY

Hierarchically Informed Engineering Models For Predictive Modeling of Turbulent Premixed Flame Propagation in Pre-chamber Turbulent Jet Ignition

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DOE program managers — Michael R. Weismiller

June 22, 2022

2022 DOE Vehicle Technologies Office Annual Merit Review Virtual Meeting

This presentation does not contain any proprietary, confidential, or otherwise restricted information

Project ID: ACE151

Overview

Timeline

Start	Jan 1, 2020
End	June 30, 2023
Budget period 2	July 1, 2021-June 30, 2022
Complete	~85% of budget period 2

Budget

Total Award	$1,093,781
Purdue	$650,000
Argonne (FFRDC)	$225,000
Cost share (20%)	$218,781
Budget period 2	$347,789

Partners

- Purdue University
- Argonne National Laboratory

Barriers

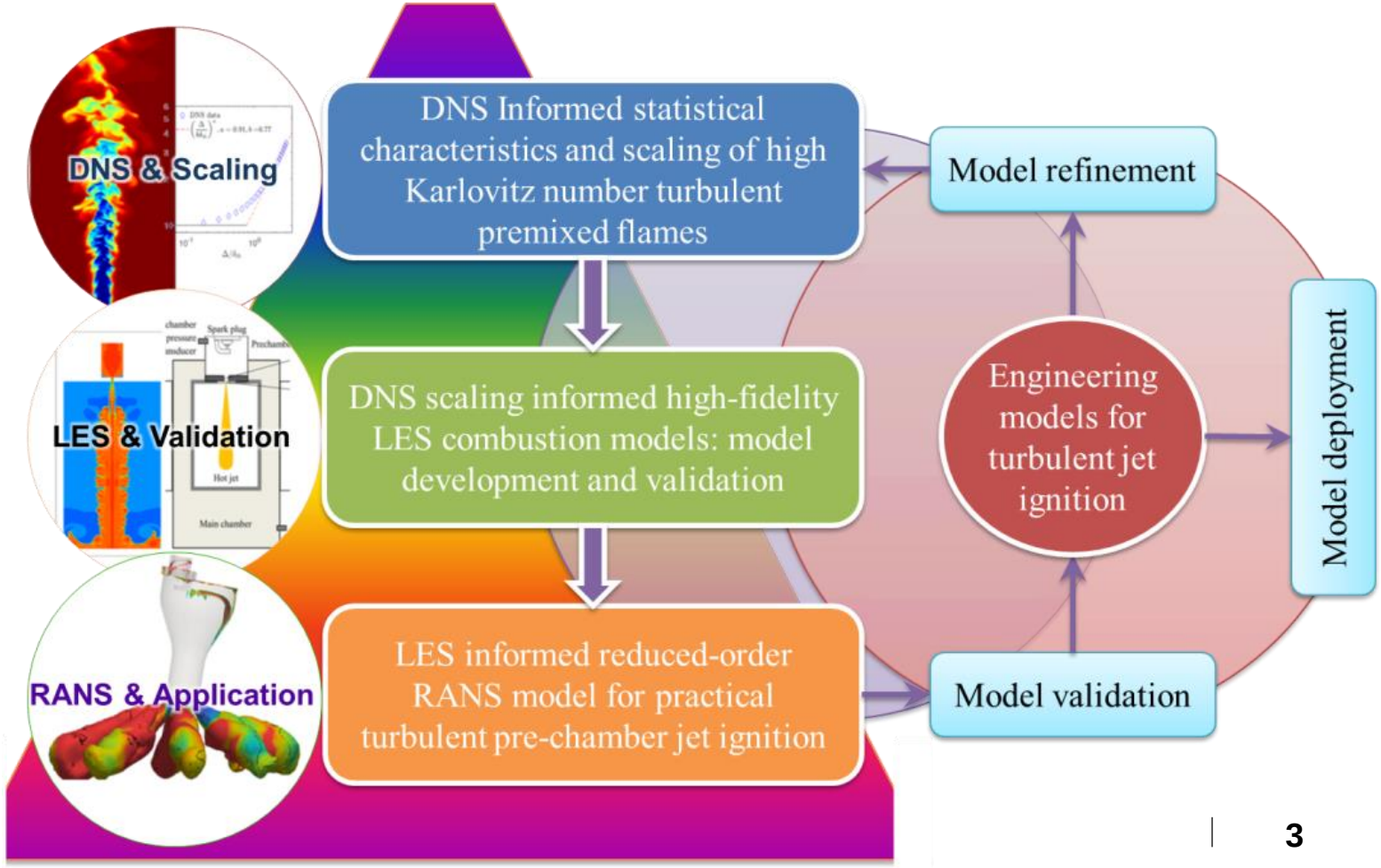
- "Understanding and robust modeling tools for rapidly screening proposed designs based on sound metrics are lacking" — U.S. DRIVE roadmaps
- "More robust ignition systems for lean and EGR, as well as boosted conditions that reduce combustion variability are needed" — U.S. DRIVE roadmaps
  - While electrification is taking over the LD/MD (maybe even HD) on-road markets, pre-chamber ignition is still an enabling technology for future ICEs for off-road, rail, and possibly even marine and (perhaps) on-road engines.
  - Pre-chamber ignition is also being evaluated as an enabling technologies for the use of H2 as an engine fuel in these sectors.
- This work overcomes these barriers by developing accurate and efficient models for turbulent flame propagation initiated by a pre-chamber turbulent jet ignition source.

Relevance

Project Goal

Significantly improve the predictive accuracy and efficiency of turbulent combustion sub-models for the simulations of premixed flame propagation initiated by pre-chamber turbulent jet ignition.

- Objective 1: Acquire statistical properties of high-Karlovitz turbulent premixed flames from direct numerical simulations (DNS) to provide theoretical basis for pre-chamber turbulent jet ignition (TJI) model;
- Objective 2: Develop high-fidelity large-eddy simulation (LES) model for TJI to yield consistency with the acquired statistical properties from DNS;
- Objective 3: Develop engineering Reynolds-averaged Navier-Stokes (RANS) model for TJI through machine learning by using data from high-fidelity LES.



A hierarchically informed engineering model for turbulent flame propagation

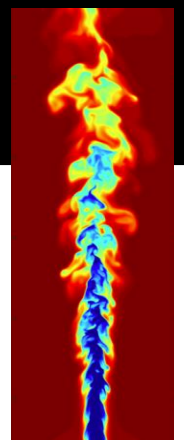
Milestones

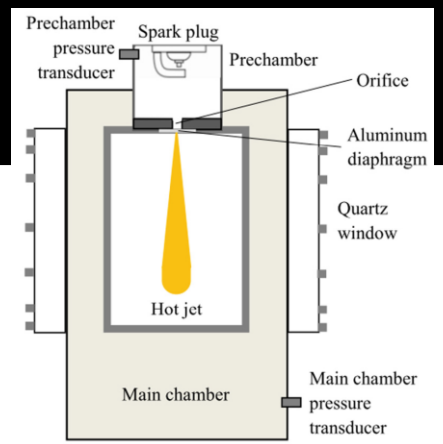
budget period 2, July 1, 2021-June 30, 2022

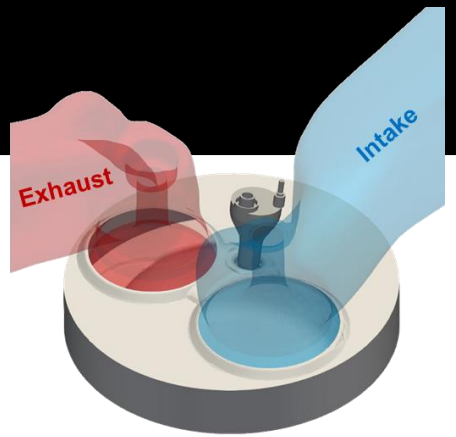
Milestone	Type	Description	Status
A posteriori testing of the mixing frequency model is complete	Technical Q1	The mixing frequency model informed by the power-law scaling observed in DNS has been incorporated in actual LES and *a posteriori* testing of the model has been completed to further validate the accuracy of the model.	95% completed
Development of high-fidelity LES model for TJI is complete	Technical Q2	The development of LES model for combustion in TJI systems has been completed.	Completed
Validation of the developed high-fidelity LES model for TJI in Purdue model TJI rig is complete	Technical Q3-Q4	The model components based on the power-law scaling have been integrated together and the model validation in the Purdue model TJI rig has been finished.	80% completed
A high-fidelity LES combustion model for TJI has been developed and validated	Go/No Go	A targeted high-fidelity predictive LES combustion model for TJI has been achieved to provide a tool for the reduced-order model development afterward. The model has been validated against the Purdue model TJI rig to reproduce the measured characteristics of the TJI rig including but not limited to the pressure rising history in pre-chamber and main chamber and the ignition timing. An overall error of the model prediction relative to the measurements within 30% is targeted.	On schedule

