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COMBUSTION
ENGINES

SAND2021-5968PE

Soot Modeling and Experiments

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Annual Merit Review, 22 June 2021, 3:45 PM EDT
Project ID: ACE168

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Overview

Task & PI	Description	FY21 Budget
S.E.07* Sjoberg	Engine experiments characterizing wall films & PM formation	270k
S.E.02* Manin	Experiments supporting PM modeling - wall film & pyrolysis	400k
L.M.01.02* Kukkadapu	Models for improved prediction of PAH/soot	200k
S.M.02.03 Hansen	Engineering PAH Model Development	100k
L.M.01* Pitz	Surrogates and kinetic models	425k
S.M.02.02* Nguyen	Flame wall interactions	50k

* Technical accomplishments shared amongst various AMR presentations

Timeline

- **PACE Started in Q3, FY19 and will end in current form in FY23**
  - We are about half-way through the program
  - Focus and objectives of various tasks will be adjusted by PACE leadership team based on needs
    - The Soot Working Group is one example of such restructuration
  - Overall PACE work plan discussed in **ACE138**

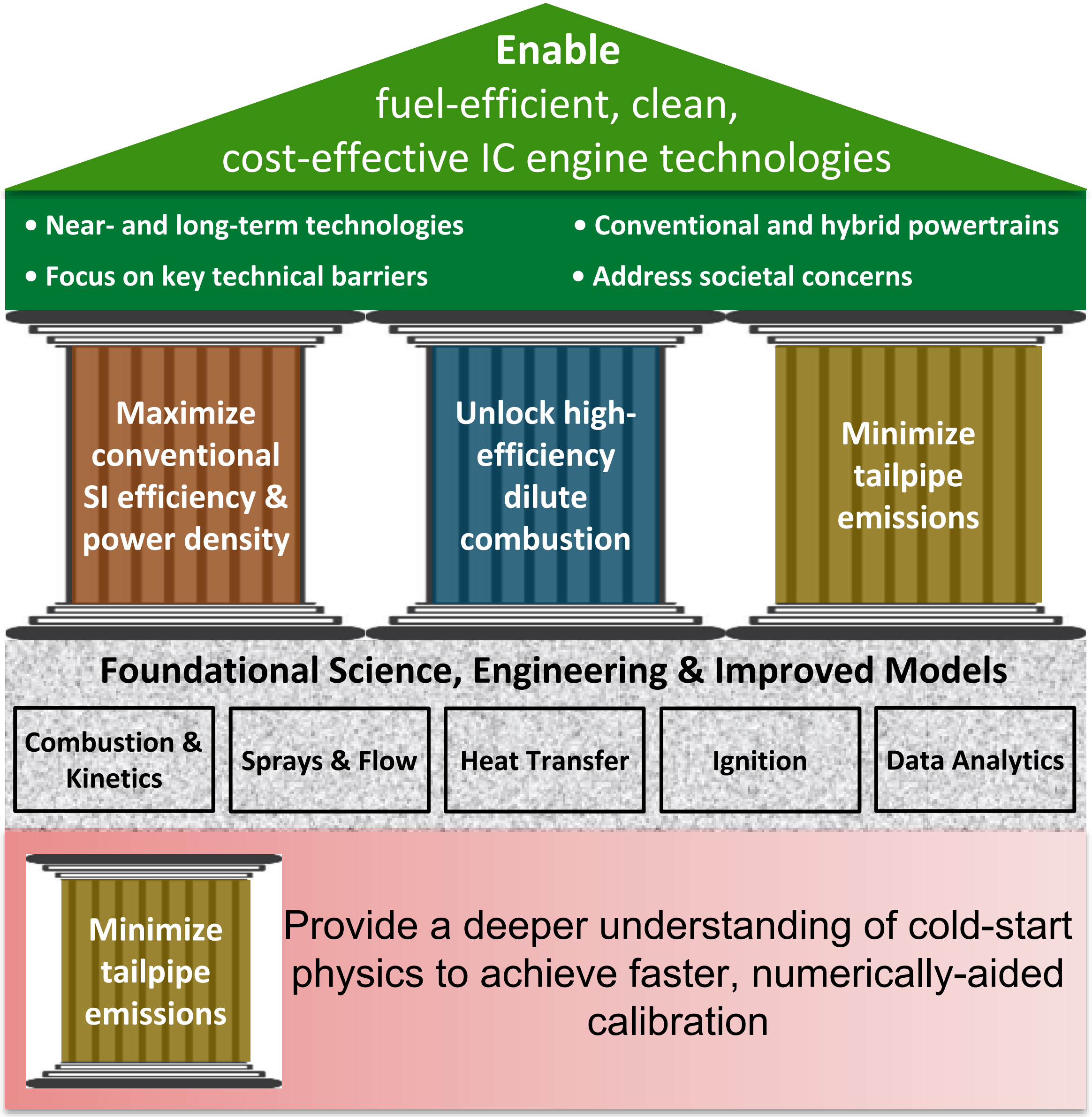
Barriers

- **US DRIVE Priority 1:**
  - **Reduced cold start emissions**
  - Understand and improve dilute combustion strategies during cold start & cold operation to reduce emissions
  - Improve modeling tools to rapidly evaluate designs based on sound metrics

Partners

- **PACE is a DOE-funded consortium of 6 National Labs. working towards a common goal (c.f. ACE138)**
  - Goals and work plan developed considering input from stakeholders including DOE, ACEC Tech Team, commercial CFD vendors, and more
- **Additional partners:**
  - 15 industry partners in the AEC MOU
  - PACE Soot Working Group coordinates tasks
  - PACE leadership team for setting directions and objectives
  - Soot activities as part of the Engine Combustion Network
  - Soot task of the International Energy Agency
  - Convergent Science Inc. software

Relevance: The role of the Soot Working Group



Relevance and Objectives of PACE MO8

- Combining unique capabilities to enhance scientific understanding/knowledge and improve engine design tools
- This will enable the OEMs to use new simulation tools and knowledge to make an engine performance breakthrough
- **Major Outcome 8:** Validated cold-start modeling capability that accurately predicts injection and spark timing trends on combustion phasing and emissions at catalyst warm-up conditions

Objectives of the Soot Working Group

- Coordinate experiments and model development aiming at better soot predictions in engines
  - Focus on cold-start, where most PM emissions come from
- Follow and provide feedback about leadership guidelines
- Work with other working groups within PACE
  - ACE139: Chemical Kinetic Models for Surrogate Fuels (Scott Wagnon)
  - ACE144: Spray Wall Interactions (Lyle Pickett)
  - ACE145: Cold Start Modeling and Experiments for Emissions Reduction (Dean Edwards)
- At the technical level, the Soot Working Group is tasked with:
  - Developing and providing kinetic mechanisms for PAH chemistry
  - Developing and providing superior yet usable soot models
  - Advanced soot measurements under atmospheric and relevant conditions
  - Comprehensive model validation procedure

Soot Working Group Organization and Technical Approach

Experiments

- Counter-flow flames
  - PAH speciation
  - Soot volume fraction
- Shock-tube data
  - PAH reactions & rates
- Spray vessel data
  - Fuel pyrolysis
  - Wall film experiments
- Engine experiment s
  - Soot sources
  - Cold-start soot emissions

- Experimental data from a variety of facilities and diagnostics to address the gaps and provide the necessary knowledge under relevant conditions
  - Structured approach from fundamental experiments to engine-out soot measurements

Kinetics and Soot model developments

- Kinetic mechanism
- Soot sectional method
- Method of moments
- Phenomenological models*

Knowledge transfer

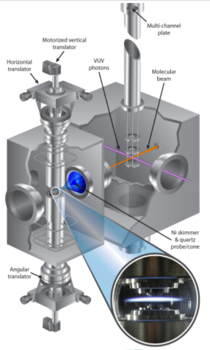
- Wall-film & flame DNS
- Pyrolysis simulations (RANS & LES)

