DEVELOPMENT OF SIMULATIONS TOOLS FOR COMPRESSION IGNITION ENGINES

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Project ID # ACE135

OVERVIEW

Timeline

Project start: FY 2012

Part of 2017 VTO Lab Call

Budget

FY 16: $ 525 K

FY 17: $ 490 K

FY 18: $ 425 K

FY 19: $ 300 K

Barriers

- "Inadequate understanding of the stochastics of fuel injection"
- "Limited understanding of analysis tools for advanced ignition systems"
- "Improving the predictive nature of spray and combustion models"
- "Incorporating more detailed chemical kinetics into fluid dynamics simulations"

Partners

Argonne National Laboratory

Leadership Computing Facility (ALCF)

Advanced Photon Source

Convergent Science Inc. (CSI) } CRADA

Cummins Engine Company } CRADA

Lawrence Livermore National Laboratory

Sandia National Laboratory

Advanced Engine Combustion (AEC)

University of Connecticut

University of Perugia (Italy)

North Carolina State University

Several more Universities involved in FOAs

OBJECTIVES AND APPROACH

In general Engine simulations involve:

- Unresolved Nozzle flow
- Simplified combustion models
- Coarse mesh => grid-dependence
- Poor load-balancing algorithms
- Simplified turbulence models

Extensive tuning to match experimental data

High-Fidelity Approach:

- Fuel spray and nozzle-flow models
- Detailed chemistry based combustion models
- Fine mesh => grid-convergence
- Improved load-balancing algorithms with METIS
- High-fidelity turbulence models: LES based

+

- Exascale Computing

Towards Predictive Simulation of the Internal Combustion Engine

- Develop reliable engine modeling capability with fewer tuning constants
- Sub-models published in open-literature and available to the industry through software packages
- Develop “engineering best practices” for industry to use these high-fidelity models

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RELEVANCE – ACCURACY, SPEED, AND AVAILABILITY*

- **Nozzle flow and Spray research**
  - Cavitation erosion continues to be a concern, and modeling tools are not predictive.
  - X-ray measurements at Argonne can now provide real injector geometry with ~1 µm resolution.
  - Approach to fully coupled nozzle flow and spray simulations developed and published.
- **Combustion modeling using detailed chemistry**
  - Tabulated Flame Model (TFM) can enable the use of full chemistry (without mechanism reduction) for compression ignition engine simulations. However, table sizes can be very large.
  - TFM is currently available through UDFs that can be ported to any academic or commercial code.
- **High-Performance Computing (HPC)**
  - Ensuring that the computational tools can scale in the next-generation exascale platforms such as Aurora (First exascale supercomputer available at Argonne in 2021)
  - Ported Converge (commercial) and Nek5000 (open-source) codes on Theta (similar hardware as Aurora) for scaling studies on engine simulations

Mira: 10 petaflops

Aurora: Exascale

* DOE-VTO workshop to identify roadmap for CFD organized by Leo Breton in 2014

SIMULATION APPROACH: SUB-MODEL DEVELOPMENT

Modeling Tool	CONVERGE
Smallest and largest characteristic grid size(s)	**Finest grid size simulations:** **2.5 µm for nozzle flow (35 million cells)** **~30 µm for GDI and diesel Sprays (20 million cells)**
Turbulence-chemistry interaction (TCI) model	**Tabulated Flamelet model (TFM) with Artificial Neural Network (ANN) for chemistry speed-up** **Homogeneous Reactor based model (HR)**
Turbulence model(s)	LES: Dynamic Structure sub-grid scale model ✓ Extensive nozzle flow and GDI spray simulations
In-nozzle Flow	**New Criteria Proposed for Cavitation Erosion** **Homogeneous Relaxation Model (HRM)** ✓ Diesel and gasoline injectors ✓ Extended for multi-component fuels
Spray models	Volume of Fluids (VOF) approach for phase-tracking **Coupled Eulerian-Lagrangian Spray Atomization (ELSA) Model** **One-way coupling approach**

Extensive validation against data from several collaborators at Argonne (C. Powell), Sandia (L. Pickett, C.J. Mueller)

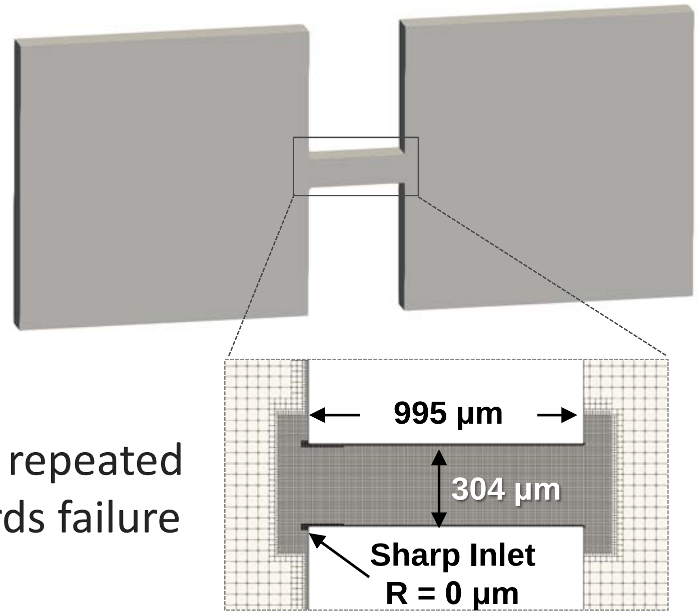
MILESTONES FOR FY 19

- Nozzle flow and Spray Research (CRADA with Cummins and CSI)
  - Develop in-nozzle cavitation erosion model within LES context for diesel injectors and validate against optical data available in literature and new data from APS {50% complete}.
- Combustion Modeling
  - Perform extensive RANS and LES calculations with detailed and reduced 5-component diesel surrogate (against optical engine data from Sandia) to demonstrate the run-time vs. accuracy trade-off of turbulence and detailed kinetic models using ANN approach {75% Complete}.
- High-Performance Computing
  - Import CONVERGE code on new architecture (theta) for the upcoming supercomputer Aurora and identify scaling bottlenecks {delayed due to CONVERGE code release issues).