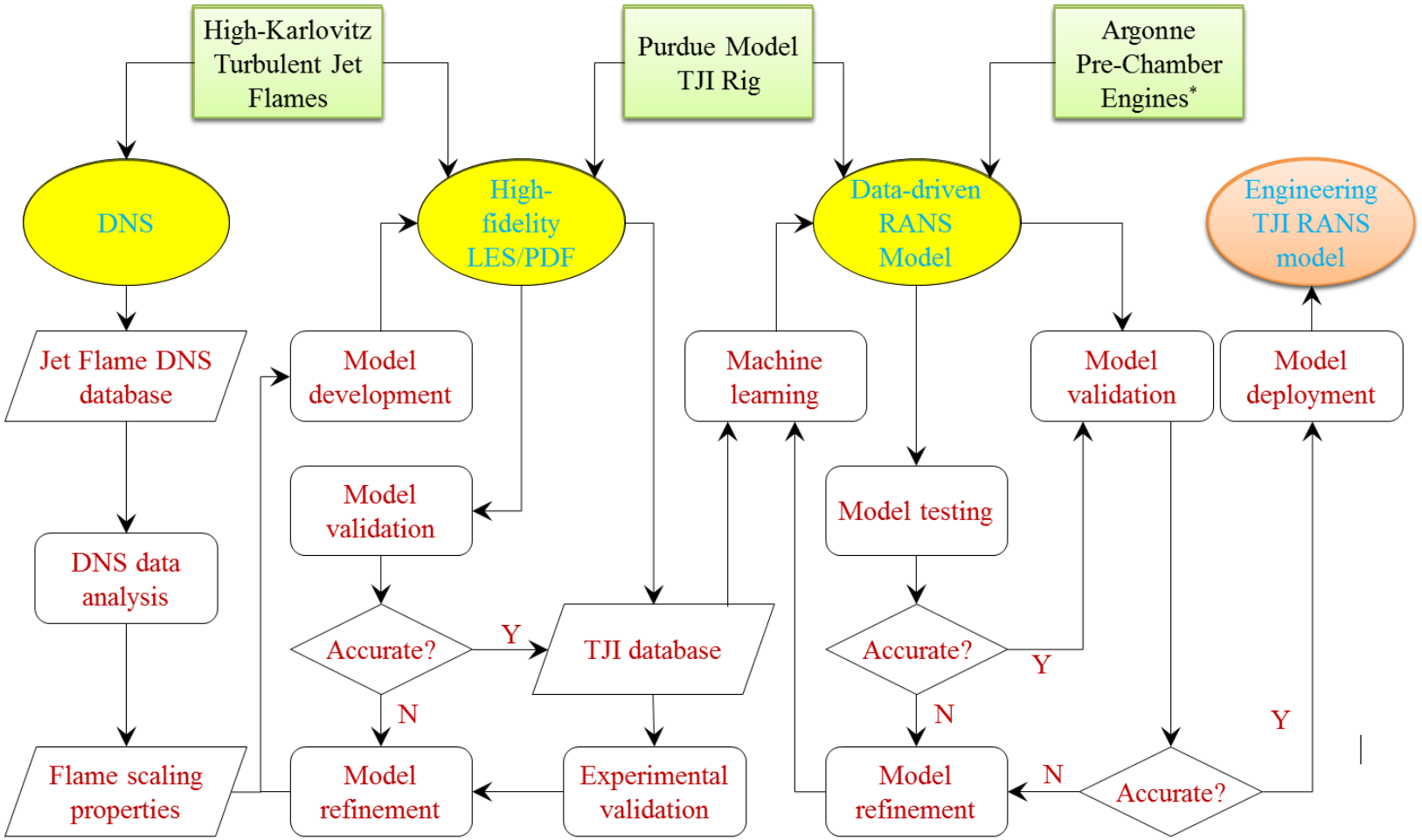
Approach

- **Three levels of model descriptions**
  - Direct Numerical Simulations (DNS)
  - Large-eddy simulations and probability density function (LES/PDF)
  - Reynolds-averaged Navier-Stokes (RANS)
- **Three levels of testing complexities**
  - Sandia premixed jet flame DNS case
  - Purdue model TJI rig
  - Argonne MD single cylinder engine with TJI
- **One model target**
  - Engineering TJI RANS model









Approach

- **Stochastic modeling of turbulent combustion with LES/PDF**
  - Detailed chemical kinetics incorporated in turbulence without modeling requirement
  - Machine learning assisted mixing model

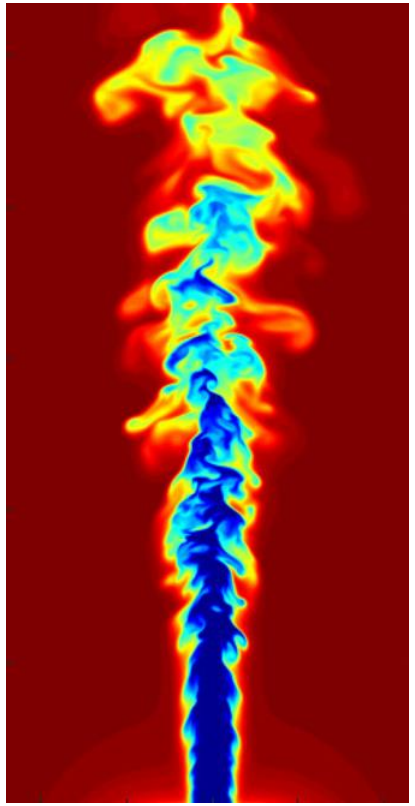
$$F = 1 + \left(\frac{\Delta}{b\delta_{th}}\right)^a$$

Empirical model:

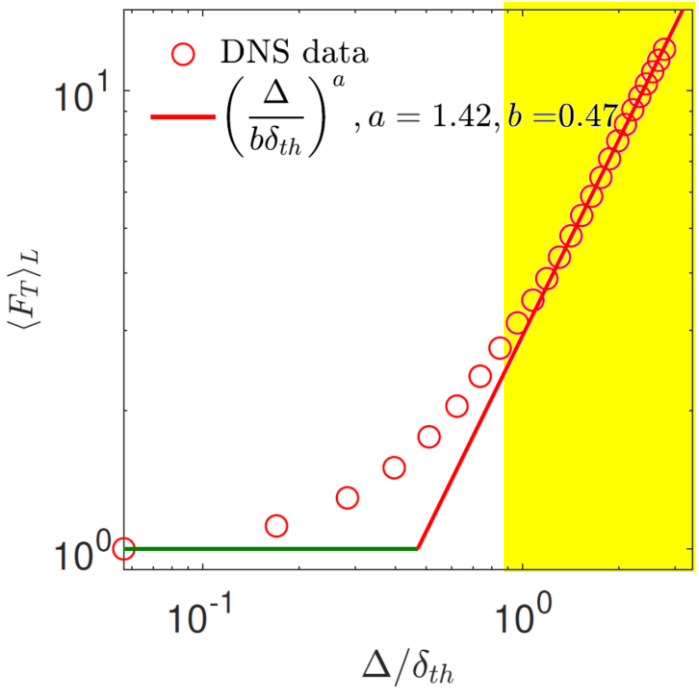
$$a = 1.72, b = \min\left(C_{b1}, \left(\frac{C_{b2}}{Ka}\right)^{\frac{1}{a}}\right)$$

Machine learning:

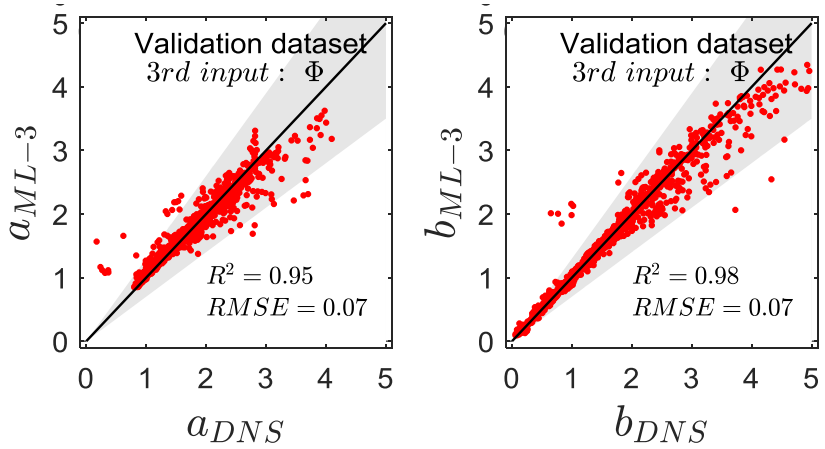
$$a \text{ or } b = f(Re, Ka, \Phi)$$

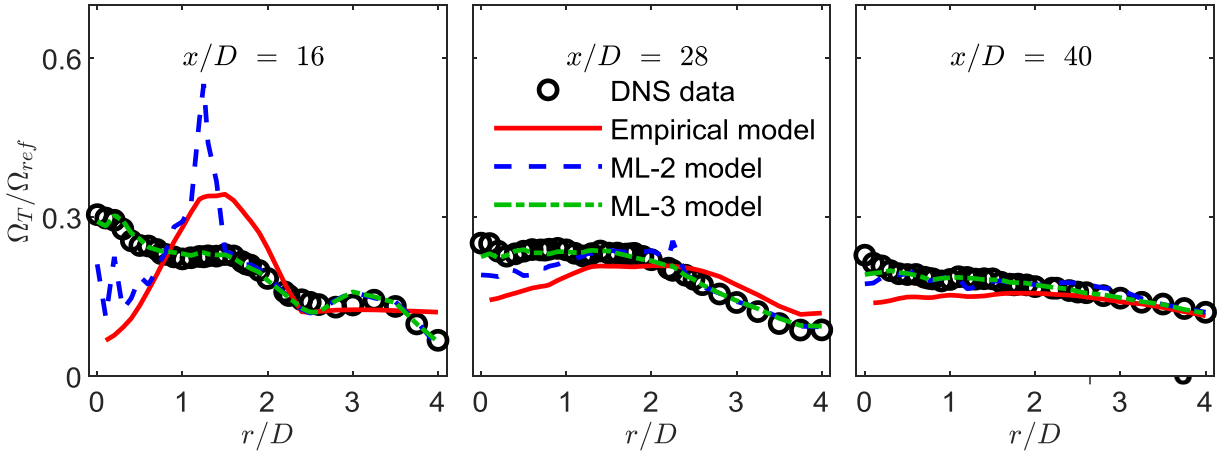


(Wang et al. Combust. Flame, 180 (2017), 110)



$$F \sim \left(\frac{\Delta}{\delta_{th}}\right)^a \quad \text{if } \Delta \gg \delta_{th}$$