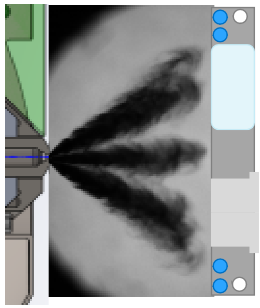
Other modeling activities

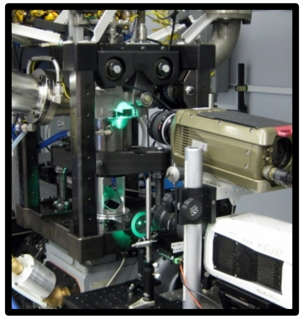
Deliverables

- Detailed & reduced PAH Mechanisms
- Sectional & Method of moments soot models

Validated "CFD-Ready" Models







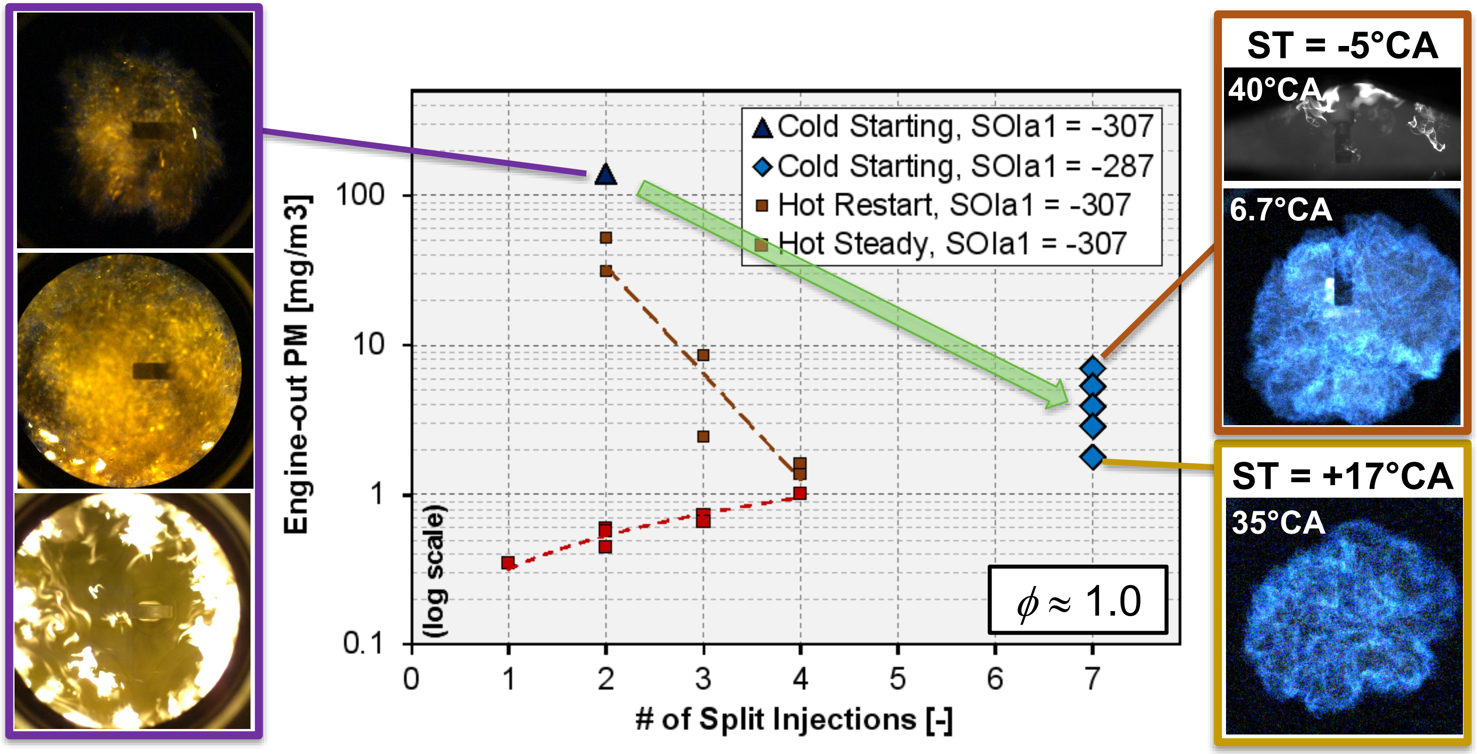
- Soot sectional method used to understand the physics needed for accurate predictions
- Knowledge transfer to "industry-friendly" method of moment model
  - Possibility to integrate knowledge into refined phenomenological models
- Modeling objectives are to capture trends and provide concentrations to within one order of magnitude across relevant conditions

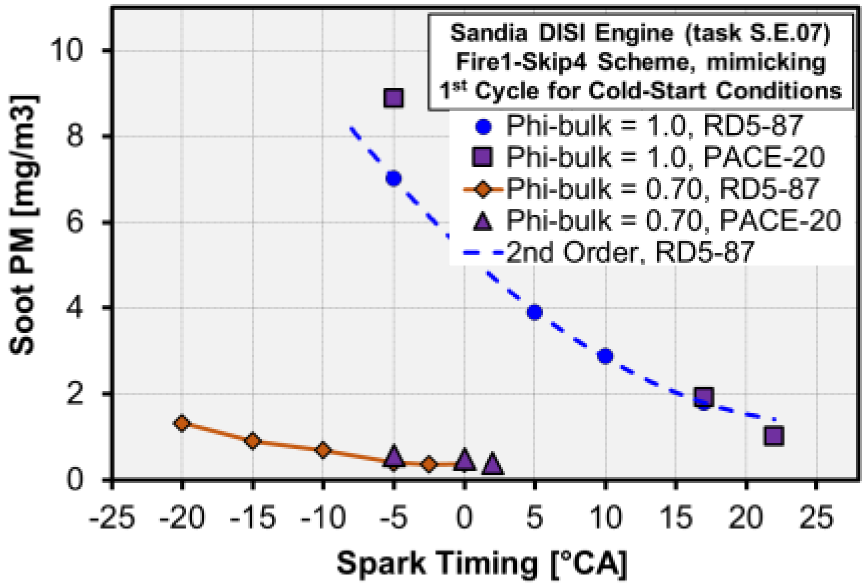
Milestones

Task & PI	Description of Milestone	Due Date	Status
S.E.07 Sjoberg	Transfer to Muhsin Ameen at ANL validation data for baseline well-mixed operating points for Outcome 5, for operation with and without 30% EGR	FY21Q2	Complete
S.E.02 Manin	Quantify soot formation rate and soot yield for various fuels and conditions relevant to GDI via fuel pyrolysis pathway	FY21Q2	Complete
S.E.02 Manin	Quantify wall film thickness, near-wall temperature distribution and soot concentration to understand film-based soot formation processes	FY21Q4	On Track
L.M.01.02 Kukkadapu	Deliver to PACE a reduced pyrolysis mechanism for TPRF + ethanol	FY21 Q1	Complete
S.M.02.03 Hansen	Develop, validate, (and publish online) the semi-empirical PAH mechanism for PACE target fuels	FY21Q4	On Track
A.01.03 Pitz	Improved model for PAH and soot predictions validated against PAH and soot measurements in premixed and counter-flow diffusion flames for neat fuels and TPRF (toluene, n-heptane & iso-octane). Also validated against soot measurements in combustion spray chamber for gasoline fuel(s)	FY20 Q2	Complete
S.M.02.02 Nguyen	DNS of end-gas ignition under boosted conditions, flame-wall interaction and soot	FY21Q4	On Track

Identification of soot sources during cold-start in engines

- All-metal experiments show that optimal injection schedule varies greatly with the thermal condition of the engine
- A typical double-injection schedule can cause excessive soot during cold start leading to:
  A. Bulk-gas soot
  B. Near-wall soot pockets (pool fires)



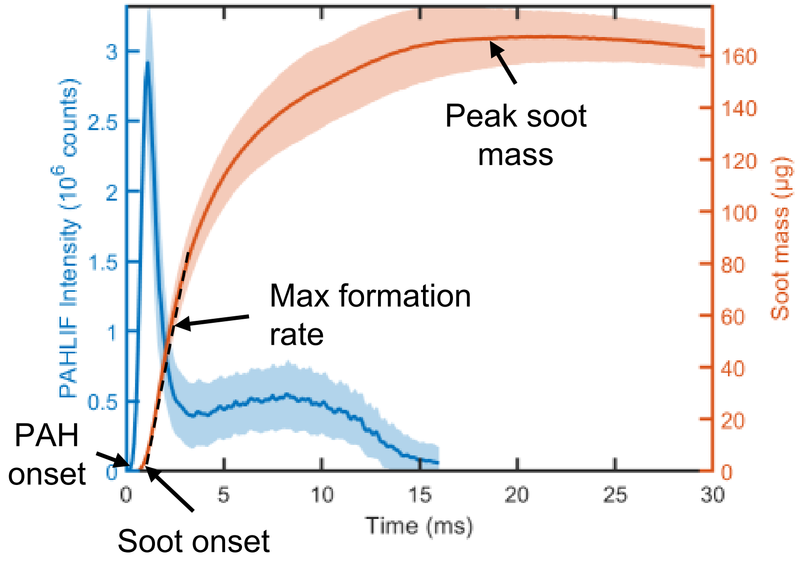


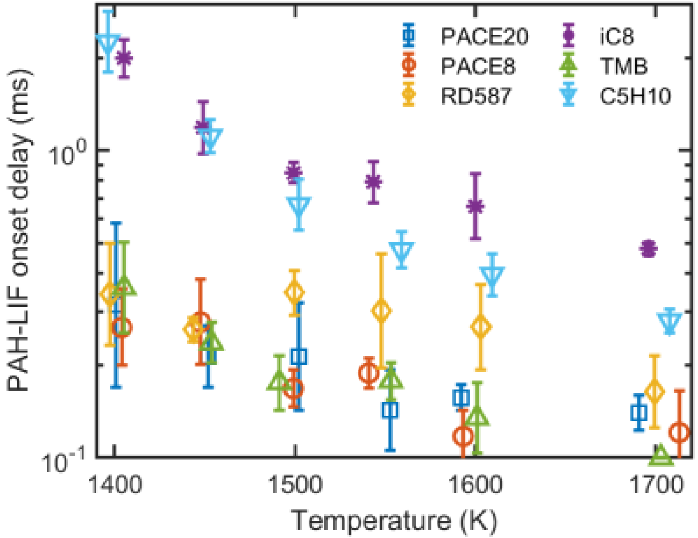
- Retarded SOI_{a1} and multiple short injections show promise to minimize soot PM for cold conditions
- Soot PM emissions depend largely on spark timing (ST) and CA50
  - Advanced ST shows diffusion flames attached to intake valve seat and injector tip
- PACE-20 surrogate fuel reproduces the soot PM trends of RD5-87 really well
  - Soot emissions for both fuels are mostly within 30 % across the tested range

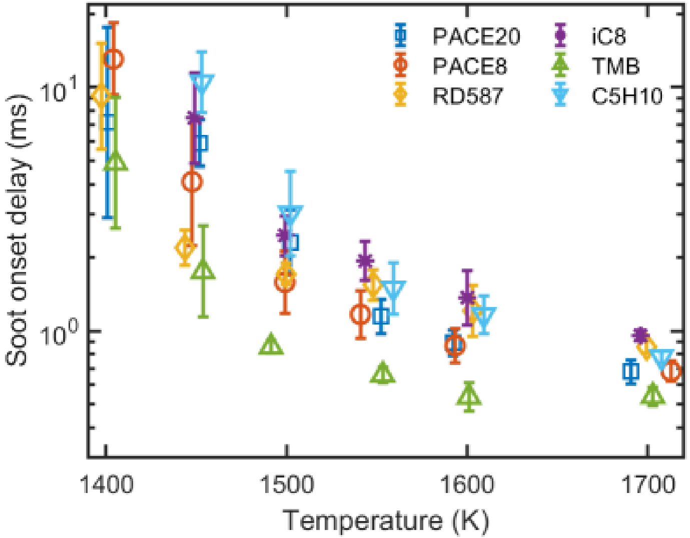
PAH and soot measurements under fuel pyrolysis conditions

- Pyrolyzing spray experiments can be used to assess sooting propensity under engine-relevant conditions
  - DBI-EI diagnostic for time-resolved soot onset, formation rate and total mass
  - High-speed 355-nm PAH LIF to simultaneously monitor PAH onset and growth
    - LIF diagnostic mostly detects 3- and 4-ring aromatics

PACE Fuels (PMI)	RD5-87 (1.68), PACE-8 (1.54) & PACE-20 (1.50)
Single-components	1,2,4-trimethylbenzene, iso-octane & cycle-pentane
Amb. pressures	38, 76 and 114 bar
Amb. temp.	1400, 1450, 1500, 1550, 1600 & 1700 K