All the newly developed models and key findings are published in journal papers and peer-reviewed conference proceedings so that academia, OEMs, and other software vendors can benefit from our work. Several OEMs and software vendors have engaged with us through the VERIFI program

APPROACH: CAVITATION EROSION MODELING

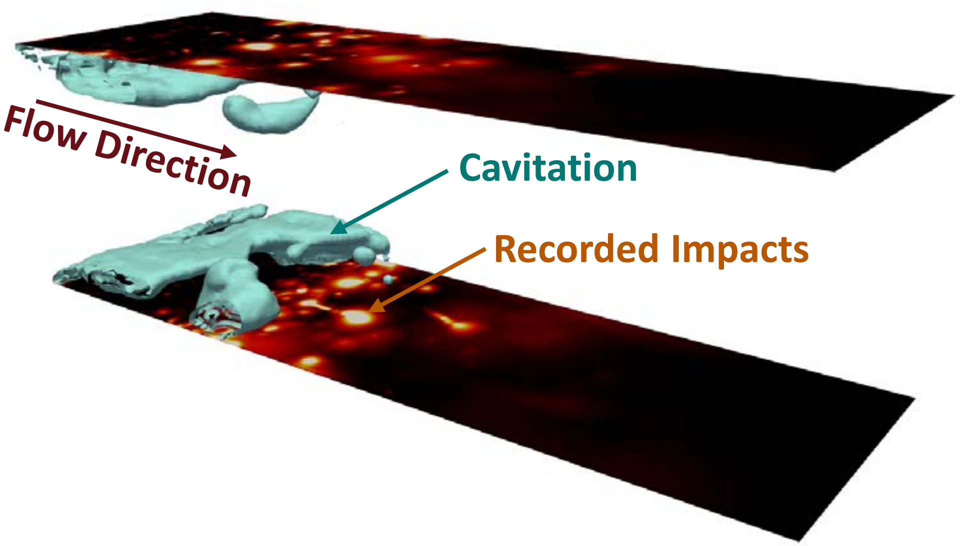
- Efficient indications of cavitation erosion are needed to identify critical flow conditions and locations.
- Rapid vapor cloud collapse can produce a shock wave, which can cause impact stresses in excess of the material yield strength on neighboring surfaces
- Linking multiphase flow predictions with propensity and severity of erosion is a challenge.



- Energy stored within the solid material[1], E_{stored}, from repeated impacts is used to efficiently represent progress towards failure
- PREVERO channel "I" geometry (Skoda et al., WIMRC 3rd Int. Cavitation Forum, 2011) modeled to study cavitation shedding and critical cloud collapse events:

$$E_{stored}(N) = \sum_{i=1}^{N} \frac{\mathcal{A}}{\rho_l c_l} \int_0^{\tau} p^2(t)dt$$

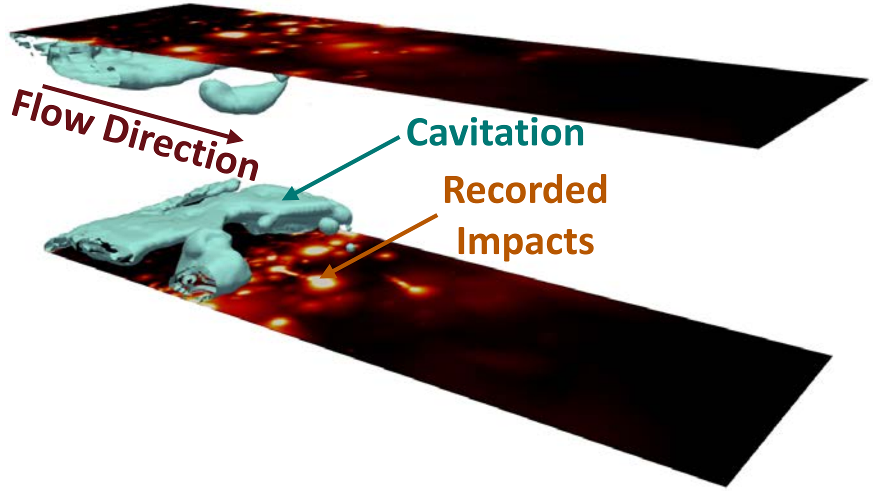
p is predicted local pressure, density ρ_l and speed of sound c_l, and acts on the surface of area $\mathcal{A}$ over a duration of time τ

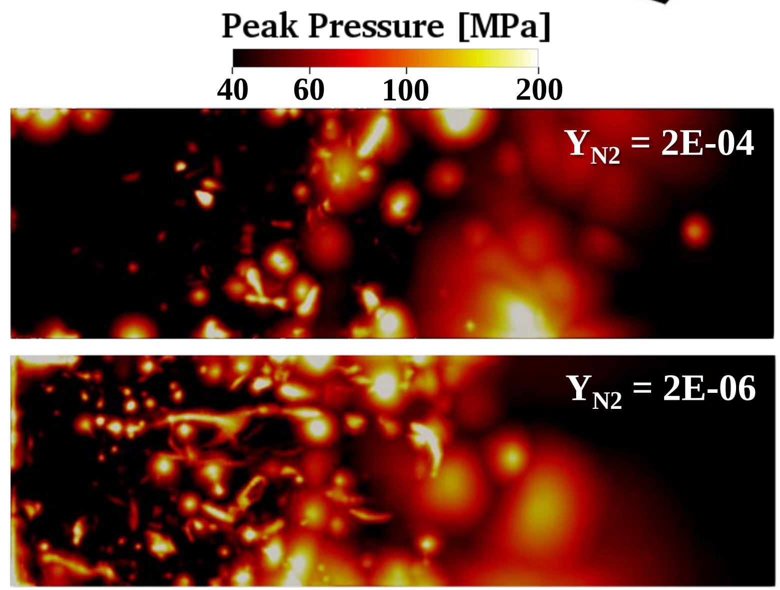


[1] Magnotti, Som et al., ICLASS 2018

ACCOMPLISHMENT: BEST PRACTICES OUTLINED FOR MODELING CAVITATION AND EROSION

- In order to identify best practices when using the newly developed cavitation erosion model, a computational study was conducted to explore the impact of numerical and thermophysical fluid properties on cavitation erosion.
- The following parameters were evaluated:
  - Grid resolution
  - Turbulence modeling approach
  - Fuel-surrogate properties
  - Non-condensable gas concentration (Y_{N2})
- Grid-converged predictions for flowfield and cavitation structure were obtained when minimum cell sizes less than 2.5 µm were employed.
- When sufficient resolution is employed, LES approach is capable of predicting cavitation formation and shedding. URANS approach may not be appropriate for modeling cavitation erosion due to inability to capture cavitation shedding.
- Accurate representation of the fuel density and viscosity are essential for predicting mass flow rate and cavitation
- Increased levels of non-condensable gas lead to decreased frequency and strength of cavitation cloud collapse events.





* Magnotti, Som et al., SAE Paper No. 2019-01-0290, *Advances and Current Practices in Mobility*, Accepted