Approach

- **Machine learning for turbulent reaction rate modeling**

A+B → C+D A:deficent

$$\frac{dY_A}{dt} = -\frac{Y_A}{\tau_c}$$

A new chemical time scale model

$$\tau_C = F \cdot \tau_A$$

τ_A: effect of chemical kinetics
F: effect of turbulence

Arrhenius reaction rate (laminar chemistry model)

$$\dot{\omega} = k[A][B] = \kappa\left(\frac{\rho Y_A}{W_A}\right)\left(\frac{\rho Y_B}{W_B}\right)$$

$$\kappa = \hat{A}T^{\beta}\exp\left(-\frac{E}{RT}\right)$$

$$\frac{dY_A}{dt} = -\frac{aW_A\dot{\omega}}{\rho} = -\frac{Y_A}{\tau_A} \qquad \tau_A = \frac{\rho Y_A}{aW_A\dot{\omega}}$$

Eddy dissipation model

$$\frac{dY_A}{dt} = -\frac{Y_A}{\tau_m} \qquad \tau_m = \frac{4k}{\varepsilon}$$

High-fidelity TJI modeling data → $F_{True} = \tau_C/\tau_A$

↓

Machine Learning → $F_{ML} \cdot \tau_A = \tau_C$

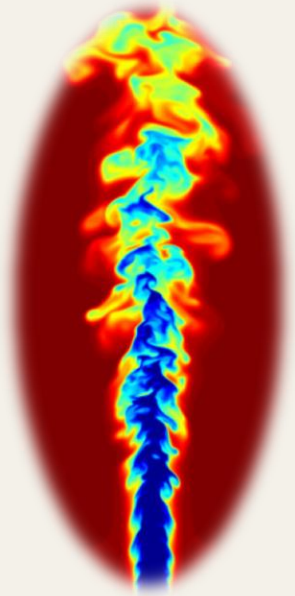
↓

TJI engineering model

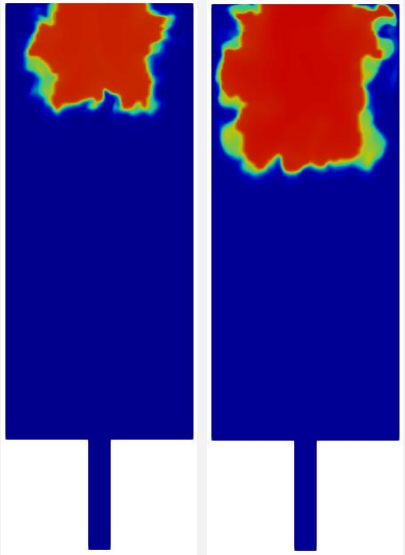
Technical Accomplishments and Progress

- **Work conducted during Budget Period 2**

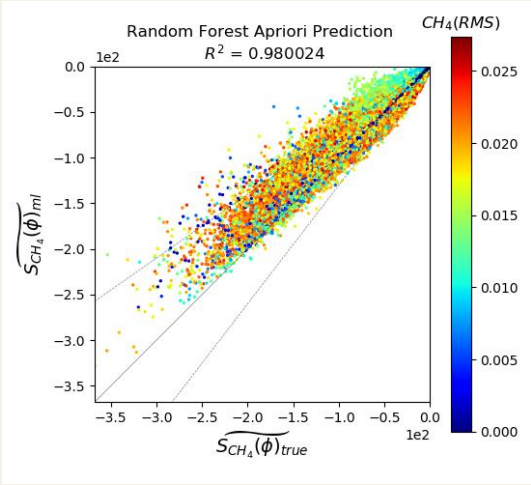
A posteriori testing of machine learning assisted mixing model



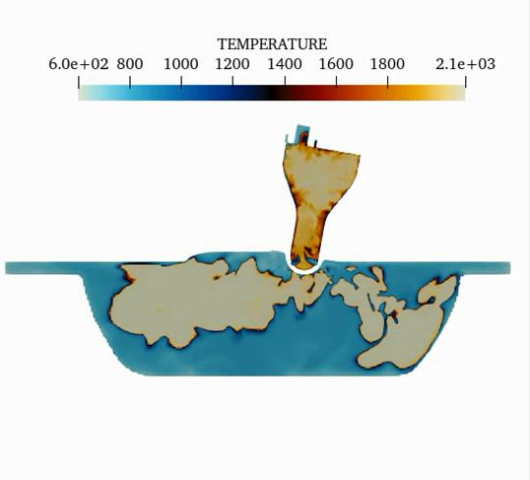
High-fidelity model validation in Purdue model TJI rig



Machine learning assisted combustion modeling

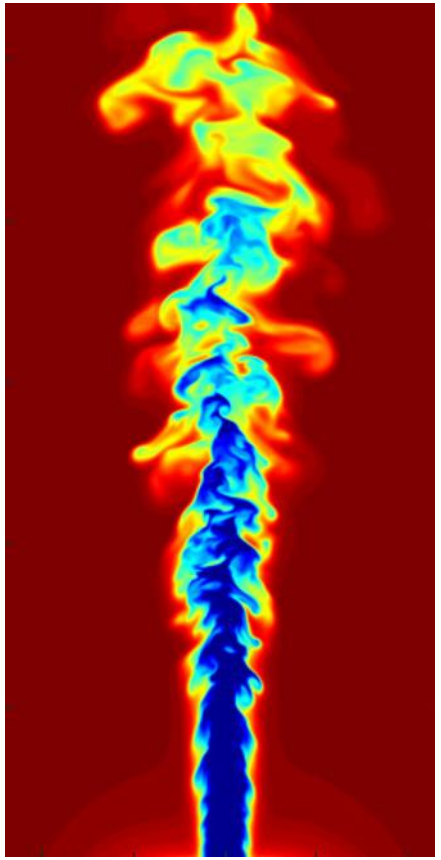


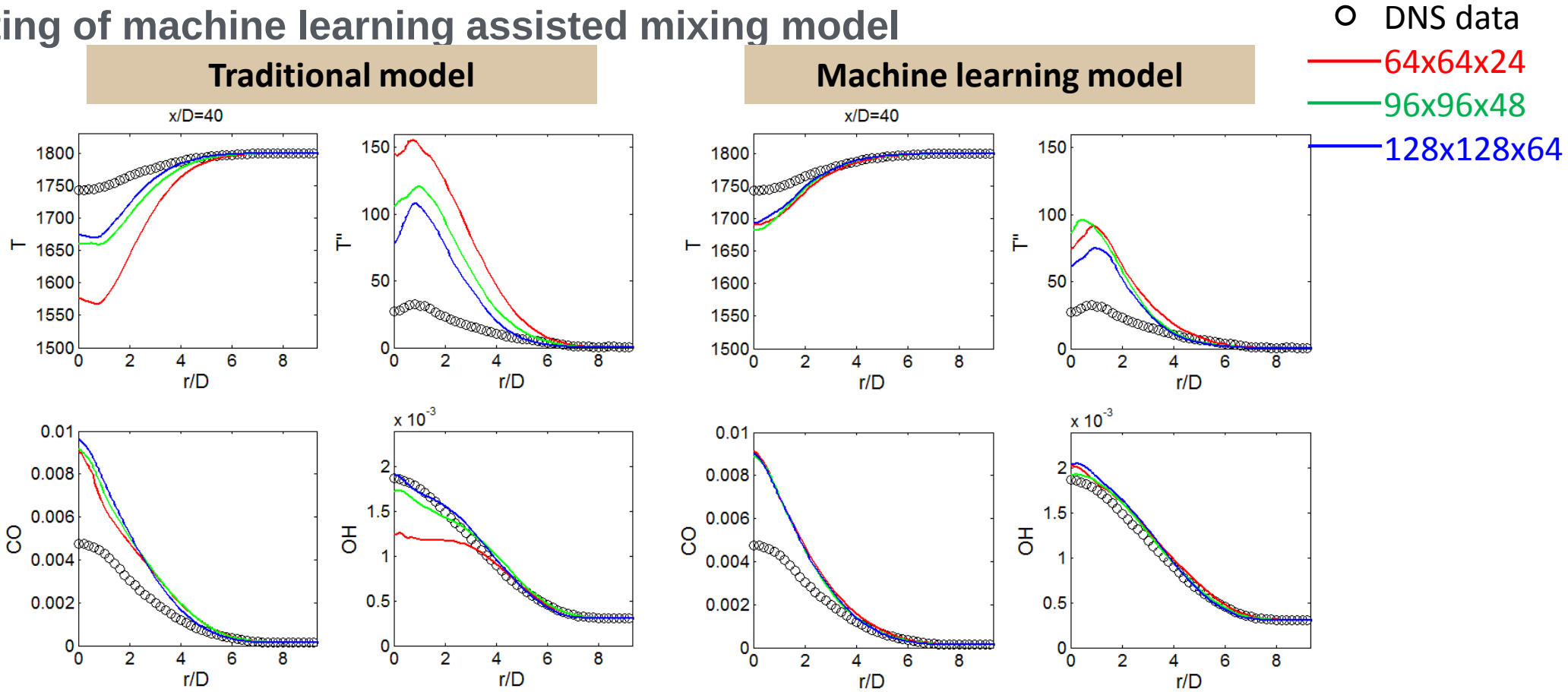
CONVERGE CFD benchmark of Argonne TJI engine