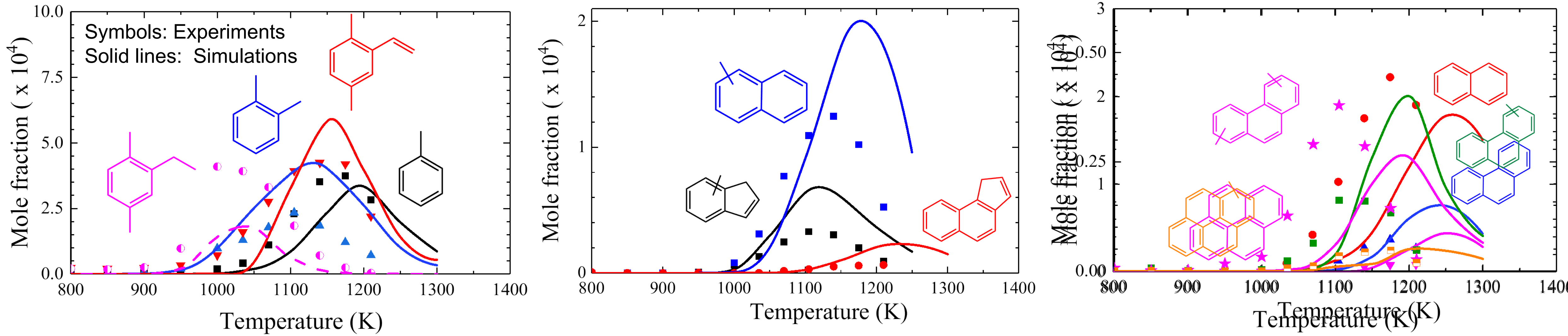


- RD5-87 target fuel and its surrogates behave almost identically in PAH and soot characteristics
- Fuels with aromatics tend to have the highest propensity to form PAHs and soot
  - Trimethylbenzene forms PAHs and soot the fastest among the studied fuels
  - Iso-octane and cyclopentane are in a slower class of PAH and soot formation compared to the other fuels
- Overall good correlations between PAH and soot onset timings for the different fuels

Improved pyrolysis chemistry of 1,2,4-trimethylbenzene helps predict sooting tendency of PACE-20

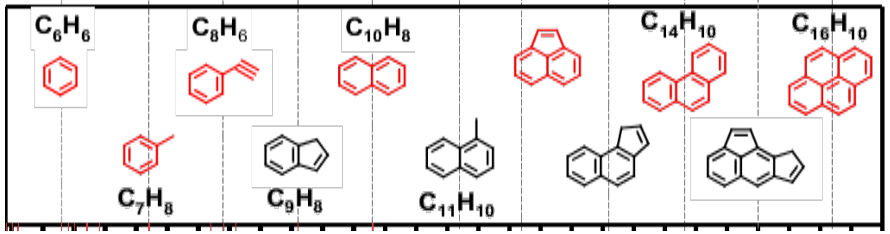
- Trimethylbenzene is a key component of PACE-20 (11.9 % by vol.)
  - It likely is the main contributor to soot formation in the blend
- Pyrolysis chemistry of trimethylbenzene is complicated primarily because of the high degree of molecular branching
  - Important pyrolysis reactions are also largely unknown

Jet Stirred Reactor measurements from USTC, China - *Data unpublished*



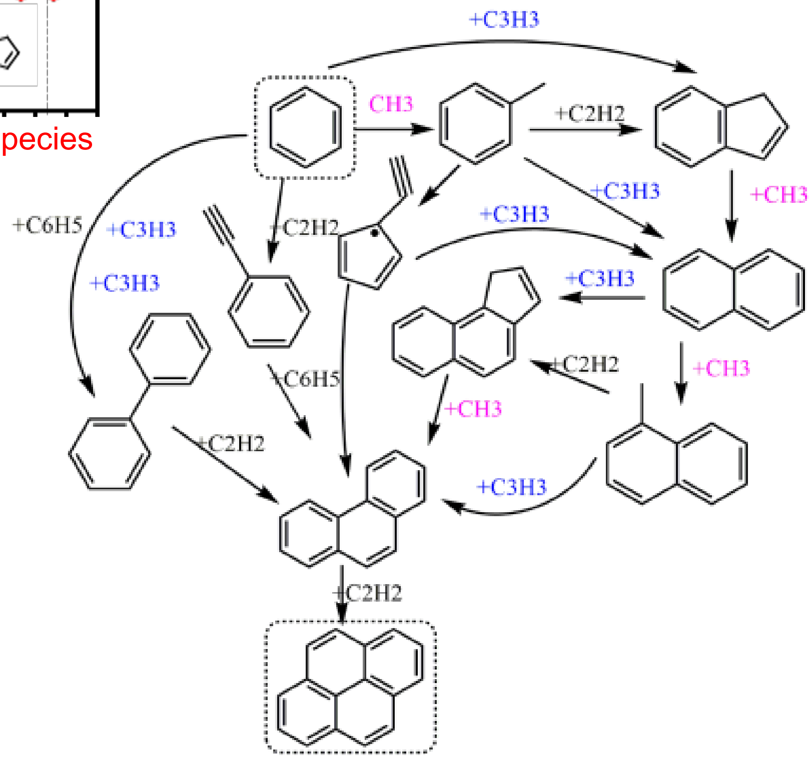
- Formation of 3- and 4-ring aromatics which link the PAH mechanism to the soot model is well captured by the newly developed detailed mechanism
- Mono- and di-methyl A3 and A4 aromatics have been detected in significant concentrations in the experiments
  - These aromatics are not generally detected in the pyrolysis of toluene, and aliphatic hydrocarbons
  - The simulation results demonstrate that the kinetic mechanism captures these species concentrations well

Reduced PAH mechanism from reaction flux analysis

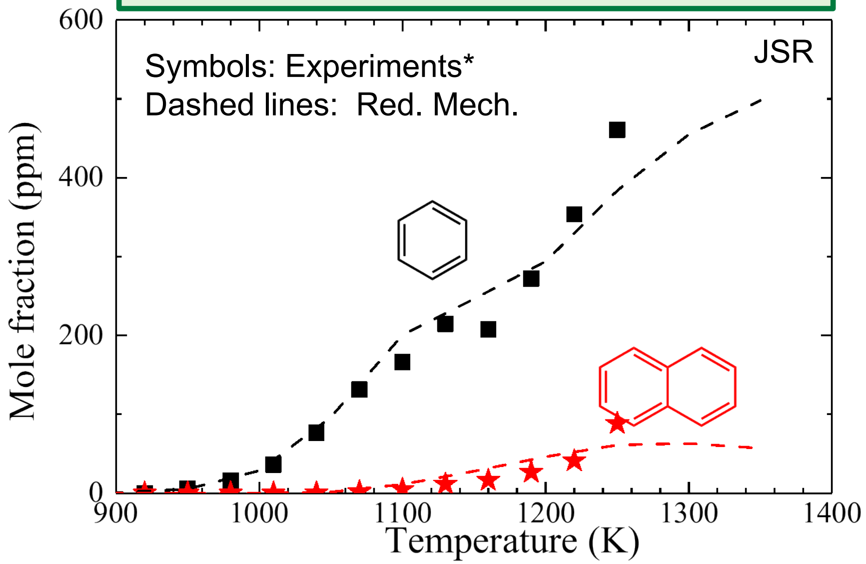


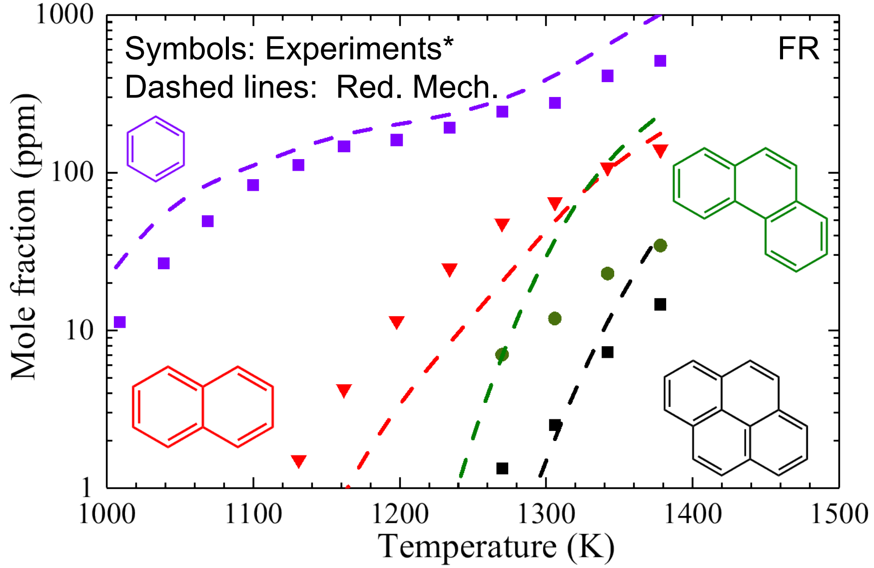
Identified stable isomer species

- Repetitive molecular growth reactions to model the formation of key 1- and 4-ring aromatics detected in flames
- Molecular growth modelled via:
  - HACA pathways
  - Radical + Radical recombination reactions
  - Ring enlargement reactions
- Reaction pathways and associated rate parameters adopted from ab-initio calculations



n-heptane/iso-octane/toluene mixture (91 RON)





- Reduced mechanism validated against jet stirred reactor (JSR) and flow reactor(FR) data
  - Pyrolysis of n-heptane/iso-octane/toluene mixtures into key PAHs is well captured by the reduced mechanism

* Experimental data from Shao et al. Proc. Combust. Inst. 2019

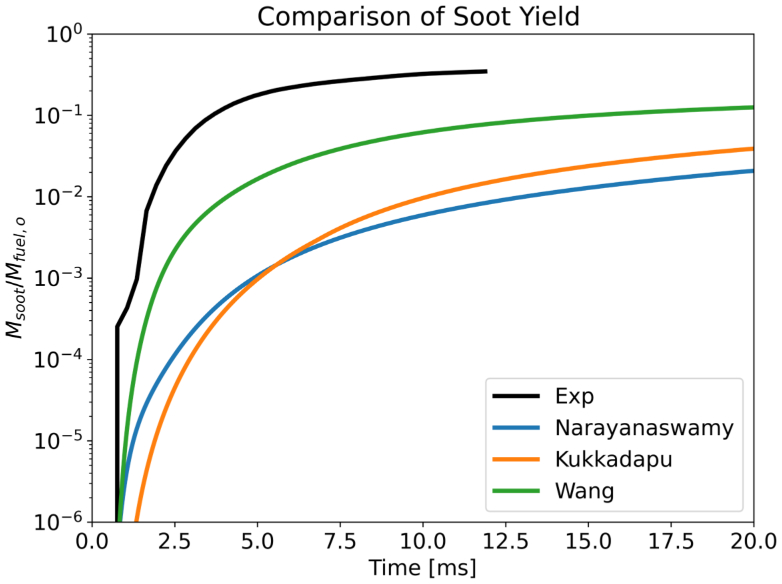
Evaluation of kinetic mechanism effects on soot formation