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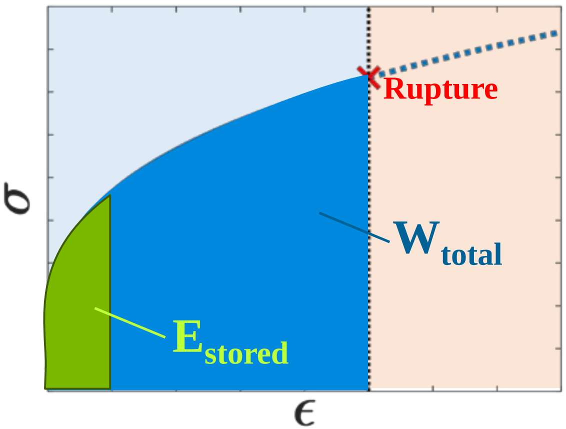
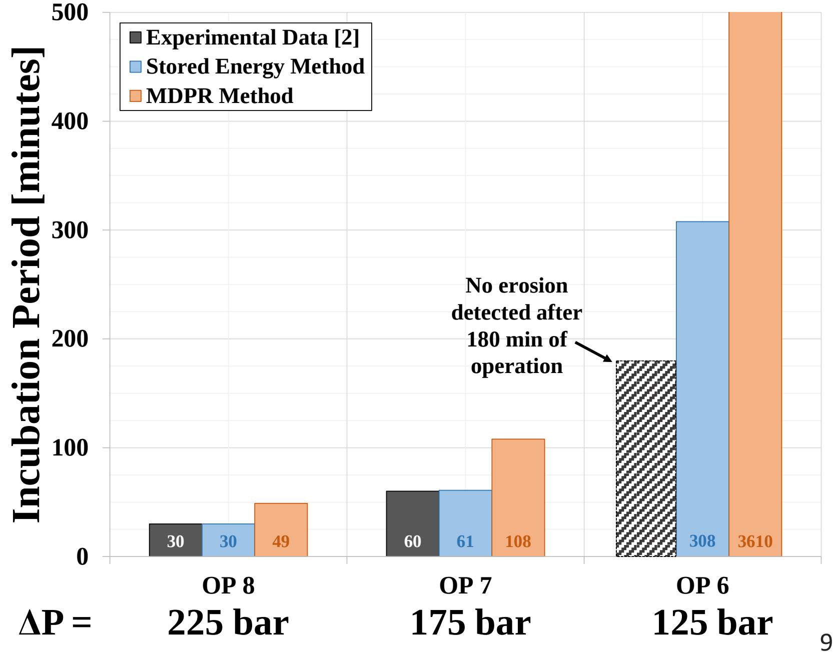
ACCOMPLISHMENT: EROSION SEVERITY ACCURATELY PREDICTED OVER SEVERAL FLOW CONDITIONS

- In order to calculate an incubation period, *T*, cavitation erosion predictions must be related to solid material properties.
- For a given material, the total work required for the solid to undergo rupture, W_{total}, can be calculated through integration of the stress-strain curve while accounting for strain-hardening effects.
- The ratio of W_{total} to the predicted E_{stored} is used to scale the simulated time, $\tau_{simulated}$, and estimate *T*.
- In the standard approach using the mean depth penetration rate (MDPR) method, the mean stress is used to characterize hydrodynamic impacts and estimate *T*.
- Evaluation of the two methods across a range of ΔP conditions highlights the improved prediction capability with the newly developed stored energy method due to its dependence on both impact strength and duration.
- Assumed level of non-condensable gas concentration has been noted to have a strong effect on the predicted incubation period and response to changes in flow conditions.



$$T \propto \frac{W_{total}}{E_{stored}} \tau_{simulated}$$



[1] Magnotti, Som et al., ILASS-Europe 2019, Under Review

[2] Skoda et al., WIMRC, 2011

APPROACH: NOVEL FLAMELET TABULATION APPROACH FOR REALISTIC FUEL SURROGATES

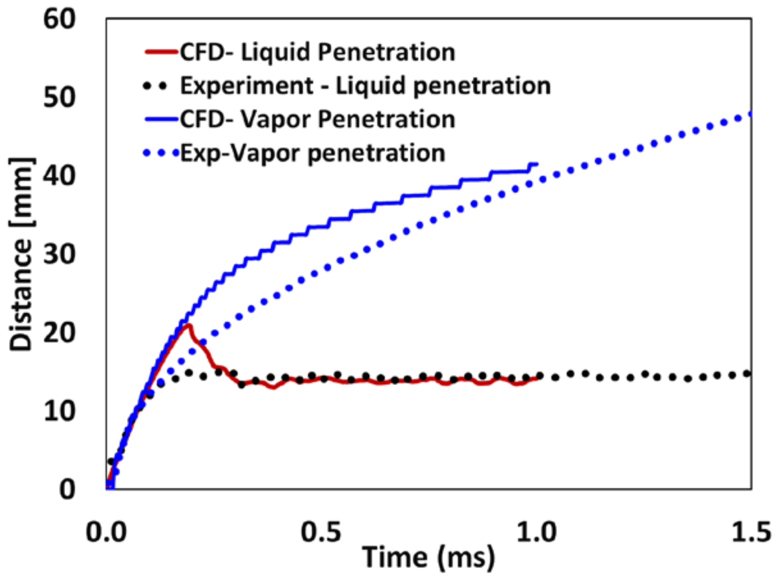
- AMR2018 talk highlighted the continued development of the Tabulated Flamelet Model (TFM) with sparse solvers and ANN for detailed mechanisms. TFM framework now enables the implementation of realistic fuel surrogates for engine simulations.
- V0a[1] is a 4 component diesel surrogate that was developed to closely match physical and chemical properties of diesel fuel.
- Presence of complex hydrocarbon components coupled with LTC leads to reaction mechanisms with more than 1000 species and 10k reactions. The previous developments with TFM and sparse solvers are ideal to bring such realistic fuel surrogates into the realm of engine simulations.
- Combustion of V0a in constant volume spray vessel was modeled using TFM and validated against experimental data.
- Reaction mechanism for V0a was developed by Goutham Kukkadapu and Bill Pitz at Lawrence Livermore National Laboratory and experimental data at engine conditions was obtained from Army Research Laboratory[2]

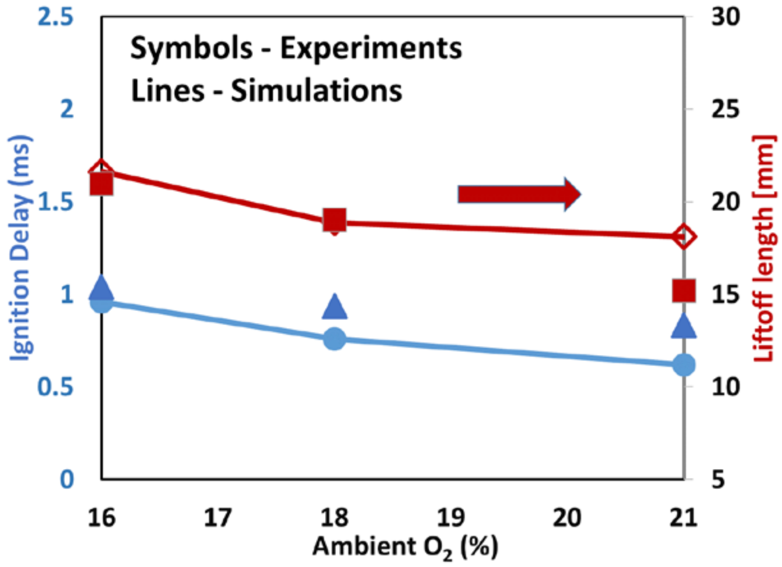
V0a components	Mole fraction
n-hexadecane	0.278
Isohexadecane	0.363
Trans-decalin	0.148
1-methylnaphthalene	0.211

Parameter	Description
Chemistry Mechanism	1544 species and 5897 reactions
Grid size	0.25 mm with AMR
Turbulence Model	RANS RNG k-epsilon
Combustion model	TFM
Presumed PDF	Beta PDF