Technical Accomplishments and Progress

A posteriori testing of machine learning assisted mixing model

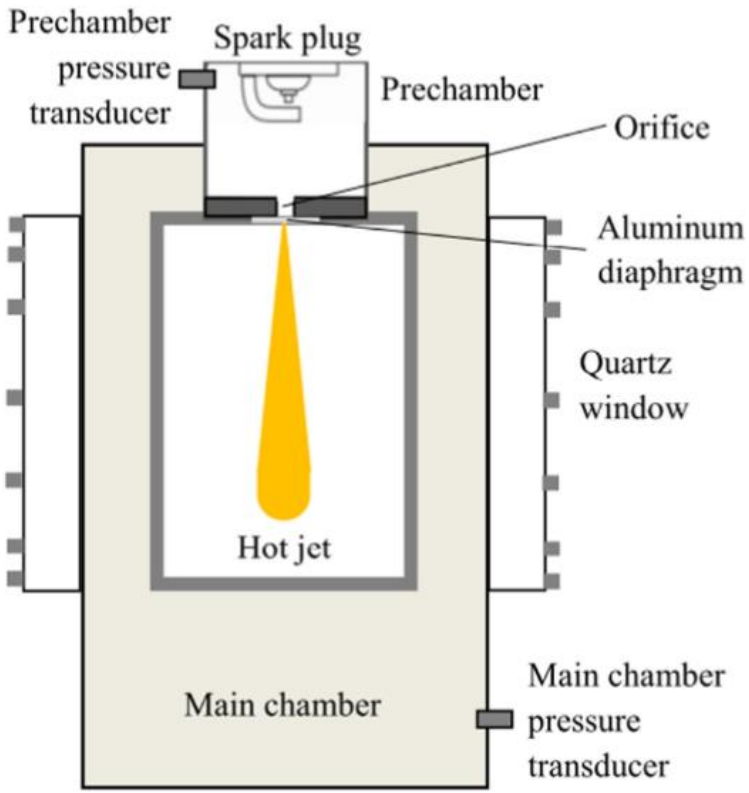




- Machine learning assisted mixing model improve coarse grid results
- Promise of the machine learning mixing model for premixed combustion modeling
- Remaining discrepancy is under-investigation.

Technical Accomplishments and Progress

Further model validation in Purdue TJI rig (under more relevant condition)



(Biswas et al. Applied Thermal Engineering, 2016, 106:925)

$$E_{spk} = \frac{\rho\epsilon}{4\pi^2\Delta_{spk}^3\tau_{spk}}\exp\left(-\frac{1}{2}\frac{\left(\vec{x}-\vec{x}_{spk}\right)^2}{\Delta_{spk}^2}\right)\exp\left(-\frac{1}{2}\frac{(t-t_m)^2}{\tau_{spk}^2}\right)$$

(Lacaze et al., C&F, 2009, 156:1993)

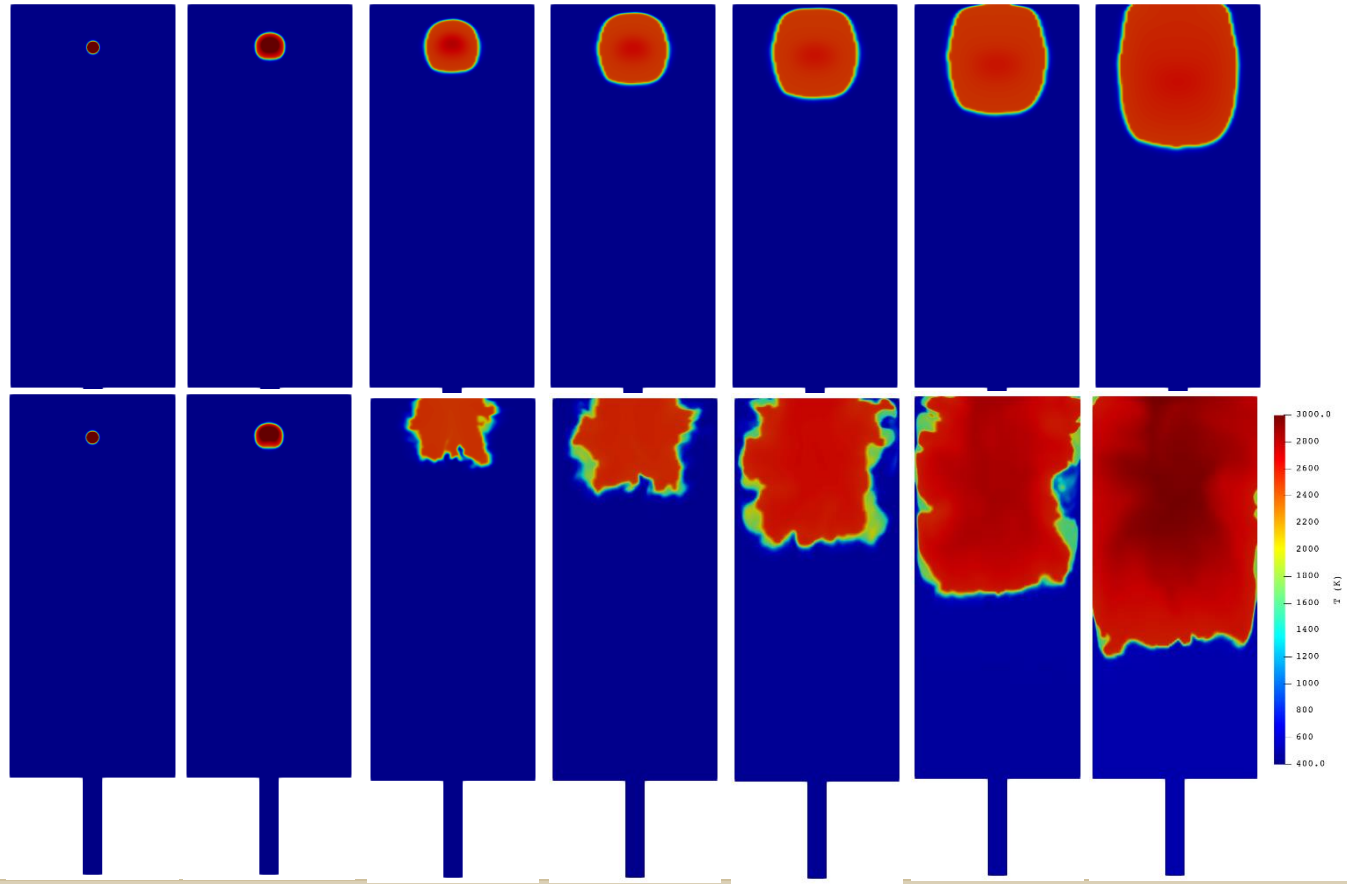
- **Numerical and model setup**
  - OpenFOAM (LES with Smagorinsky turbulence model)
  - Transported PDF method (stochastic fields)
  - IEM mixing model
  - Machine learning assisted mixing model
  - Global chemistry CH4+2O2➔CO2+2H2O
  - Spark model: energy deposition model
  - Pre-chamber simulation (reported here)
  - Main chamber simulation (in-progress)
  - Unstructured grid (1 million cells for pre-chamber, 3.5 million total)

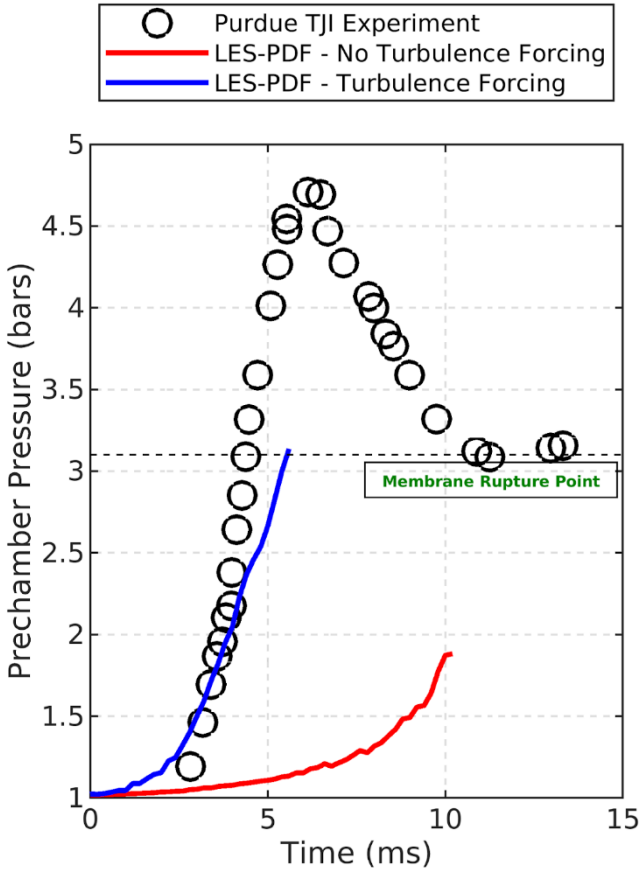
Technical Accomplishments and Progress

Further model validation in Purdue TJI rig

W/O turbulence forcing

With turbulence forcing



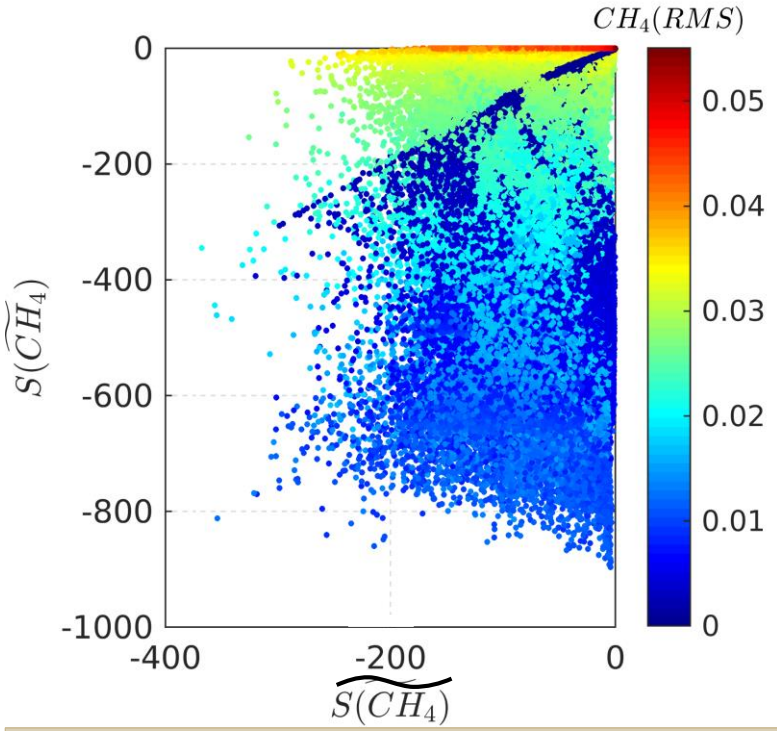


- Turbulence forcing is needed to allow transition from quiescent to turbulence (due to the limitation of turbulence model and spark model)
- The flame propagation is more plausible after turbulence forcing.
- The pressure growth is reasonably captured with turbulence forcing.