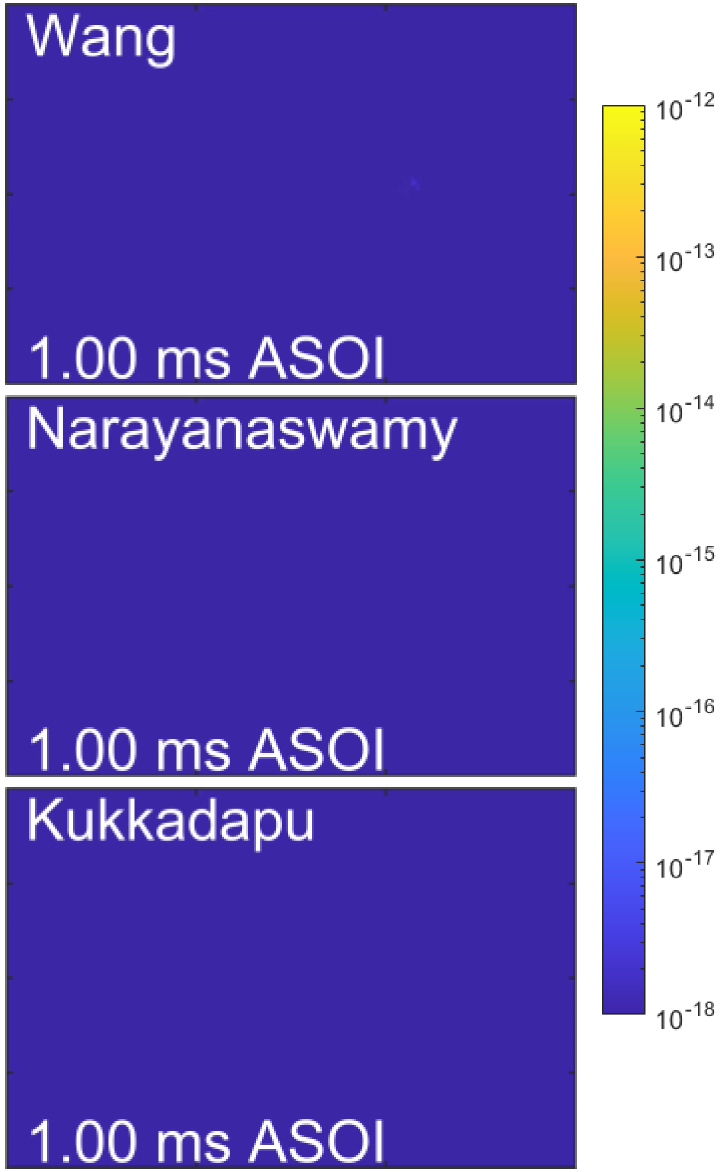
- 3-D RANS CFD simulations of soot formation via pyrolysis with different kinetic mechanisms
  - Sectional method model in CONVERGE (Particulate Size Mimic)
  - N-dodecane fuel, P_{amb} = 76 bar, T_{amb} = 1500 K, 0% O_2
  - Short injections (<200 µs) to isolate chemistry from evaporation and mixing

Mechanism	Nb of Species	Nb of Reactions	Soot Precursor
Wang	100	432	A_4
Narayanaswamy	255	1509	A_4
Kukkadapu	872	5611	A_4R5

A_4: 4-ring aromatic (pyrene)
A_4R5: Cyclopentapyrene

- Consistent simulation results and good visual agreement with the experiments
- Soot mass (or yield) is largely underpredicted
  - Significant differences between kinetic mechanism, both in formation rate with time and peak soot yield
  - Even the most detailed kinetic mechanism is over an order of magnitude below
  - Details about the kinetics leading to soot formation are paramount

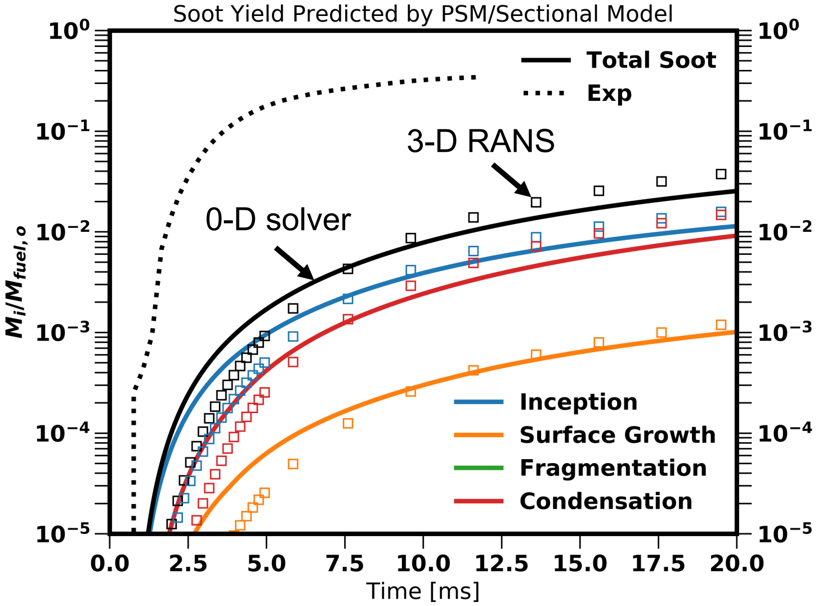




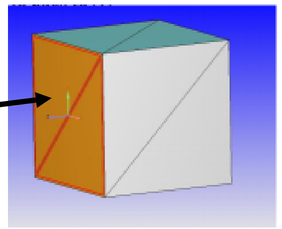
Detailed examination of soot models via 0-D simulations

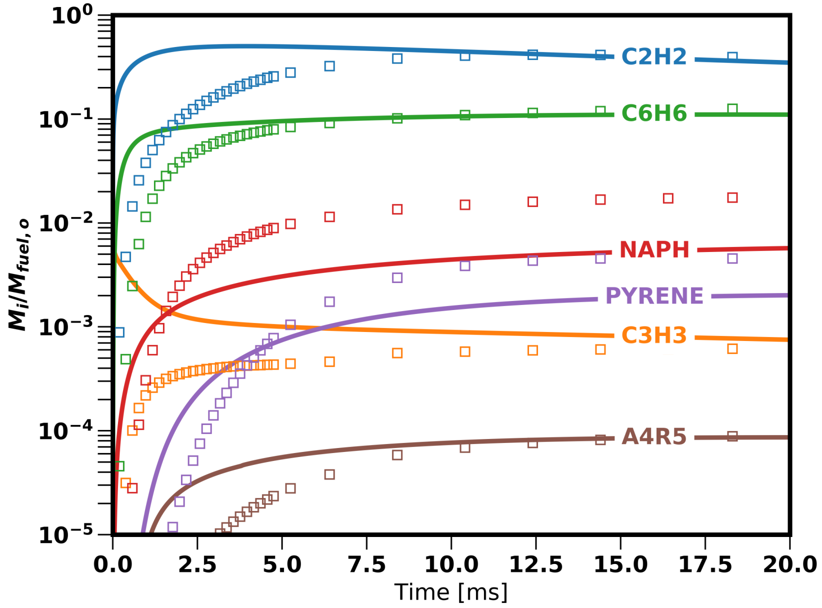
- Even with RANS-based calculations, 3-D CFD simulations are still very expensive
  - Existing 0-D or 1-D commercially-available chemical solvers are computationally inexpensive, but do not include advanced soot models
- A 0-D* approach was introduced using a simple cubic (8 cells) domain to convert CONVERGE CFD into a constant pressure 0-D solver
  - About a million times cheaper than typical 3-D calculations but similar fidelity
  - Virtually all kinetic mechanisms can be accommodated
  - Offers the ability to perform longer simulations or large parametric studies