1. CRC AVFL-18a
2. Experimental data from ARL (M. Kweon, J. Temme, and V. Coburn)

ACCOMPLISHMENT: INCORPORATING REALISTIC FUEL SURROGATES FOR ENGINE SIMULATIONS

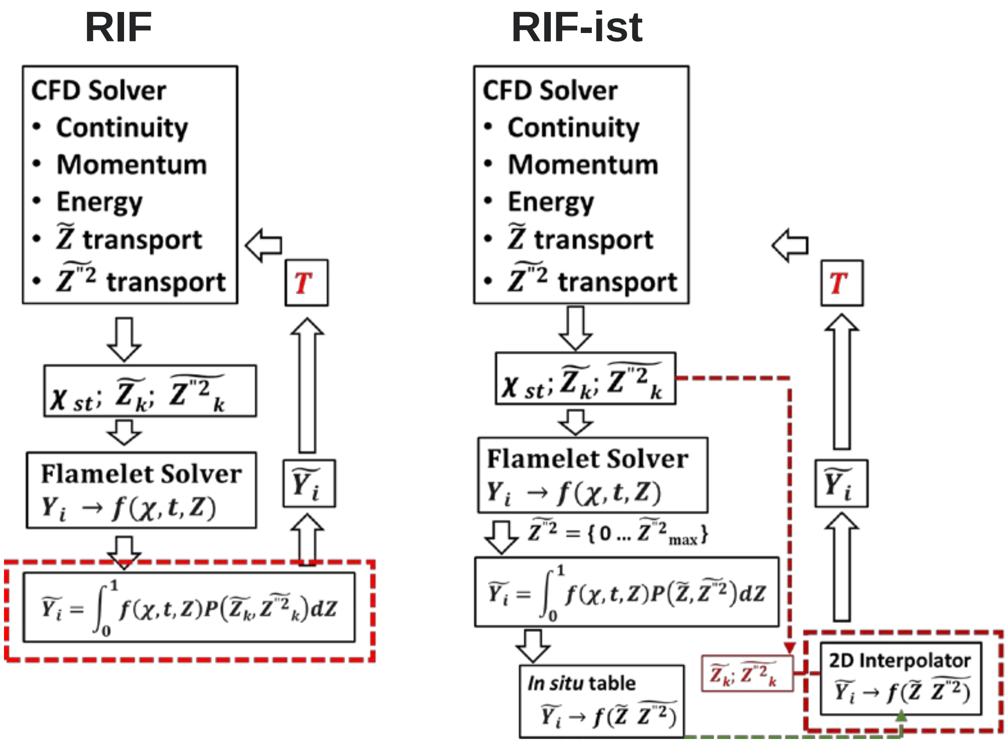




- Lagrangian spray model setup and validations carried out against non-reacting experimental data.
- Ignition delays and flame liftoff lengths are significantly large for these conditions.
- The fuel surrogate exhibits a 2 stage ignition process signifying the role of low temperature chemistry.
- TFM is able to capture the ignition delay and flame liftoff lengths accurately at the low oxygen concentrations and the overall trend.
- Future work: Diesel engine simulations with V0a as surrogate.

APPROACH: HYBRID FLAMELET TABULATION CONCEPT

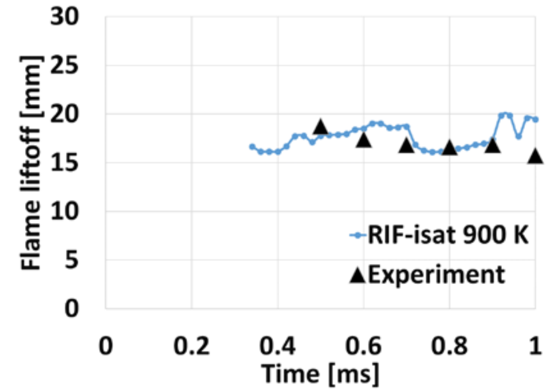
- New *in-situ* unsteady flamelet tabulation approach (RIF-ist) combines the computational efficacy of pre-tabulated models and accuracy of online flamelet solvers.
- Multiple flamelets are injected as per the original RIF formulation and flamelet tables are generated at each time step for each flamelet.
- This algorithm bypasses the cost of presumed PDF integration at each cell.
- It was implemented in CONVERGE and initially validated against a partially premixed gas jet flame*. Comparisons were carried out against temperature and species measurements. The model is able to capture the transient processes accurately.

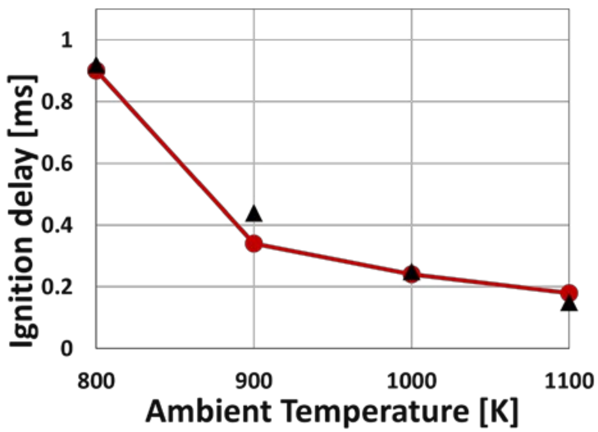


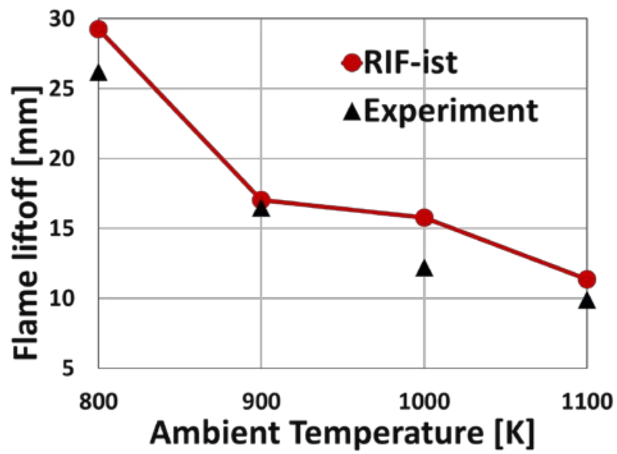
* Kundu et al., A Novel In Situ Flamelet Tabulation Methodology for the Representative Interactive Flamelet Model. *Combustion Science and Technology*, 2018 pp.1-25.