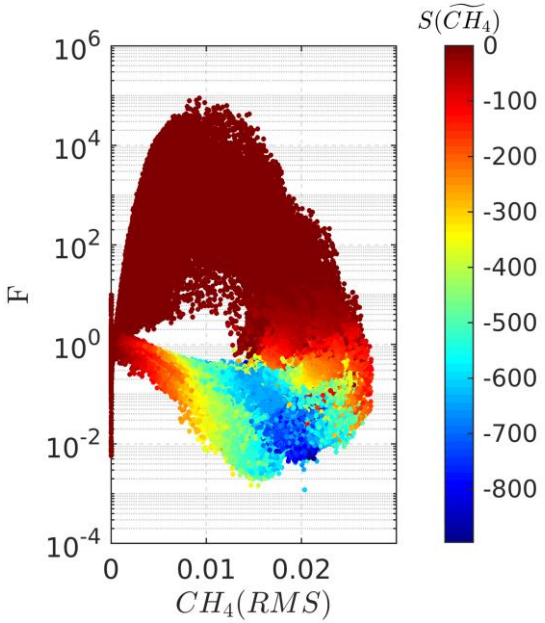
Technical Accomplishments and Progress

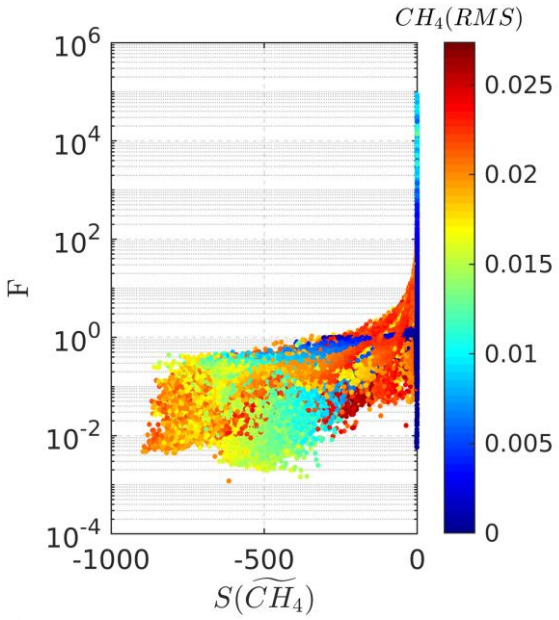
Machine learning assisted combustion modeling: a preliminary analysis

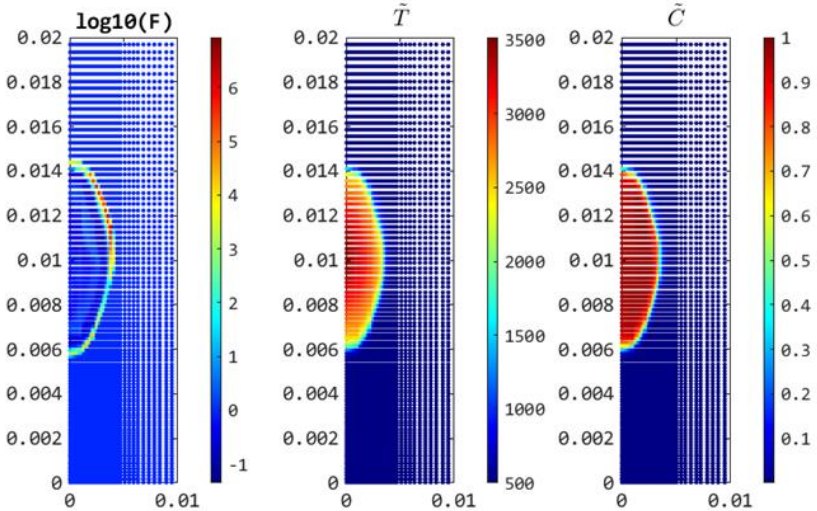
LES/PDF pre-chamber simulation



$$F_{True} = \frac{S(\widetilde{CH_4})}{S(\widetilde{CH_4})}$$





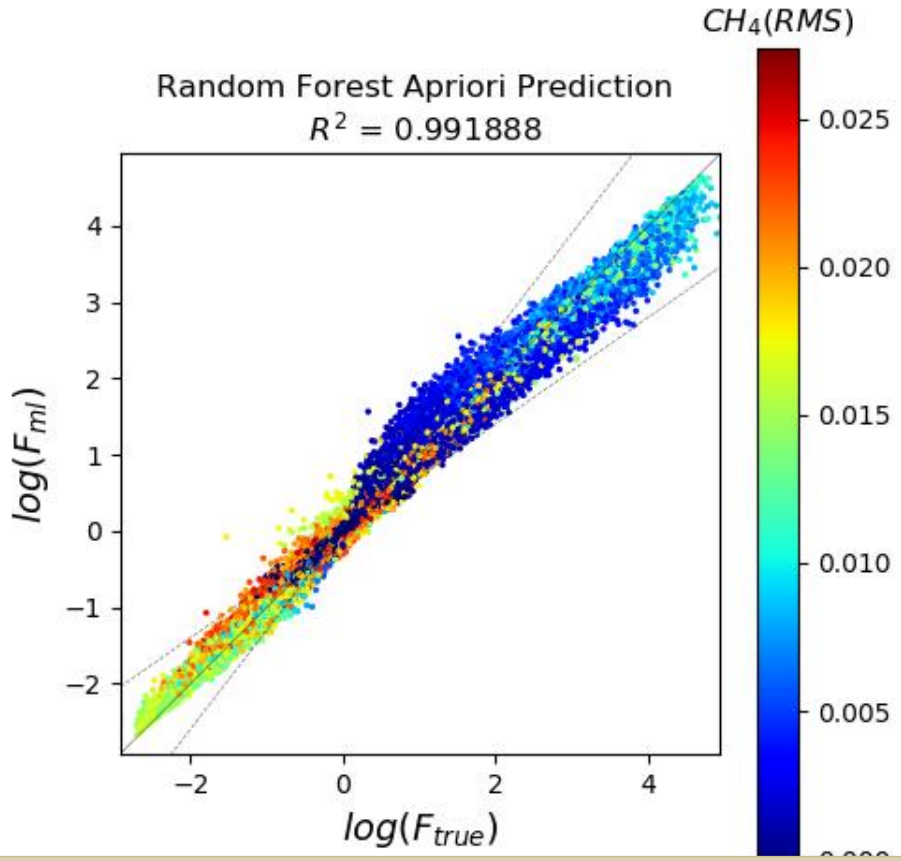


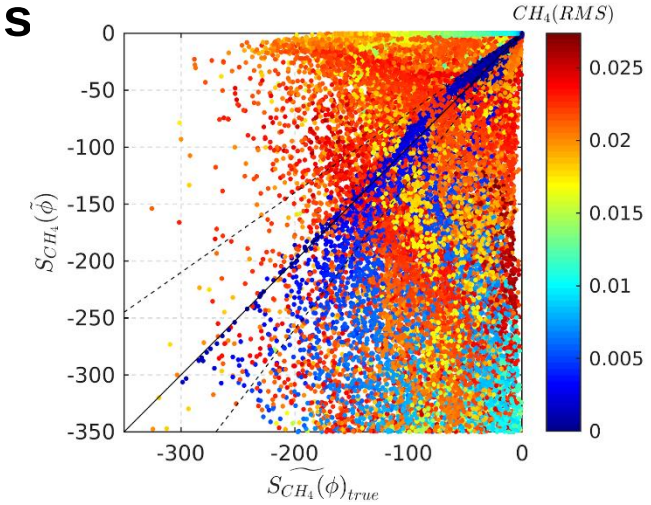
- Laminar chemistry model $S(\widetilde{CH_4})$ is very problematic
- F varies significantly (eight orders of magnitude difference)
- The variation is mainly near the flame front in a narrow region where turbulence-chemistry interaction is strong