Kukkadapu (872-species) mechanism



Constant Pressure

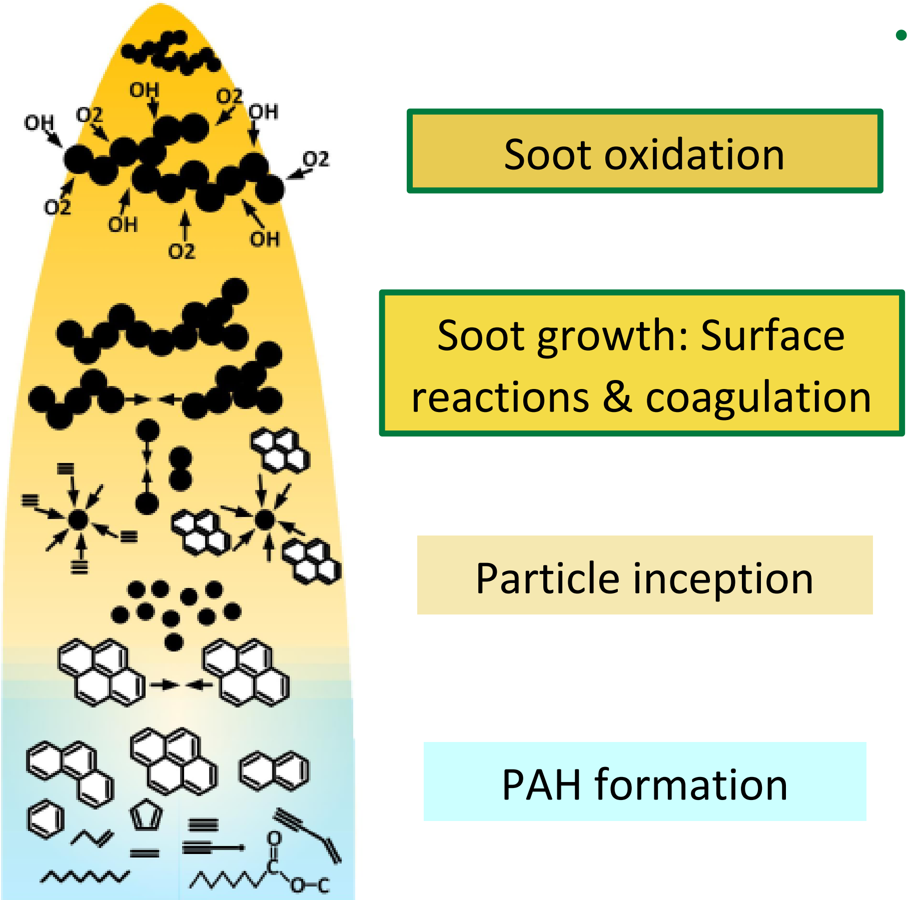




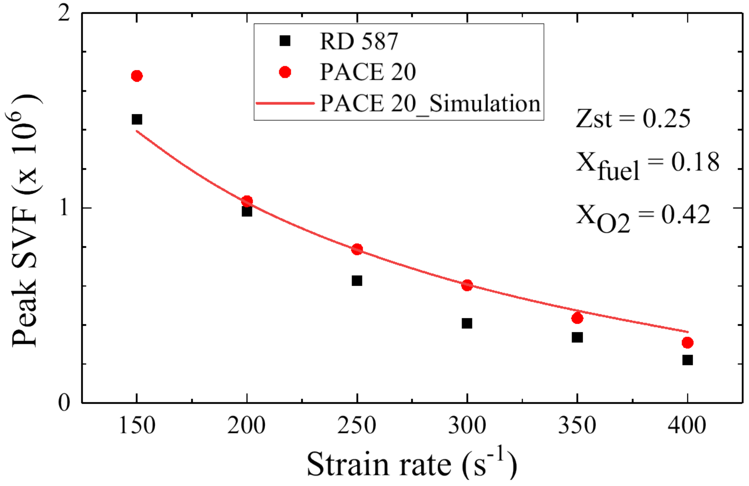
- Comparisons to 3-D RANS calculations for soot processed show good agreement
- A closer look at the kinetics related to soot formation reveals well matched quantities
  - Noticeable variations in formation rates at relevant time scales
- Comparisons to the experiments regarding PAH and soot onset timing or formation rate suggest that commonly used precursors may not be appropriate
  - The results strongly support the importance of kinetic mechanisms (especially for PAHs)

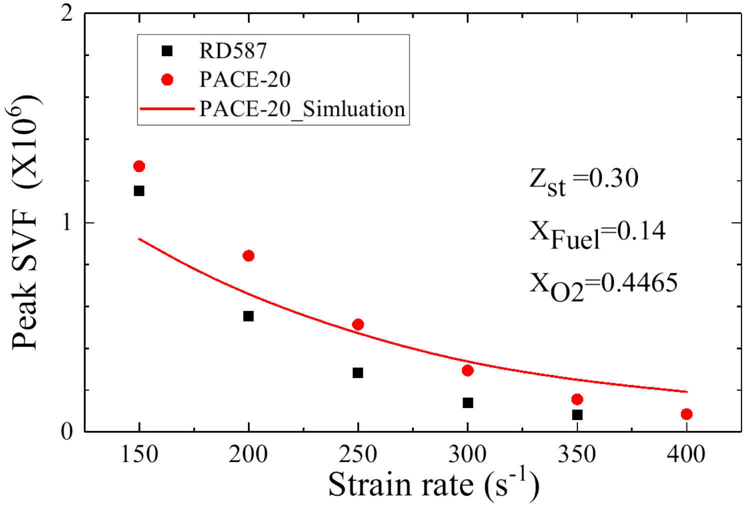
* 0-D solver approach was proposed by Adam Dempsey (Marquette University)

Sooting tendencies of RD5-87 and PACE-20 are well captured by newly developed soot model



- New soot model is based on an advanced sectional scheme
  - Designed to work in conjunction with the PAH mechanism
  - Advanced sectional method keeps track of detailed molecular information (such as H/C) to more accurately describe total soot mass
  - Improvements made to describe
    - Surface growth
    - Oxidation of soot particles using information from ab-initio reactions of PAH radicals with oxygen, acetylene and propargyl radical
  - Future work will focus on improving key steps such as nucleation and coagulation of soot

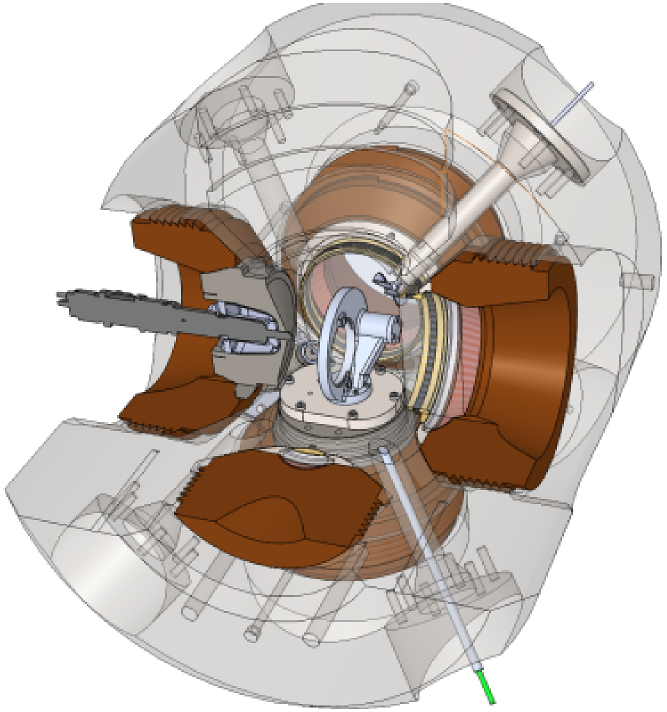




- Comparisons to the experiments demonstrate that soot volume fraction predictions are within a factor of two across the validation range
  - Also validated against counter-flow flame data from ethylene, n-heptane, iso-octane, toluene, TPRF fuels and showing good agreement
  - Next step is to benchmark the soot model against soot experiments at high pressure conditions

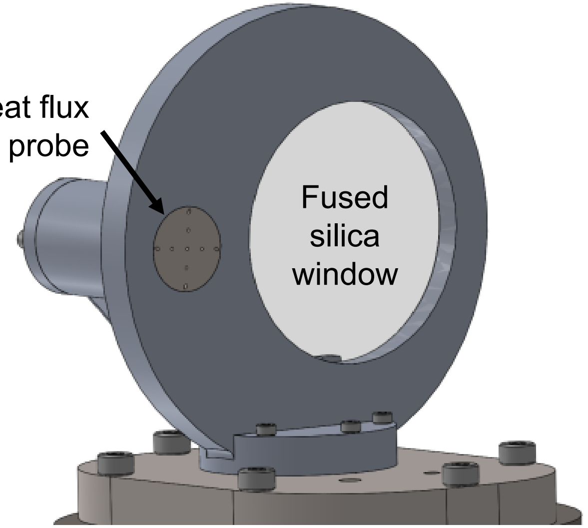
LLNL sub-contract with UCONN
Data unpublished

Experimental approach and temperature-controlled wall

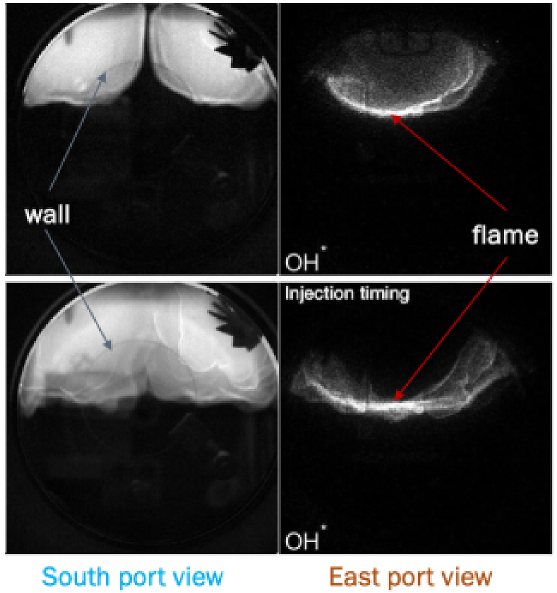


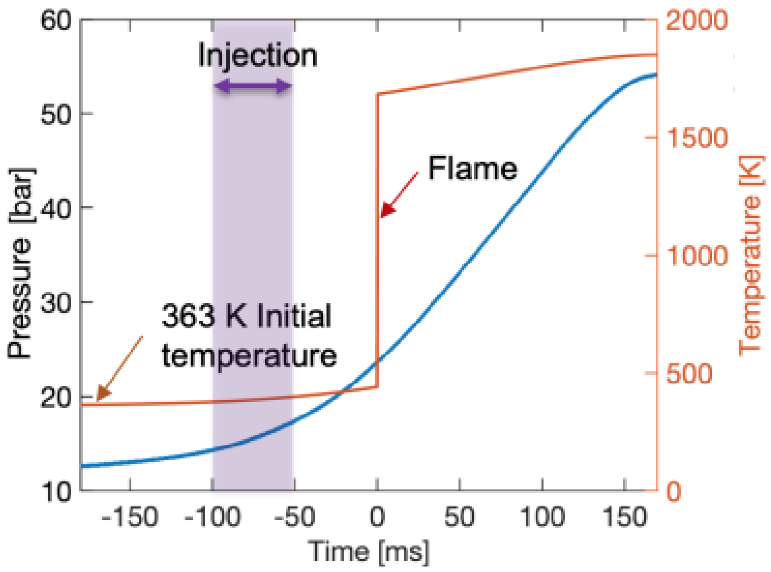
- Upgraded facility can produce films of varying thickness
  - Accurate control of fuel and ambient temperature, as well as ambient pressure
  - Temperature-regulated optical wall with heat-flux probe
  - Defined PACE target conditions can be met

Parameter	Value
Amb. temp.	20 - 188°C
Amb. density	6 - 12 kg/m^3
Wall temp.	20 - 188°C
Wall distance	40 (60) mm
Fuel temp.	20 - 90°C