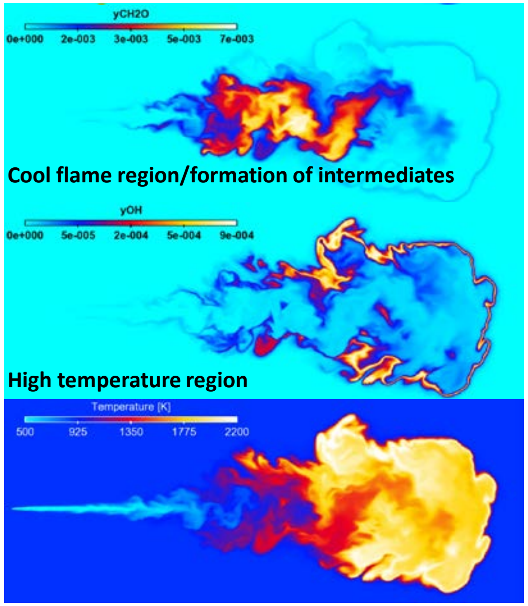
ACCOMPLISHMENT: VALIDATION OF RIF-IST APPROACH AT ENGINE CONDITIONS

- The RIF-ist model was validated against ECN* Spray A experiments over a range of ambient temperatures in a LES framework.
- The model is able to capture the two stage ignition process and flame stabilization over a range of ambient temperatures.









Flame stabilization - ECN Spray A conditions (900 K)

Advantages of RIF-ist approach

- In-situ approach recovers the same solution as traditional RIF.
- 67% reduction of computational cost for LES with higher savings for finer grids.
- LES with unsteady, multi-flamelet RIF approach now within the realm of engine simulations.

* Engine Combustion Network (https://ecn.sandia.gov/)

ACCOMPLISHMENT: DETAILED SOOT MODELING

Coupling with in-situ tabulation strategy

- Detailed soot modeling approach accounting for particle inception, coagulation, condensation and surface growth using the method of moments.
- Moment equations and PAH chemistry[1] solved for flamelets[2].
- Coupled in-situ flamelet tabulation code with detailed soot model with 4 moment equations in CONVERGE code.
- Initial validations carried out against ECN Spray A in a RANS framework over a range of temperatures.
- The model is able to capture accurate trends in soot inception and formation locations without tuning of model parameters.
- Under-predictions observed in transient soot mass formation.
- High fidelity - low cost approach for soot predictions in RANS framework.
- Future work:
  - Extension to larger PAH mechanisms and LES using previously developed LSODES framework
  - Extension to multiple injections

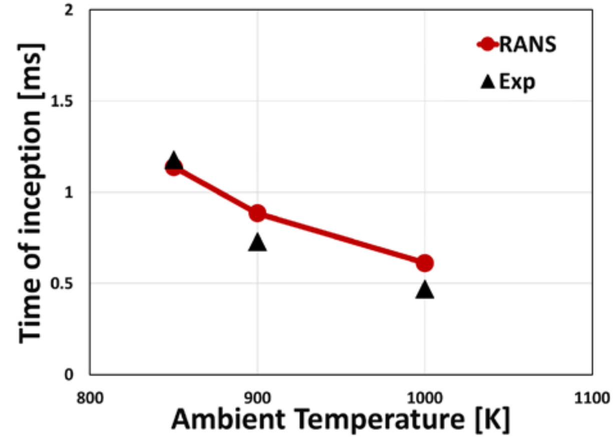
$$\rho\frac{\partial Y_i}{\partial t} = \rho\frac{\chi}{2}\frac{\partial^2 Y_i}{\partial Z^2} + \dot{\omega}_i$$

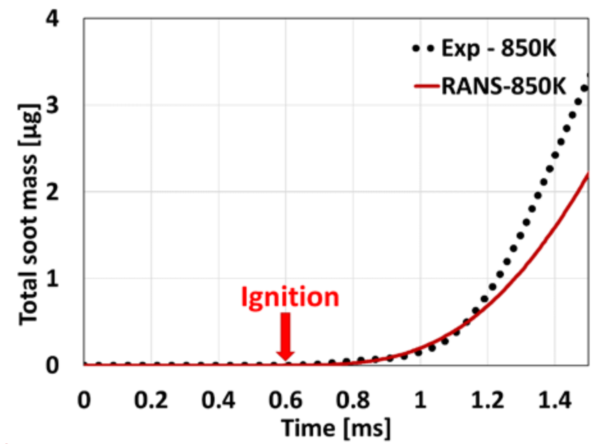
$$\rho\frac{\partial T_i}{\partial t} = \rho\frac{\chi}{2}\frac{\partial^2 T_i}{\partial Z^2} + h_i$$

Flamelet equations

$$\rho\frac{\partial M_r}{\partial t} = \rho\frac{\chi}{2}\frac{\partial^2 M_r}{\partial Z^2} + s_r$$

r^{th} Moment equation





1.Wang, H., et al., Development of a reduced n-dodecane-PAH mechanism and its application for n-dodecane soot predictions. Fuel, 2014.
2.Mauss et al. Aspects of modeling soot formation in turbulent diffusion flames, 2006 Combustion Science and Technology.

COLLABORATIONS

Argonne National Laboratory

- **Engine and Emissions Group: (Provide data for model validation)**
- **Leadership Computing Facility (Improving Scalability of CONVERGE, HPC resources)**
- **Advanced Photon Source: (Nozzle flow and Spray Data)**

Convergent Science Inc. (Algorithm and code development in CONVERGE)

Cummins (Provide experimental data, alpha testing of new models)

Sandia National Laboratory (Provide experimental data on several projects)

Lawrence Livermore National Laboratory (Mechanism development)

University of Connecticut (Mechanism Reduction)

University of Perugia (In-nozzle Flow Simulations)

North Caroline State University (Turbulent Combustion Modeling with ANN)

Presentations at Advanced Engine Combustion (AEC) Working group

Engine Combustion Network Participation and Data Contribution

***Simulation Toolkit Team* in "Co-Optima" is leveraging our developments**

Three University FOAs are leveraging our developments

COLLABORATIONS THROUGH VERIFI

- Based on the capabilities developed under this program, we have established the Virtual Engine Research Institute and Fuels Initiative (VERIFI).
- VERIFI is designed to provide HPC solution for industrial problems of interest using either clusters of leadership class supercomputer such as Mira.
- > 70 attendees for the 3rd workshop from light and heavy duty engine OEMS, software vendors, oil and energy companies, and Supercomputing solutions companies.

4th workshop in June 2019

Ignition Processes in Internal Combustion Engines

FY 18 & 19

Cummins

CONVERGENT SCIENCE

HPC4 MANUFACTURING

U.S. DEPARTMENT OF ENERGY | Energy Efficiency & Renewable Energy
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RESPONSE TO PREVIOUS YEAR REVIEWER COMMENTS

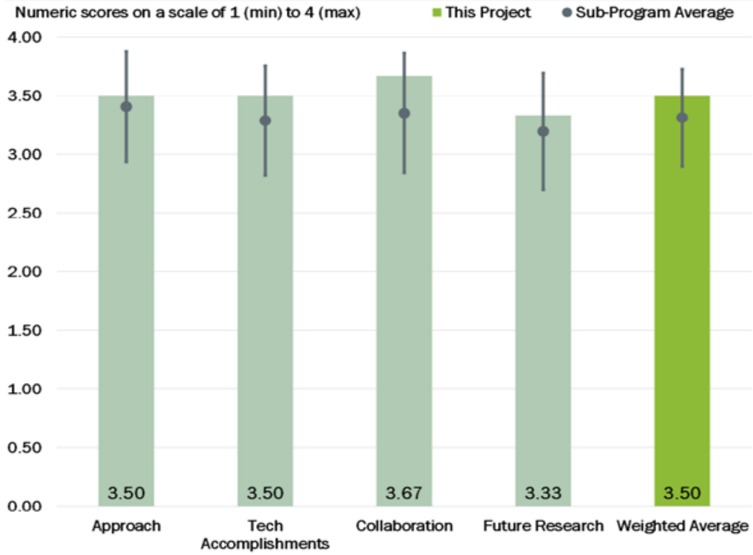
Overall the reviewers were positive about the progress of the project

The reviewer said that this project has made excellent progress. Regarding the ELSA model, the reviewer questioned what was new about it, because it has been around a decade now with number of demonstrations.