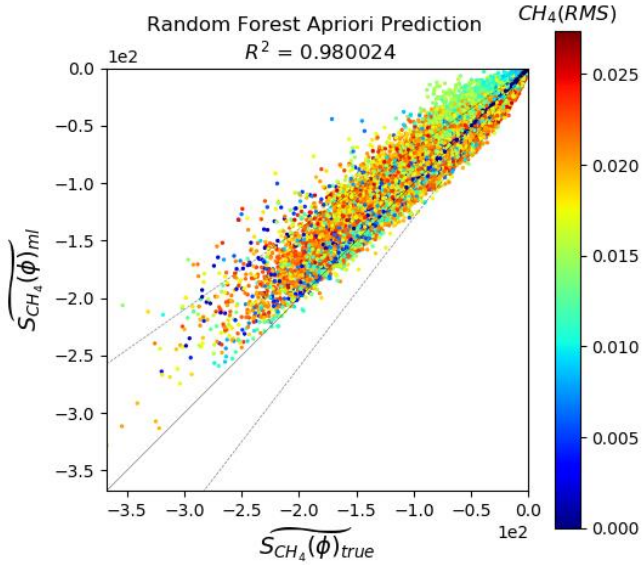
Technical Accomplishments and Progress

Machine learning assisted combustion modeling: a preliminary analysis

- **Machine learning approach for modeling F**
  - Random forest algorithm
  - Input features (15 parameters)
  - Pre-chamber data for the preliminary analysis







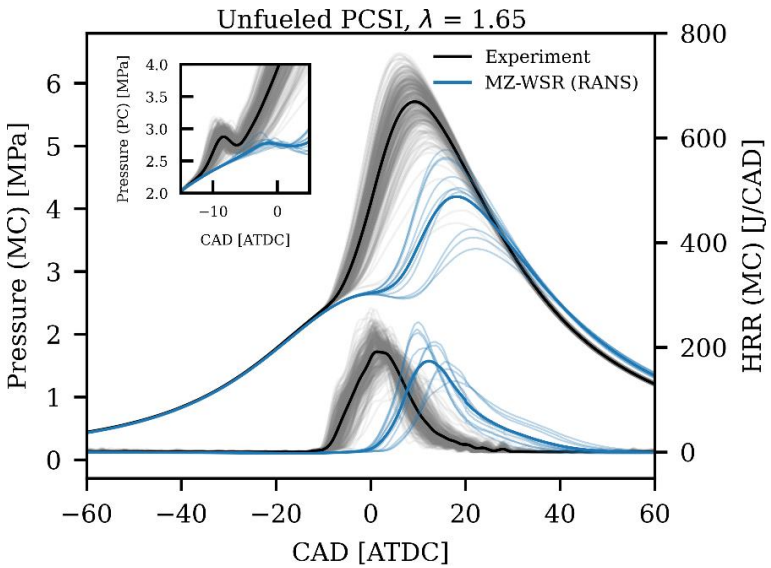
- Promising to use machine learning to produce better prediction for turbulent reaction rate (compared to laminar chemistry model)
- ML error ~ $\pm 30\%$
- Add ~10% computational cost to laminar chemistry model

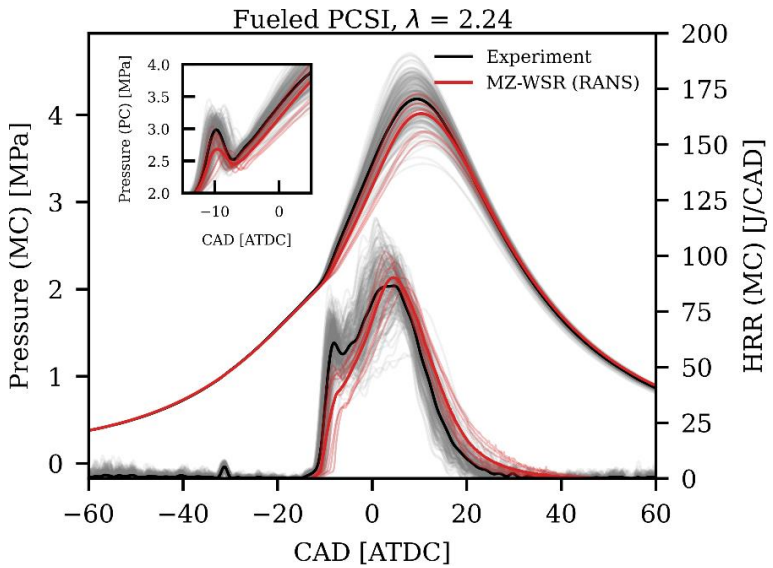
Technical Accomplishments and Progress

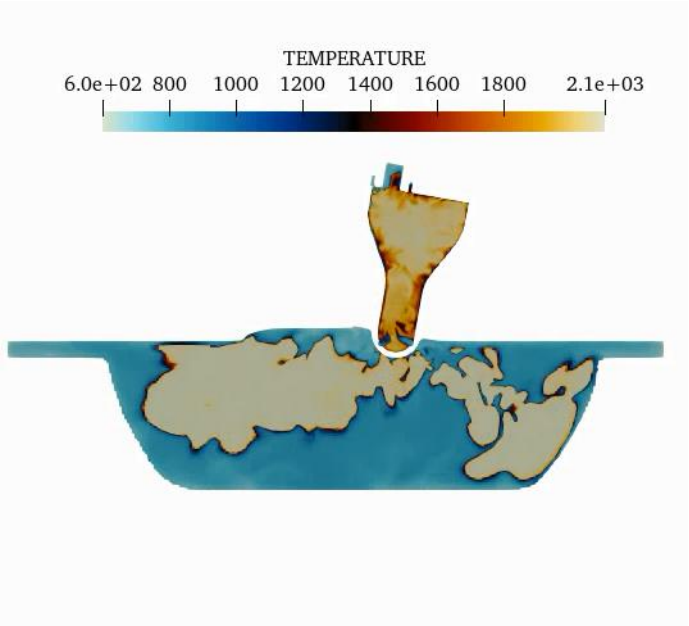
Benchmark CFD simulations completed for both active (fueled) and passive (unfueled) PCSI conditions

		Unfueled PC		Fueled PC	
Engine speed	rpm	1200			
Intake boost pressure	bar	1.16		1.04	
Exhaust back pressure	bar	0.98		0.98	
Spark ignition timing	CAD aTDCf	-17		-17.5	
Excess-air ratio (λ_{intake})	-	1.50	1.65	1.91	2.24
Fuel ratio of PC/Intake	%	-	-	2.2, 4.1, 6.6	7.7
Engine load (nIMEP)	bar	8.1	7.6	5.4, 5.5, 5.7	4.7

- Benchmark RANS simulations performed using the commercial solver CONVERGE CFD.
- Good agreement between simulations and engine data for fueled PC conditions.
- PC combustion rate under-prediction was observed for unfueled PC conditions.



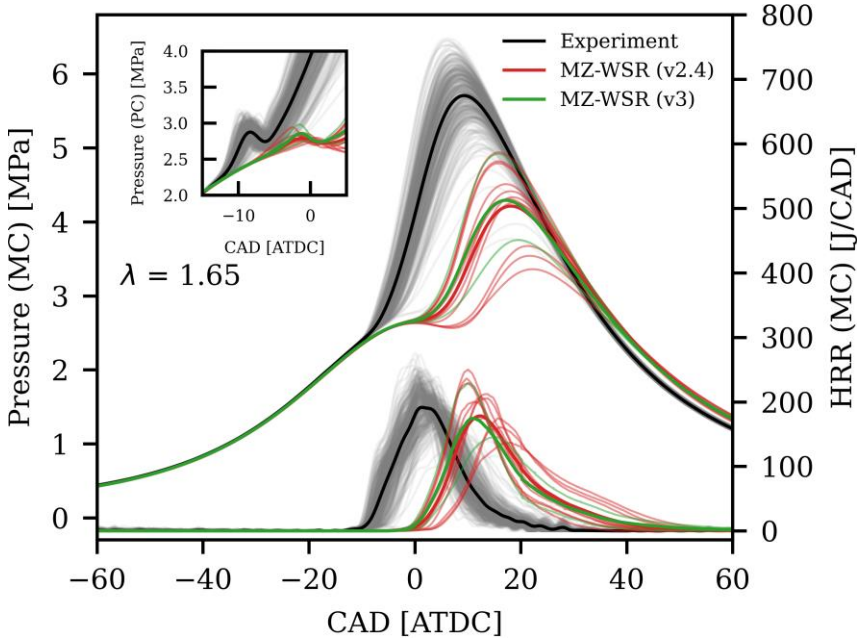


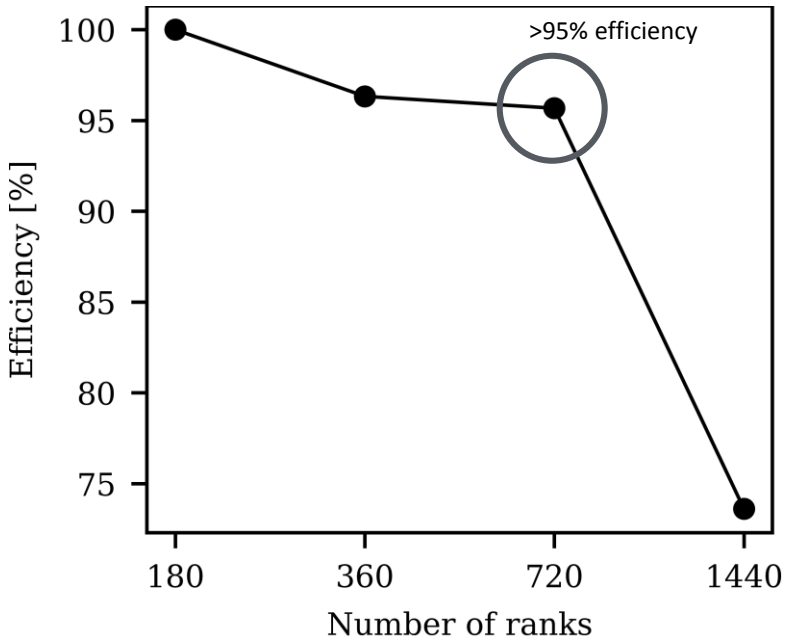


Technical Accomplishments and Progress

Updates to the existing CFD framework

- CONVERGE CFD v3.0 was utilized with improved computational performance and scaling.
- Similar simulation results were obtained with respect to v2.4, with x4 performance increase:
  - **V2.4:** 42-82 hrs/cycle (unfueled-fueled). **V3.0:** 9-20 hrs/cycle (unfueled-fueled).
  - Scaling performance around 95% was observed for up to 720 processors with v3.0.
- User Defined Function (UDF) structure changed to v3.0 for future model implementation.