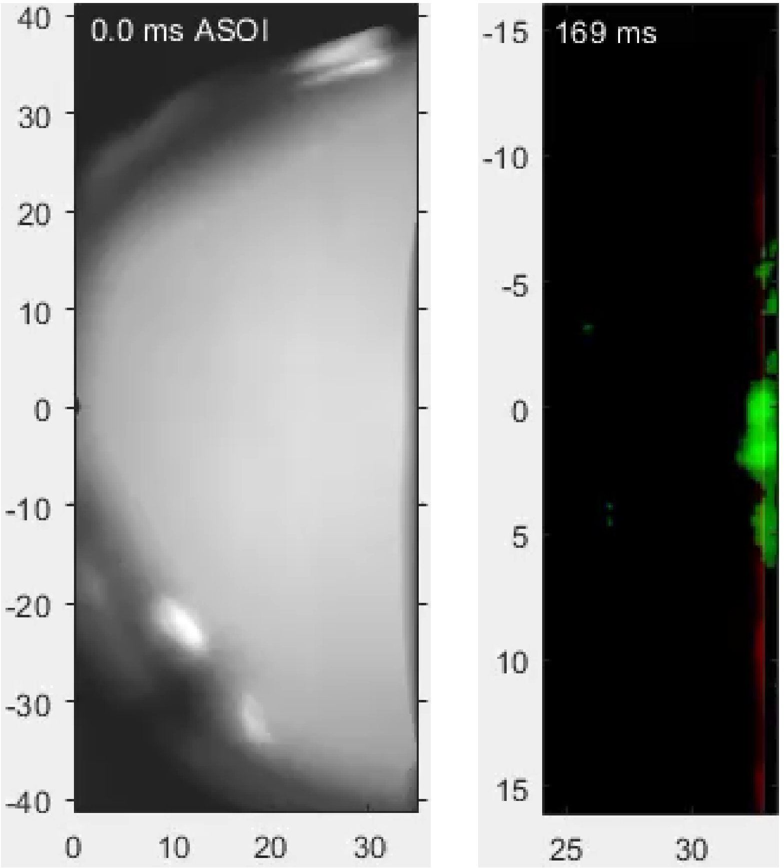
- Stoichiometric mixture is spark-ignited above the wall
  - Flame development characterized via pressure measurement and high-speed chemiluminescence
- Flame develops and propagates, increasing pressure and temperature
  - Temperature increase is location-dependent, while pressure increase is global and gradual
  - Injection is timed over a range with respect to the flame





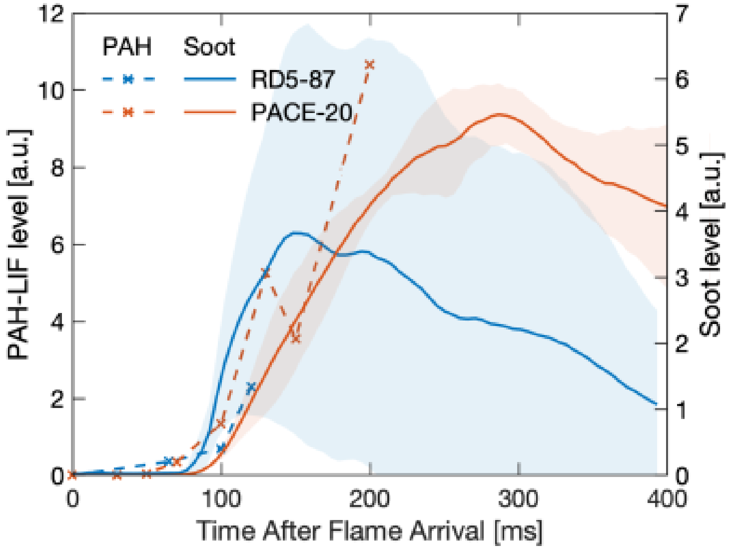
c.f. ACE144 (Lyle Pickett) about spray-wall impingement and film formation

Measurements of PAH and soot from wall-film experiments



- Buoyancy-induced convective flow promotes turbulence, film evaporation and soot formation
- Soot levels in the field of view indicate that soot production increases with time
  - Soot production rate appears to scale with liquid film evaporation
  - Gradual rise in pressure and temperature is likely to enhance soot production and increase soot yield
- The soot formation process is slow compared to what is typically observed in engines
  - Soot formation extends hundreds of milliseconds after the flame
  - Ambient conditions such as temperature (higher temperatures) or oxygen concentration (non-zero) may need to be explored

- Simultaneous high-speed PAH LIF measurements highlight the transition from PAHs to soot in a spatio-temporal manner
  - PAH LIF signal is observed long before any soot is detected (in relative time-scales)
  - There is a clear passage from PAH to soot
  - PAHs are also detected throughout the time soot is formed



Spray A-3 single-hole injector
90°C fuel, wall & amb. temp.
32-mm wall distance

Responses to Previous Year Reviewers' Comments

S.E.07 Sjoberg	This task was reviewed in two FY20 AMR presentations and received generally positive comments. Reviewer 1 for *ACE149* commented on the approach: "However, it is not certain if soot modeling can be accurate for a wide range of cold-start operation as the current surrogate fuel showed a big difference with the reference fuel RD5-87 in higher exhaust heat flux range". Response: During FY21, cold-start experiments with the finally selected PACE-20 surrogate revealed that it can reproduce both soot PM and PN trends of the RD5-87 gasoline as shown in the Accomplishments for this task (Slide 6).
S.E.02 Manin	This research was presented in *ACE144* in FY20. It was well received, and reviewers had overall very positive comments and feedback about this work.
L.M.01.02 Kukkadapu	This task was part of *ACE149* for FY20. Reviewer 5 raised concerns about the poor performance of the kinetic model for tetralin: "Yield sooting index (YSI) measurement validation is "complete," but the simulated YSI for tetralin, a key component planned for use to represent heavy, high boiling point components, is off by nearly 35% from the experimental measurement. It is not clear how this is a successful validation, given the offset and importance of this molecule to the PACE surrogate". Response: We will work on tetralin in the upcoming quarters, and are talking to our collaborators about acquiring datasets for validation of tetralin pyrolysis chemistry. Trimethylbenzene was identified as a key component related to soot and significant effort has been dedicated to improving its pyrolysis chemistry.
S.M.02.03 Hansen	This is a new task and no related task was presented last year.
L.M.01 Pitz	This research, presented in *ACE149* in FY20, was split into two tasks for FY21. The reviewers' comments about the work related to PAHs and soot are being addressed in L.M.01.02 (Kukkadapu).
S.M.02.02 Nguyen	This is a new task and no related task was presented last year.

Collaboration and Coordination with Other Institutions

S.E.07 Sjoberg	• Co-Optima AED Team Lead, which includes multiple efforts pertaining to fuel effects on soot formation, development of fuel sooting propensity metrics, as well as methods for curtailing in-cylinder soot formation.
S.E.02 Manin	• Lead or co-lead on soot activities the Engine Combustion Network and the International Energy Agency • Collaborating with nearly 10 institutions on problems related to soot formation in gasoline and diesel • Co-lead of PACE Soot Working Group • Working with engine research groups at SNL (Sjöberg) and ORNL (Jatana) to study the effects of cold-start condition on soot
L.M.01.02 Kukkadapu	• Co-lead of PACE Soot Working Group • Collaboration with 4 National Labs as part of the work related to PACE • University collaborations: King Abdullah University of Science and Technology (KAUST), National University of Ireland – Galway (NUIG), University of Connecticut (UCONN), University of Central Florida (UCF), Advanced Industrial Science and Technology (AIST, Japan), Univ. of Science and Tech. of China (USTC)
S.M.02.03 Hansen	• Collaborating with researchers in National Laboratories such as SNL, LLNL, and ANL as part of PACE • Collaborations with RWTH Aachen (Germany), University of Hawaii
L.M.01 Pitz	• Collaboration with 4 National Labs as part of the work related to PACE • University collaborations: King Abdullah University of Science and Technology (KAUST), National University of Ireland – Galway (NUIG), University of Connecticut (UCONN), University of Central Florida (UCF), Advanced Industrial Science and Technology (AIST, Japan)
S.M.02.02 Nguyen	• Collaborate with LLNL to evaluate detailed chemical kinetics and their impacts on soot models • Collaborate with IFPen to validate their new Sectional Soot Model

Remaining Challenges and Barriers

S.E.07 Sjoberg	• Current DISI engine has somewhat limited optical access for diagnosing soot formation associated with fuel films on the outer portions of the piston top
S.E.02 Manin	• Optical arrangement and complexity limits the reach of advanced diagnostics to study fundamental aspects at relevant conditions • Limited range of applicability of LIF diagnostic for PAHs because of laser attenuation, signal trapping and LII signal from soot • Large experimental variability in film evaporation and soot formation related to in-chamber temperature distribution and flow
L.M.01.02 Kukkadapu	• Better understanding of pyrolysis chemistry of tetralin • Understanding of pressure, temperature on nucleation and coagulation of soot
S.M.02.03 Hansen	• Fuel-structure dependence of the importance of formation pathways of larger PAHs • Developing a physical-chemical understanding of soot nucleation
L.M.01 Pitz	• Current state-of-the-art in soot modeling for engine applications is still missing key physics to reliably capture soot formation
S.M.02.02 Nguyen	• Uncertainty with the correct PAHs to soot dimerization process in engines • 0-D approach generate TBs of dataset across all conditions, making detail analyses of all soot relevant chemistry very time consuming • The link between 0-D model to reacting high speed spray with soot formation is still unclear

Future Research

S.E.07 Sjoberg	• Perform additional measurements for MO8 (cold-start), now without intake tumble plate • Identify and measure key in-cylinder soot formation processes and how those are affected by the intake-generated flow field • Enhance the optical access to the outer regions of the piston top
S.E.02 Manin	• Soot film experiments and pyrolysis with variation in ambient oxygen concentration (0 – 3%) • Soot measurements from non-wall sources, such as dribble at the end of injection • Develop diagnostic to measure film temperature and assess evaporation rate
L.M.01.02 Kukkadapu	• Improving the pyrolysis chemistry of neat components: tetralin • Validation of the PAH and soot model against spray chamber experiments from Sandia • Validation of the soot model against engine data under normal and cold start conditions • Transferring features of the sectional soot model to in-built models in Converge
S.M.02.03 Hansen	• Reducing this mechanism even further while maintaining reliability and carrying the necessary inception species • Collaborate with CFD modelers to simulate soot measurements from reacting sprays
L.M.01 Pitz	• Explore various soot models with 3-D RANS/LES for both pyrolysis and oxidizing conditions • Test the pyrolysis simulations with reduced kinetic models and improved inception mechanism
S.M.02.02 Nguyen	• Examine how each and all soot precursors (A1, A2, A3, A4) affect the soot inception process • Derive new soot inception rates based on experimental measurements provided by Manin • Extend the 0-D approach to include oxidizing condition • Extend 0-D approach to 1D configuration to understand strain effect on soot model