ELSA has been existence for a decade now and has been largely applied to single hole academic injectors for validation purposes. Also, the transition from Eulerian to Lagrangian remains largely ad-hoc. The PI has successfully demonstrated that ELSA can be applied to multi-hole fuel injectors with improved predictions compared to one-way coupling approach.

The reviewer commented that many sophisticated models are used within this project. The reviewer wondered if they really need to be so complex. It might be possible to devise simpler models to explore the detailed processes such that engineers can use them an effective tool. If so, then it will be an outstanding accomplishment.

Reviewers comments are notes. Data-driven modeling approaches are being pursued by the PIs as well. However, complicated physical models are necessary to capture the multi-scale, multi-physics nature of combustion engines. It should be noted that although simulations are becoming more expensive, computational resources are also more readily available and most of these simulations can actually be run on clusters available to industry and academia.



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REMAINING CHALLENGES AND BARRIERS

- Cavitation Erosion: Extremely disparate time scales between cavitation and material fatigue leading to erosion. Collaborating with material scientists may provide insight into the appropriate coupling between CFD predictions and material behavior.
- Real Geometry: Computations with real geometry are extremely memory intensive and time-consuming regardless of the computational tool being used.
- Computational resources: Coupling large chemistry with LES turbulence modeling can increase the computational resources needed to perform these simulations.
- High-fidelity experimental engine data: We need dedicated experiments to validate some of our models and at times this dataset is not available and needs to be generated. Also, we need uncertainties in measured data. Simulations do not account for the experimental uncertainties that can be significant at times.
- Uncertainty Quantification (UQ): Rigorous UQ has not yet been applied to engine CFD simulations to understand the relative importance of uncertainties from experimental boundary conditions vs. chemical kinetics vs. sub-model constants.
- Soot modeling: It is extremely challenging to capture soot formation in CFD simulations in a predictive fashion. It requires the accurate modeling of a large number of coupled processes, incorporation of detailed PAH chemistry and detailed soot models. The highly disparate chemical time scales associated with intermediate species, high temperature species and slow forming PAH species render traditional flamelet tabulation approaches to be inaccurate.

PROPOSED FUTURE WORK

Cavitation erosion modeling: CRADA project with Cummins and CSI

- Extend cavitation erosion modeling framework by integrating material properties into the erosion criteria and perform more quantitative validation against available measurements.
- Understand and evaluate potential sources of variability in erosion characteristics and injector wear (e.g. variations in injector geometry, needle motion, and fuel properties on cavitation and erosion propensity and severity).
- Development of fluid structure interaction model to predict needle transients and identify fuel property effects on needle motion: validation against x-ray measurements of needle lift and wobble.
- Develop "engineering best-practices" to expedite internal nozzle flow simulations and enable industry to use the "real-geometry" from injectors.

Turbulent combustion modeling:

- Extensive validation of flamelet models (TFM and RIF-ist) soot models for multiple injections in constant volume vessel and optical engine experiments.
- Incorporation and validation of detailed PAH chemistry models for diesel surrogates in engine simulations developed at LLNL.

SUMMARY

- **Objective**
  - Development of predictive spray, turbulence, and combustion models aided by HPC tools and comprehensive validation.
- **Approach**
  - Coupling expertise from DOE Office of Science on fundamental chemical kinetics, industrial partners, and HPC resources for development of robust engine models.
- **Collaborations and coordination**
  - With industry, academia, and national laboratories.
  - Through VERIFI collaborations with light-duty, heavy-duty, software vendors, and energy companies.

- **Technical Accomplishments**
  - Cavitation erosion model used to characterize erosion propensity and severity within canonical channel geometries and a practical off-the-shelf injector.
  - Guide the use of the new erosion model, best practices for modeling cavitation and erosion outlined in terms of turbulence and fluid thermophysical properties.
  - Relating erosion predictions with solid material properties allowed for erosion severity to be quantified and accurately predicted within 2% of experimental measurements.
  - Use of ML tools (Artificial Neural Network) further enabled the implementation of full chemistry (without mechanism reduction) in engine simulations.

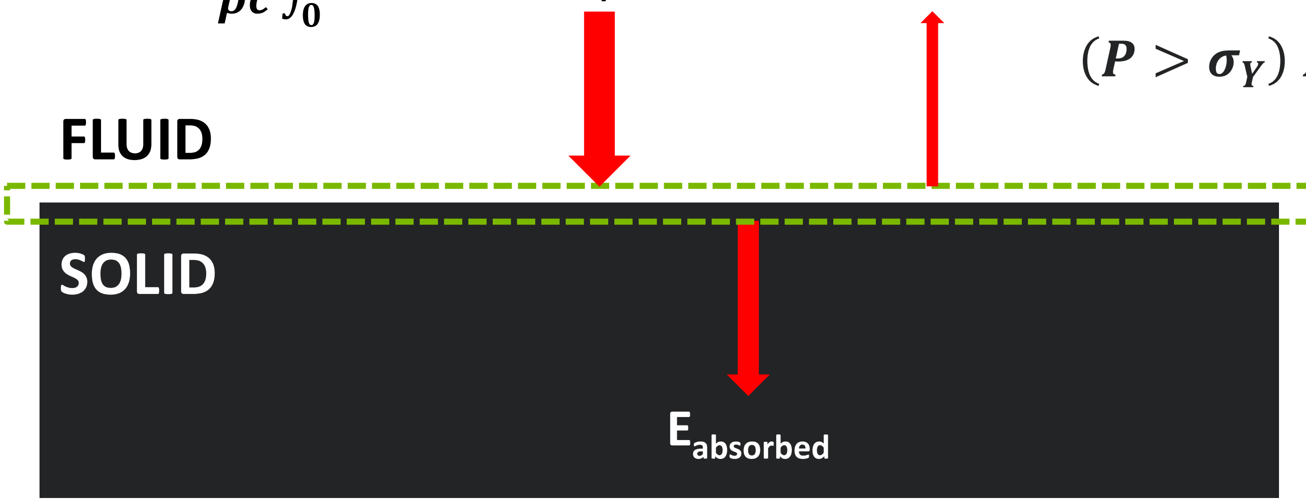
Technical Back-Up Slides

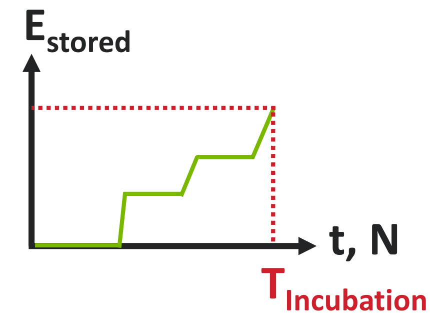
APPROACH: CAVITATION EROSION MODELING[1]

$$E_{impact,i} = \frac{\mathcal{A}}{\rho c}\int_0^{\tau} p^2(t)dt$$

$$(P < \sigma_Y)\ E_{reflected} = E_{impact}$$

$$(P > \sigma_Y)\ E_{reflected} = 0$$





$$E_{stored}(N) = \sum_{i=1}^{N} E_{impact,i} = \sum_{i=1}^{N} \frac{\mathcal{A}}{\rho_l c_l}\int_0^{\tau} p^2(t)dt$$