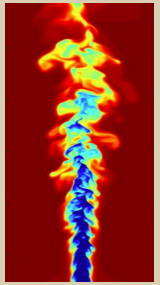


Responses to Previous Year Reviewers' Comments

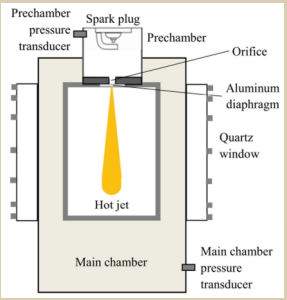
- This project was NOT reviewed last year but in 2020
- "*the newly developed model should be validated based on experimental results, in addition to DNS.*" The simulations for the Purdue TJI rig and the Argonne engine will be validated against the available experimental data.
- *"will the proposed power-law scaling account for turbulence-chemistry interaction in the RANS framework?"* Yes, it will.
- "*feedback for each simulation to improve the sub-models being investigated was lacking.*" (1) the use of machine learning to enhance power-law scale mixing model; (2) prototype model will be tested in Argonne test case to grain feedback for iterative improvement.
- *"how much more effort should we be putting into RANS model?"* The ultimate model is a RANS model and will be tested in CONVERGE. It will be the focus of Budget Period (BP)3.
- *"It would be good to show a comparison of predictions of a flame with and without the addition of the power-law scaling."* This is done in the current BP2.
- *"most engine combustion conditions are under high pressure … The power-law scaling model seems to be overly simplified, …"* C&F 2021(231): 111500
- "*Sandia is also listed a partner… How do they fit in*" The collaboration with Sandia is mainly the use of the DNS database for high-Ka flame for this study (BP1).
- *"Strengthen the collaborations with the auto OEMs or other companies who are working on TJI."* Will encourage more OEM users when the targeted model is deployed.
- "*See some alternate development pathways*" feasibility of the proposed model is much higher compared 2 years ago
- "when work with the engineering level simulation will be undertaken?" BP2 and BP3, especially the later.
- "Will ANL also simulate the TJI rig?" No, the TRI rig will only be used to validate high-fidelity model. The targeted RANS model will be tested in the Argonne engine by ANL.
- *"In order to improve the sub-model development, experimental data validation at high pressure and high EGR conditions is needed for DNS."* We do have experimental data to validate LES and RANS models

Collaboration and Coordination with other Institutions

Sandia National Lab (J.H. Chen)
Zhejiang University (H. Wang)
University of New South Wales (E.R. Hawkes)

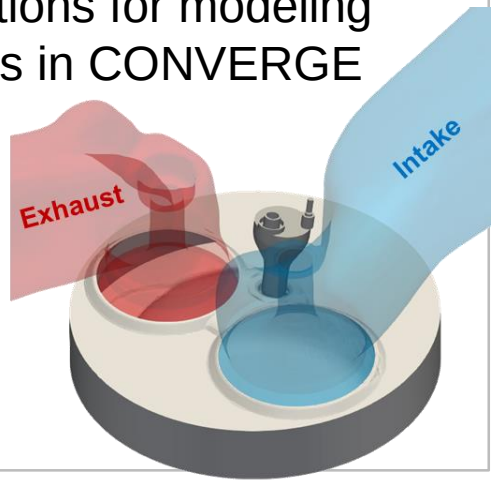


Purdue University (L. Qiao)



Argonne National Lab (R. Scarcelli)

- Supply experimental validation data for the Argonne MD engine
- Conduct model validation
- Work done or being conducted
  - Identified test conditions for modeling
  - Setting up simulations in CONVERGE CFD



		Unfueled PCSI		Fueled PCSI		
Engine speed	rpm	1200				
Intake boost pressure	bar	1.16		1.04		
Exhaust back pressure	bar	0.98		0.98		
Spark ignition timing	CAD aTDCf	-17		-17.5		
Excess-air ratio (λ_{intake})	-	**1.50**	**1.65**	**1.91**		**2.24**
Fuel ratio of PC/Intake	%	-	-	2.2,	4.1, 6.6	**7.7**
Engine load (nIMEP)	bar	8.1	7.6	5.4,	5.5, 5.7	4.7

Pick one of the two

Pick one of the three

Engine data: courtesy of A. Shah and M. Biruduganti, ANL

Remaining Challenges and Barriers

- Remaining challenges and Barriers for Budget Period 2
  - Remaining discrepancy in the a posteriori testing of machine learning assisted mixing model in the high-Ka DNS flame
  - Model validation of high-fidelity LES/TPDF model in Purdue TJI case including both pre-chamber and main chamber
- Remaining challenges and Barriers for Budget Period 3
  - Generation of machine learning training data
  - Development of machine learning assisted combustion model
  - Testing and validation of machine learning assisted combustion model in Purdue TJI rig
  - Validation of machine learning assisted combustion model in Argonne engine

Proposed Future Research

Following the project plan in Budget Periods 2 and 3

- Development of high-fidelity predictive LES model for the entire cycle of TJI combustion.
- Validation and refinement of the high-fidelity LES combustion model in Purdue model TJI rig
- Development and testing of data-driven engineering RANS model for TJI

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- Implementation of the Purdue model into the commercial solver (CONVERGE) used for final demonstration
- Validation of data-driven engineering RANS model for TJI in an MD/HD natural gas engine

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

SUMMARY

- The goal of project is to improve the predictive accuracy and efficiency of turbulent combustion sub-models for the simulations of premixed flame propagation initiated by pre-chamber turbulent jet ignition.
- A hierarchical approach is developed to deduce accurate and efficient engineering models for TJI.
- A machine learning assisted power-law scaling mixing model has been developed and has shown promise for premixed flame predictions.
- Validation of high-fidelity LES/PDF simulations for Purdue TJI rig is conducted for pre-chamber simulations.
- Machine learning model for turbulent reaction rate is explored for its feasibility and potential.
- A model validation framework based on CONVERGE is established for the targeted engineering model testing.

Technical Backup Slides

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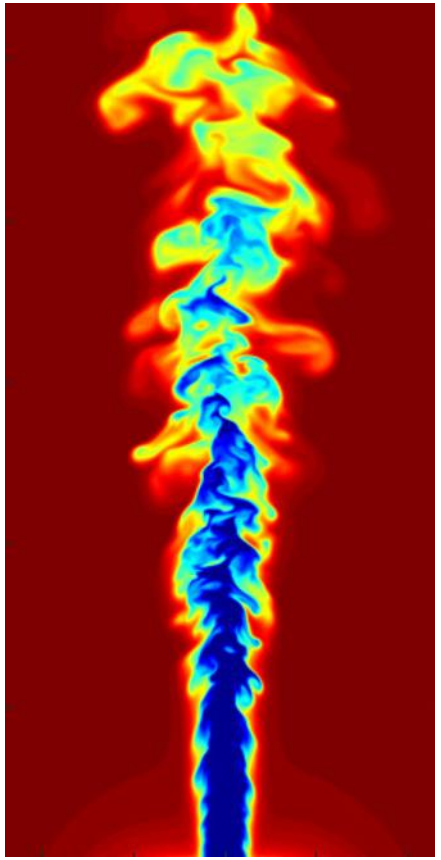
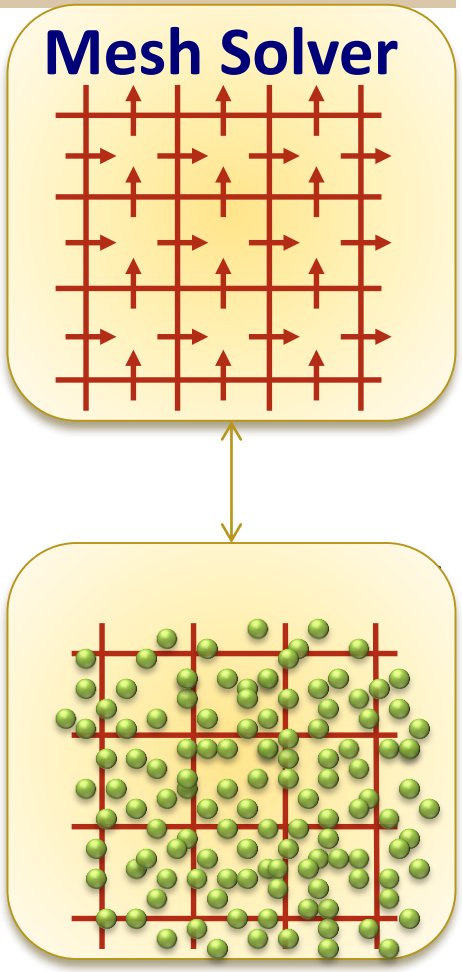
Technical Backup Slides