Summary

S.E.07 Sjoberg	• The in-cylinder soot formation varies greatly with both the injection schedule and the thermal state of the engine • By tailoring the injection schedule, it is possible to achieve relatively clean combustion during a cold-start sequence • The PACE-20 surrogate reproduces the engine soot PM and PN trends of RD5-87 well, making it suitable for further experiments and modeling efforts
S.E.02 Manin	• RD5-87 target fuel and its surrogates behave almost identically in PAH and soot characteristics under fuel pyrolysis conditions • Preliminary experiments about wall-film soot formation shows that soot forms long after flame passes over film, as fuel vapor undergoes pyrolysis • Good correlation between PAHs and soot for both free spray fuel pyrolysis and wall-film soot formation
L.M.01.02 Kukkadapu	• Developed Reduced ETPRF mechanism to model oxidation and pyrolysis of TPRF + ethanol fuels needed for DNS simulations • Improved pyrolysis chemistry of trimethylbenzene, one of the major source of soot for PACE-20 • Developed an improved sectional model for soot which captures soot levels within a factor of two in laminar diffusion flames of PACE-20 and RD5-87
S.M.02.03 Hansen	• Repetitive chemical reaction sequences are used to develop a chemical mechanism for PAH formation • The reduced mechanism shows promising performance when compared to fundamental flame experiments
L.M.01 Pitz	• Soot formation is highly dependent on the kinetic mechanism • Even state-of-the-art models soot models fail at predicting soot formation under high-pressure fuel pyrolysis conditions
S.M.02.02 Nguyen	• 0-D model provides a computationally-efficient tool to systematically evaluate detailed chemical kinetics in combination with engine-relevant soot models

Soot Modeling and Experiments

Technical Back-Up Slides



Complete PACE Budget FY21

Code and Work Flow Development

		Lab	PI	FY20	FY21
A.M.05.01	Spray and Combustion model implementation	ANL	Ameen	350k	340k
A.M.05.02	Gridding, validation, and workflow development	ANL	Ameen	350k	300k
A.M.05.04	MO1 Integration	ANL	Som		75k
A.M.05.05	MO5 Integration	ANL	Scarcelli		75k
L.M.05.01	Accelerated multi-species transport in engine simulations	LLNL	Whitesides	275k	250k
L.M.05.02	Improved chemistry solver performance with machine learning	LLNL	Whitesides		250k
L.M.05.04	Scalable performance and CFD integration of ZERO-RK	LLNL	Whitesides	275k	75k
L.M.05.06	Mechanism Reduction	LLNL	Whitesides		75k
L.M.05.07	Accelerate Mechanism Reduction Tools	LLNL	Whitesides		75k

Cold Start

		Lab	PI	FY20	FY21
O.E.07	Multi-cyl Cold Start & surrogate testing	ORNL	Curran	350k	350k
S.E.07	Engine experiments characterizing wall films & PM formation	SNL	Sjoberg	270k	270k

Combustion and Emissions

		Lab	PI	FY20	FY21
O.E.02	Effectiveness of EGR to mitigate knock throughout PT domain	ORNL	Szybist	220k	175k
S.E.02	Experiments supporting particulate modeling -- wall film & pyrolysis	SNL	Manin	500k	400k
L.M.01	Improved Kinetics for Ignition Applications	LLNL	Pitz	150k	
S.M.02.01	DNS and modeling of turbulent flame propagation & end gas ignition	SNL	Chen	50k	50k
S.M.02.02	Flame wall interactions	SNL	Nguyen	150k	50k
S.M.02.03	Engineering PAH Model Development	SNL	Hansen		100k

Data Analytics

		Lab	PI	FY20	FY21
O.E.08	Machine Learning and Nonlinear Dynamics	ORNL	Kaul	200k	200k

Flows and Heat Transfer

		Lab	PI	FY20	FY21
O.E.06.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	100k	100k
O.E.06.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	200k	200k
O.M.06	Conjugate heat transfer	ORNL	Edwards	350k	350k
LA.M.06.01	Heat Transfer through Engine Metal - - -	LANL	Carrington	200k	
LA.M.06.02	Heat Mass Transfer in Liquid Species - - -	LANL	Carrington	200k	

Flows and Heat Transfer

		Lab	PI	FY20	FY21
O.E.06.01	Neutron diffraction for in situ measurements in an operating engine	ORNL	Wissink	100k	100k
O.E.06.02	Neutron Imaging of Advanced Combustion Technologies	ORNL	Wissink	200k	200k
O.M.06	Conjugate heat transfer	ORNL	Edwards	350k	350k
LA.M.06.01	Heat Transfer through Engine Metal - - -	LANL	Carrington	200k	
LA.M.06.02	Heat Mass Transfer in Liquid Species - - -	LANL	Carrington	200k	

Fuel Kinetics and Surrogates

		Lab	PI	FY20	FY21
A.E.01	Measurements of autoignition fundamentals at dilute gasoline conditions	ANL	Goldsborough	280k	252k
L.M.01	Surrogates and Kinetic Models	LLNL	Pitz	500k	425k
L.M.01.02	Models for improved prediction of PAH/soot	LLNL	Kukkadapu	200k	200k

Ignition

		Lab	PI	FY20	FY21
A.M.03	Advanced Ignition Modeling Tools	ANL	Scarcelli	400k	370k
N.M.03	ML based LES ignition model	NREL	Yellapantula	275k	275k
S.M.03.01	DNS of early ignition kernel development	SNL	Chen	100k	100k
S.M.03.02	Physics based flame-kernel LES modeling	SNL	Nguyen	100k	100k
A.E.03	Fundamental Ignition Experiments	ANL	Rockstroh	380k	342k
S.E.03.01	Advanced Ignition to Enable Alternative Combustion Modes	SNL	Ekoto	420k	420k
S.E.03.02	Fundamental ignition experiments	SNL	Ekoto	420k	420k

LSPI

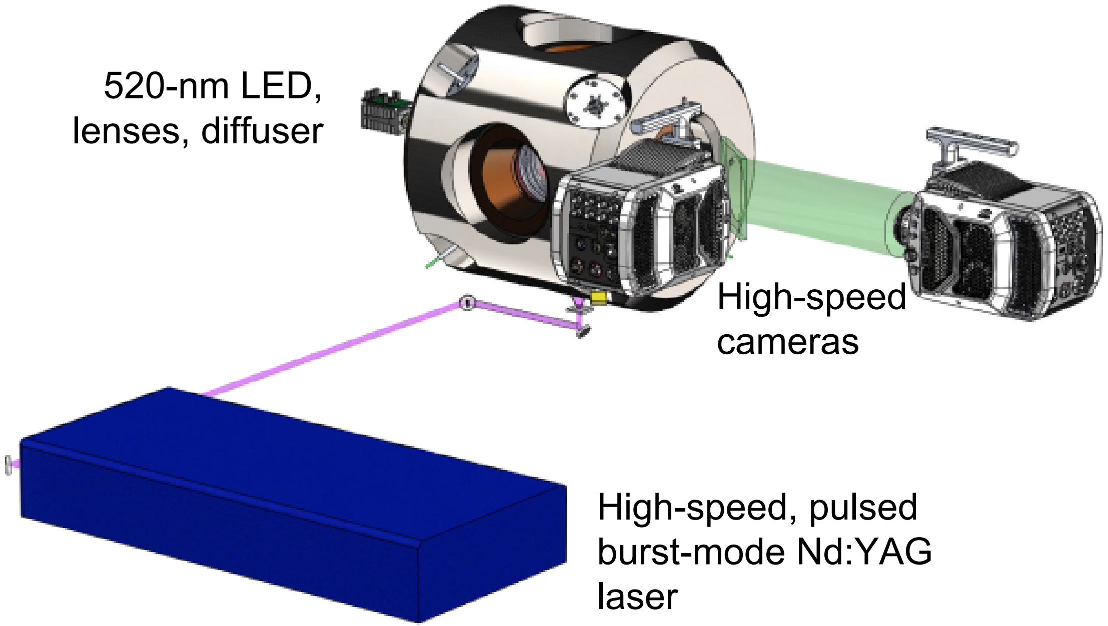
		Lab	PI	FY20	FY21
O.E.09.01	Fuel spray wall wetting and oil dilution impact	ORNL	Splitter	220k	220k

Sprays

		Lab	PI	FY20	FY21
A.E.04	X-Ray Studies of Fuel Injection and Sprays	ANL	Powell	490k	441k
O.E.04.01	Injector Characterization & Distribution	ORNL	Wissink		125k
S.E.04	Spray Experiments	SNL	Pickett	380k	380k
S.E.04.03	GDI sprays leadership & data sharing	SNL	Pickett	140k	140k
A.M.04	Towards Predictive Simulations of Sprays in Engines	ANL	Torelli	300k	220k
A.M.04.01	Improved free spray and spray-wall interaction modeling	ANL	Torelli		125k
LA.M.04.01	Simulate free sprays in chamber and engines - - -	LANL	Carrington	200k	
S.M.04.01	Free spray modeling	SNL	Nguyen	50k	50k
S.M.04.02	Free spray modeling addition	SNL	Tagliente		125k

High-speed diagnostics for fuel pyrolysis and wall-film experiments [S.E.02]

- High pressure and temperature experiments in constant-volume chamber
  - Denso (ECN) Spray A-3 injector (single-hole, 0.094 mm diameter)
  - Ambient temperature: 1400 – 1700 K
  - Ambient pressure: 3.8 – 11.4 MPa
  - Ambient oxygen concentration: 0 %
  - Injection pressure: 40 MPa (ΔP)
  - PACE fuels: RD5-87, T4-B1 and PACE # 8
  - Single-component fuels (PACE surrogate): 1,2,4-trimethylbenzene, iso-octane & cyclo-pentane