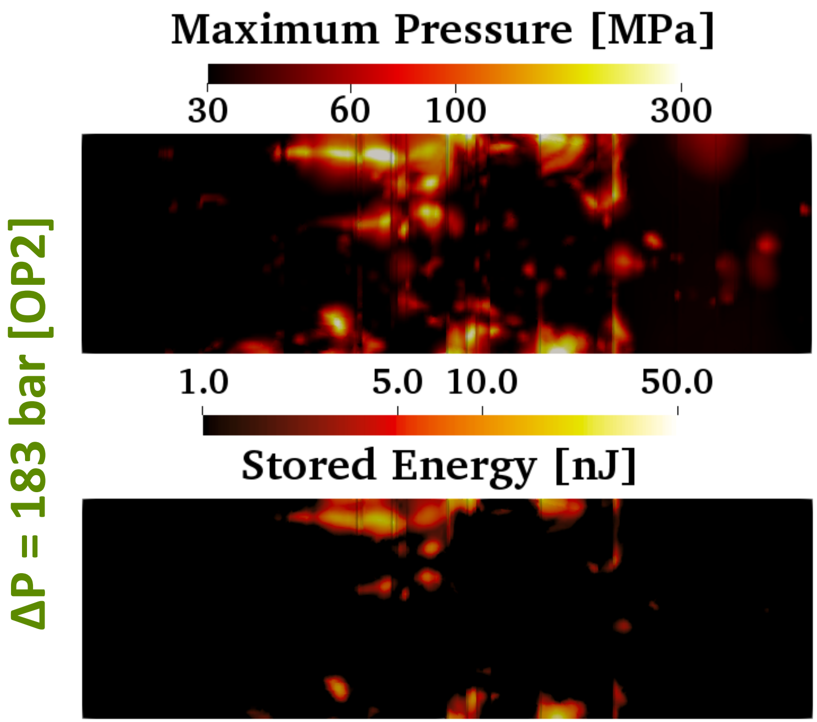
p is predicted local pressure, density ρ_l and speed of sound c_l, and acts on the surface of area $\mathcal{A}$ over a duration of time τ

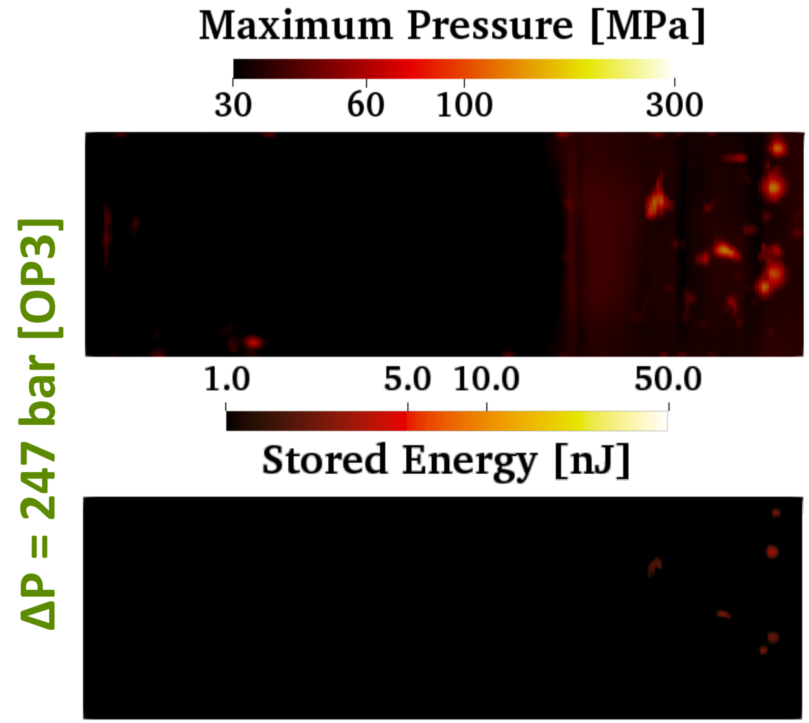
- Cavitation erosion model is premised on an energy balance at the fluid-solid interface
- This modeling framework allows for the influence of both single and repeated impact events to be related to the progress towards material failure
- E_{stored} can be used as either a qualitative or quantitative measure of cavitation erosion propensity and severity
- Qualitatively, E_{stored} provides a relative measure for the strength of hydrodynamic impacts based on its dependence on the impact load, p, and duration, τ
- By relating the impact energy to solid material properties, the time before first material removal, known as the incubation period, $T_{Incubation}$, can be quantified[2] and compared with experimental measurements

[1] Magnotti, Som et al., ICLASS 2018
[2] Magnotti, Som et al., ILASS-Europe 2019

ACCOMPLISHMENT FY18: FLOW AND CRITICAL EROSION LOCATIONS FAIRLY WELL PREDICTED

- Onset of choked flow condition at ~200 bar is well captured along with the mass flow rate* at all ΔP
- Comparison of the predicted stored energy distributions for the “OP2” and “OP3” conditions provide a qualitative assessment of relative erosion severity and time before material failure
- The larger average stored energy for the OP2 condition in comparison to the OP3 condition suggests that the incubation period would be shorter under the OP2 condition. This result is consistent with the experimental findings*, where the incubation period for the OP3 condition was found to be relatively longer
- These findings using the newly developed cavitation erosion metric highlight its utility in quantifying both the energy of single impact events, as well as the influence of repeated impacts on the incubation period before material rupture



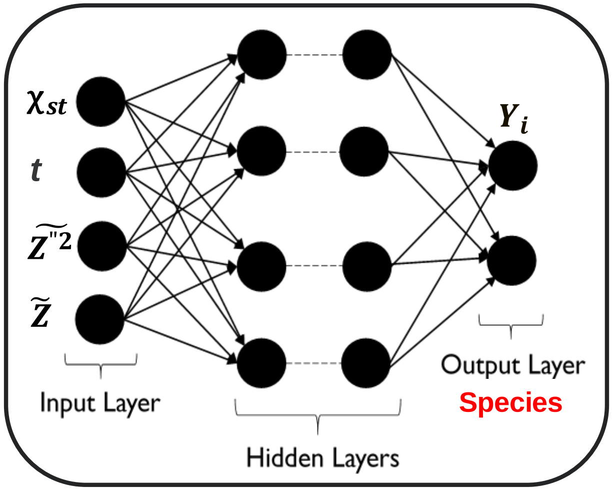


* Skoda et al., WIMRC 3rd Int. Cavitation Forum, 2011.