A posteriori testing of machine learning assisted mixing model



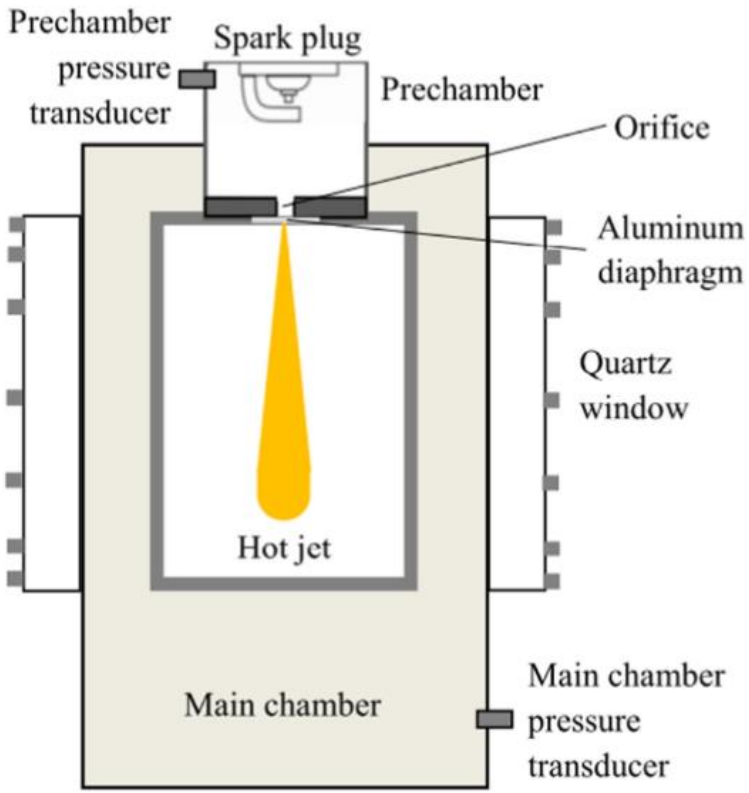
Simulation setup

- Large-eddy simulations for flow and turbulence
- Transported probability density function (PDF) method for scalars
- Hybrid mesh/particle solver
- Dynamic Smagorinsky model
- Modified Curl micro-mixing model
- DRM 19 species reaction mechanism for CH4 oxidization
- In Situ Adaptive Tabulation (ISAT) for chemistry calculation



Technical Backup Slides

Further model validation in Purdue TJI rig (under more relevant condition than DNS)



(Biswas et al. Applied Thermal Engineering, 2016, 106:925)

- **Numerical and simulation setup**
  - Numerics - Second order in Space and Time
    - ✓QUICK scheme for reacting scalars
    - ✓Central differencing for velocity field
  - Time step size - adaptable based on maximum allowed Courant number of 0.3
  - Prechamber initial conditions:
    - ✓T = 500 K
    - ✓P = 1 bar
    - ✓Equivalence ratio = 1.0
  - Eulerian Stochastic Field
    - ✓Number of stochastic fields = 8
    - ✓Mixing model = IEM
    - ✓Mixing constant = 3.0
    - ✓Consistency Model = EMCF-O

Technical Backup Slides

Machine learning assisted combustion modeling: a priori analysis

- **Machine learning approach for modeling F**

Machine Learning Algorithm	
Model	Random Forest
Number of Trees	200
Source Code	MATLAB Libraries
Bootstrapping of training sample?	Yes
Minimum sample size for split	5
Number of Input(n_i)/Output(n_o)	15/1
Maximum Features for Split	$n_i/3$

Machine Learning Input Variables

Physics	Variables
Combustion	$\hat{T}, C, \nabla\hat{T}, \nabla C, \nabla^2\hat{T}, \nabla^2 C, \hat{T}^2, C^2, S(\tilde{\phi}), \omega$
Turbulence – Resolved	∇U
Turbulence – Sub-filter	Γ_{sgs}, Γ
Pressure	$\hat{p} = p/\rho U^2, \nabla\hat{p}$

Technical Backup Slides

Collaboration and Coordination: Argonne Engine Test Facility

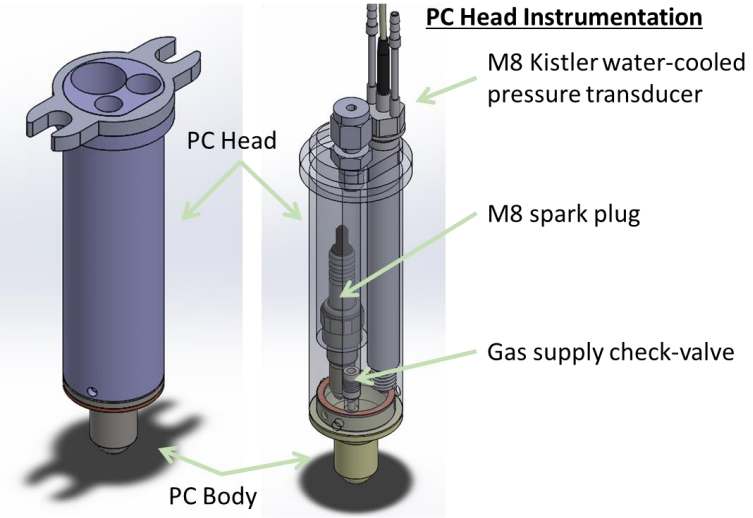
- Single Cylinder Engine setup (Hyundai based)
- Port fuel injected gaseous fuel
- Altronics CD-200 spark ignition system
- Full exhaust emission analysis capability
- Possibility of using NG or pure gaseous fuels

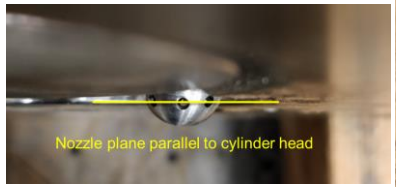
Number of cylinders	1
Number of intake/exhaust values	1/1
Bore [mm]	130
Stroke [mm]	140
Displacement [L]	1.85
Compression ratio	11:1
Fueling system	
Method	Fumigation, well-mixed
Natural Gas	Piped NG (~ 93% CH4 v\v%)

Courtesy of A. Shah and M. Biruduganti, ANL

Pre-chamber Igniter with active fueling capability

- In-house, modular pre-chamber design for flexibility needed for fundamental studies
- Relatively simple to change PC volume, nozzle geometry, number, and orientation
- Close collaboration with SNL and NREL to achieve “common PC design”





Technical Backup Slide

CFD Modeling Setup

CFD Code	CONVERGE v2.4-v3.0
Grid	main-chamber: 1 mm (w/ AMR 0.5 mm) pre-chamber & jet region: 0.25 mm
Turbulence	***RANS*** RNG k-ε
Ignition	energy deposition w/ spherical source
Combustion	**MZ-WSR** direct chemistry SAGE solver
Chemical kinetics	1. GRI Mech 3.0 2. Aramco 1.3 skeletal

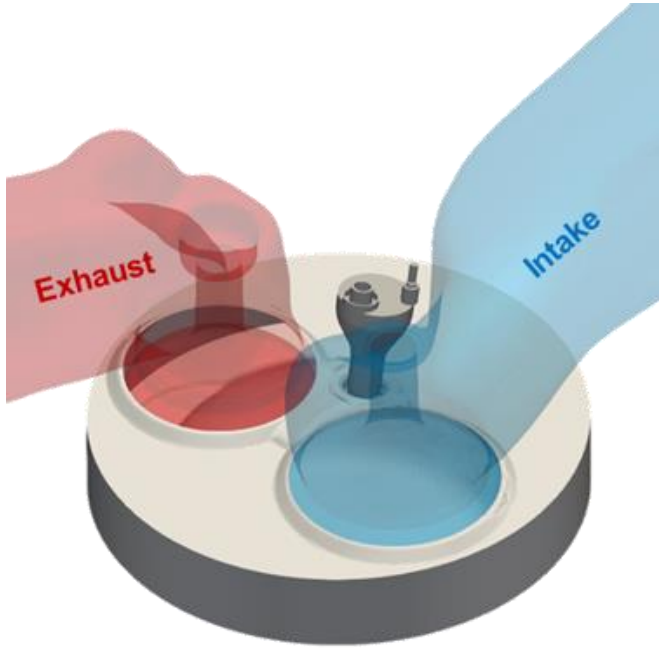
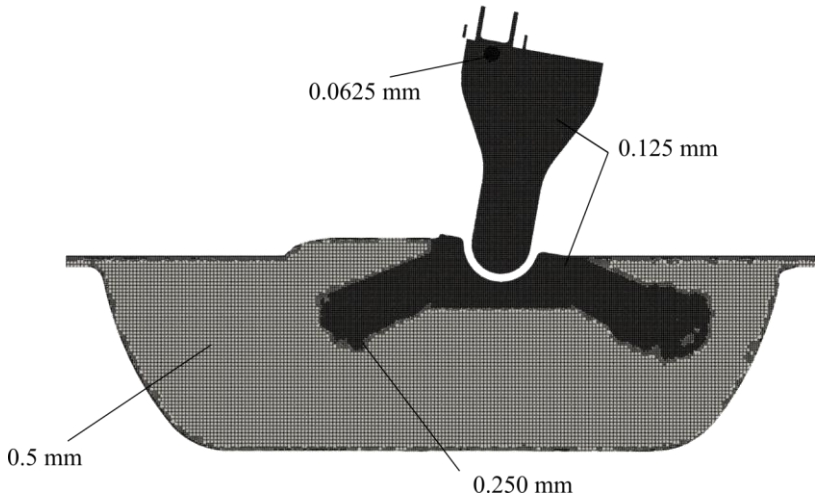
Un-fueled PCSI

GRI-Mech 3.0
(53 sp, 253 rxn)

* inaccuracy of IDT, LFS at fuel-rich branch

Fueled PCSI

AramcoMech 1.3
(253 sp, 1542 rxn)

DRGEPSA

Skeletal mechanism
(46 sp, 274 rxn)