ACCOMPLISHMENT FY18: ANN IMPLEMENTATION & VALIDATION

ANN algorithm

Use multidimensional flamelet manifold to train a Deep Neural Network

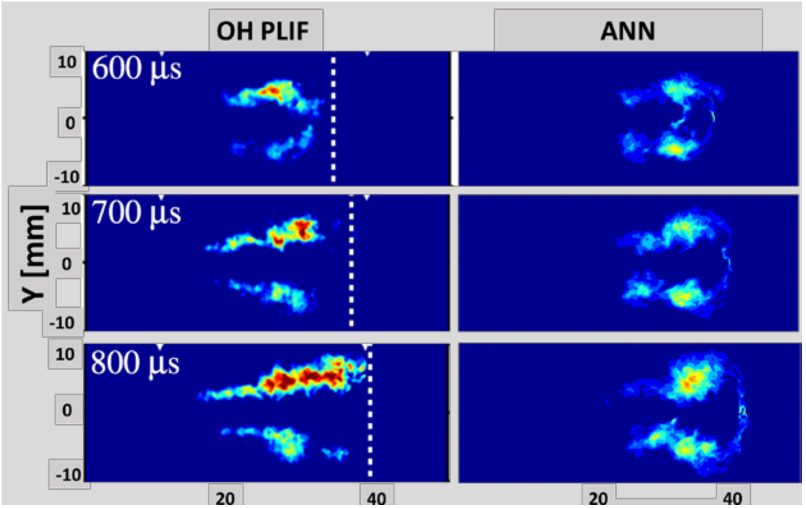


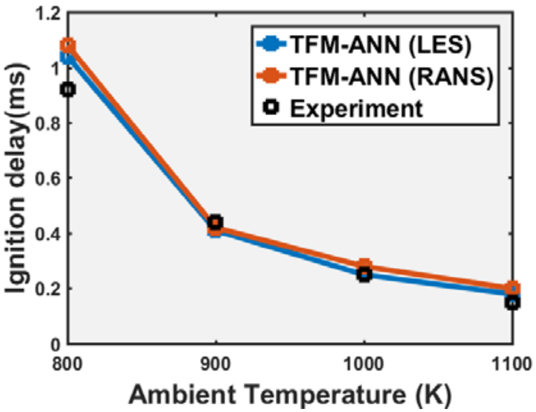
ANN features

- Novel bifurcation algorithms for multi-dimensional manifolds. Automated bifurcation of species.
- **1 GB flamelet table can be replaced by 85 KB ANN**
- Elimination of multi-dimensional interpolation

Validation: ECN Spray A data from Sandia

- LES with 22 million cells and 60 µm grid
- 103 species n-dodecane mechanism
- Ambient temperature range: 800 K – 1100 K
- Same ANN algorithm used over the entire range
- 4D flamelet table Y_i - $(\chi, t, \widetilde{Z''^2}, \tilde{Z})$





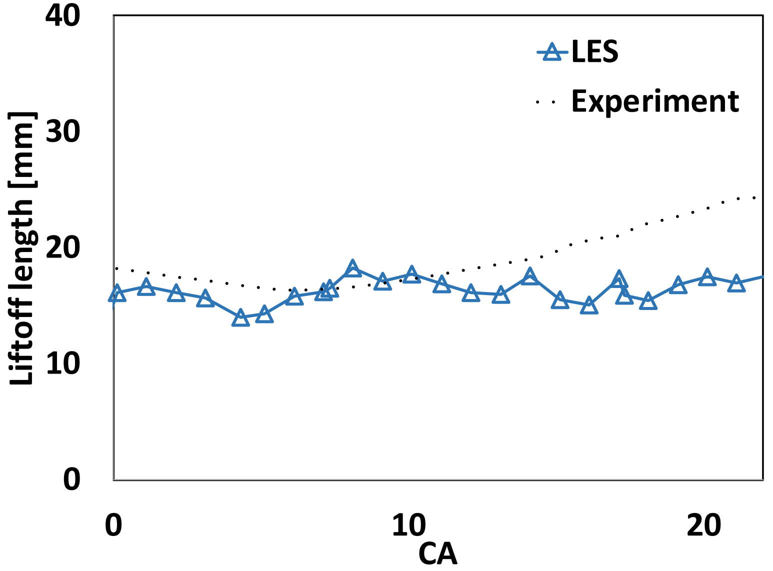
Ignition delay and flame lift-off length (LOL) along with the flame structure is well captured!

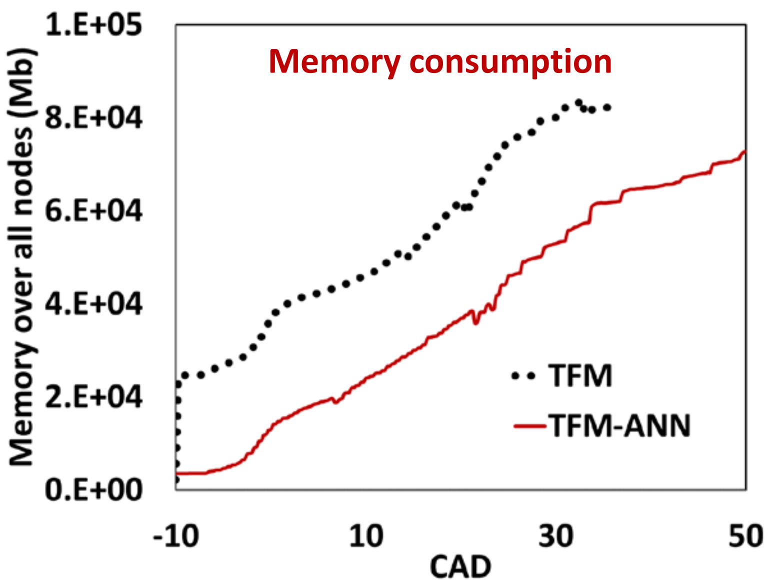
ACCOMPLISHMENT FY18: VALIDATION WITH ENGINE DATA

Experimental data: Mueller's Optical Engine @ Sandia National Lab.

Simulation Details:

- Open cycle engine simulation with LES.
- Min. cell size: 90 µm grid; 25 million cells.
- Fuel: Methyl Decanoate ($C_{11}H_{22}O_2$)
- Full mechanism without reduction: 3299 species, 10804 reactions
- 5D flamelet table Y_i - $(P, \chi, t, \widetilde{Z''^2}, \tilde{Z})$.
- Simulation time: 160 Hours on 480 processors.





- ANN is able to capture the ignition delay and flame liftoff across different conditions.
- Accurately captures the onset & cool flame regions.

Advantages of ANN

- Lower memory footprint.
- **40 %** reduction in CPU costs.
- Higher savings for higher dimensional manifolds.
- Can be used with any tabulation methodology.