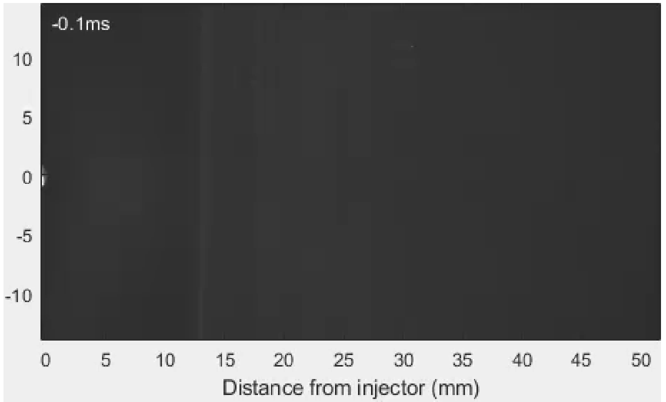


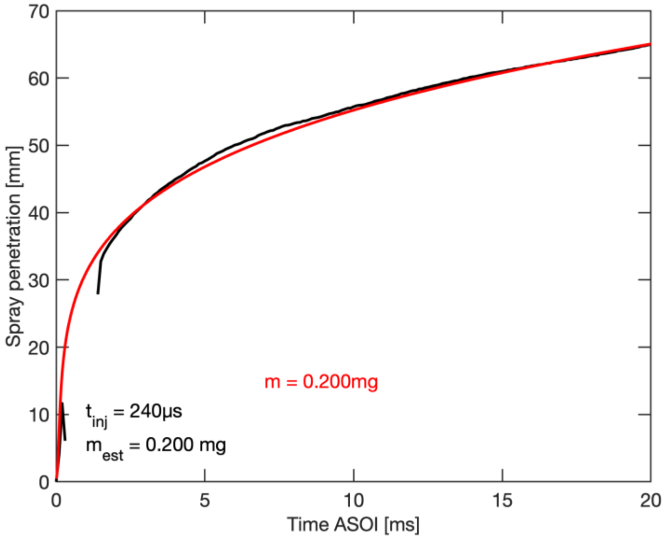
- Planar laser-induced fluorescence (PLIF) imaging measurements
- Pulse burst-mode 355-nm (THG) Nd:YAG laser
  - 10 kHz repetition rate, 50 mJ/pulse
  - 20-ms long burst
- High-speed CMOS camera with appropriate optics and filters

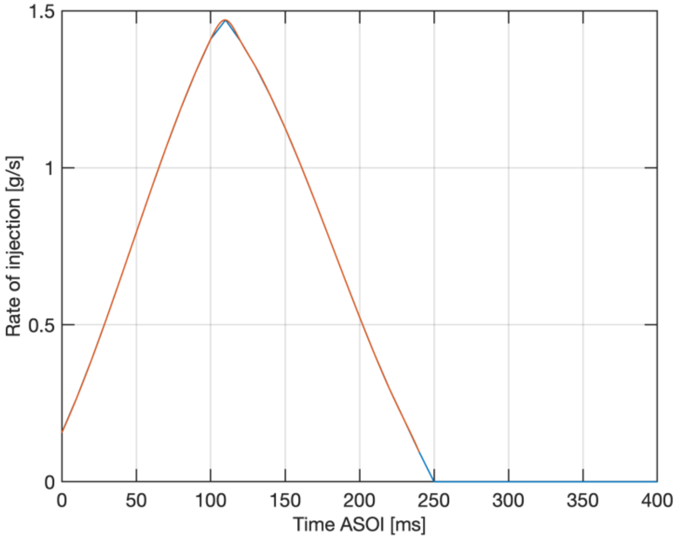
- High-speed diffuse back illumination extinction imaging to measure liquid length and quantify soot
  - High-speed CMOS camera, lens and filters
  - Pulsed violet/UV (centered at 520 nm) LED illumination
  - Skip-pulsed arrangement (10 kHz effective) for hot soot incandescence correction
- Dichroic beam-splitter for spectral separation and efficient collection

Boundary conditions for 3-D simulations of pyrolysis experiments [L.M.01]

- Injection characteristics such as Rate of Injection (ROI) and injected mass are estimated using a combination of internal flow simulation and 1-D jet model results
- Validation against experimental measurements show good agreement
  - Tip penetration rate
    - Injection duration and mass
  - Planar laser Rayleigh scattering imaging measurements
    - Mixture fraction comparisons to 3-D predicted mixing fields





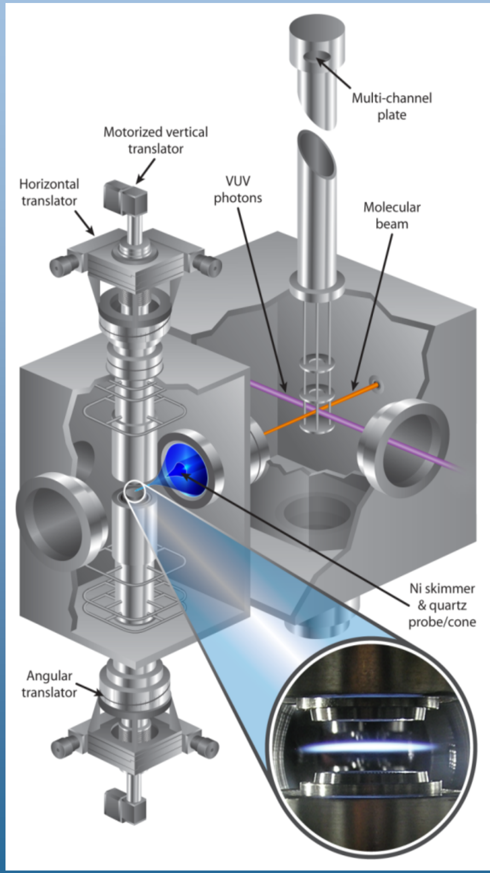


Numerical Set Up	
CFD Code	CONVERGE v3.0.17
Turbulence	RANS $k-\varepsilon$ STD
Minimum Cell Size	62.5 μm
Spray model	Lagrangian parcel
No. of parcel injected	200,000
Break-up model	KH-RT
Droplet drag and vaporization	Corrected Distortion Model
Droplet collision	No time counter (NTC)
Droplet dispersion	O'Rourke
Injection Method	Blob
Plume cone angle	21
Initial TKE	0.00502*

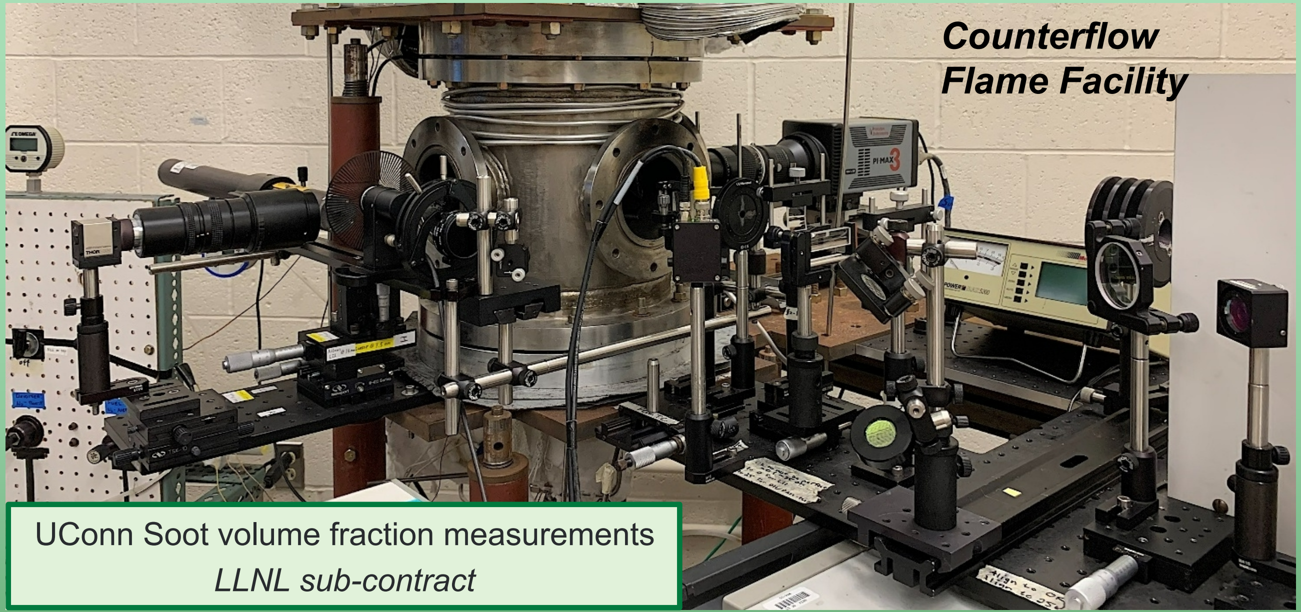
PACE PARTNERSHIP TO ADVANCE COMBUSTION ENGINES

Counterflow flame experiments to validate new soot model [L.M.01.02]

- Counter-flow diffusion flame experiments at Sandia will focus on identifying key PAHs contributing to soot formation



Sandia: PAH measurements
Nils Hansen



UConn Soot volume fraction measurements
LLNL sub-contract

- Validation experiments were conducted with RD5-87 target and PACE-20 surrogate fuels
  - LII calibrated via laser extinction and OH* chemiluminescence experiments
- UCONN Soot volume fraction measurements in counterflow diffusion flames
  - Aromatics/alkane blends, RD5-87 and PACE Surrogate
  - Pressure: 1 to 3 atm.
  - O_2 concentration, Strain rate

Soot Modeling and Experiments

Reviewer-Only Slides

Publications & Presentations

S.E.07 Sjoberg	• The engine work related to soot processes has not been presented or published yet
S.E.02 Manin	• Manin, J. Pickett, L.M., Skeen, S.A. & Frank, J.H. "Image processing methods for Rayleigh scattering measurements of diesel spray mixing at high repetition rate", Applied Physics B 127:79, 2021 • Killingsworth, N., Nguyen, T. M., Brown, C., Kukkadapu, G., & Manin, J. "The role of chemical mechanism in simulations of high-pressure n-dodecane spray pyrolysis",12th U. S. National Combustion Meeting, May 2021 (Virtual) • Wan, K., Manin, J., Sim, H.-S. & Dempsey, A. "Soot and PAH formation from gasoline surrogate fuels in high pressure spray pyrolysis", AEC Program Review Meeting, Feb. 2021 • Nguyen, T. M., Manin, J., Tagliante, F., Killingsworth, N., Kukkadapu, G., Demsey, A. "Assessment of chemical kinetics for soot model development using Zero D simulations", AEC Program Review Meeting, Feb. 2021
L.M.01.02 Kukkadapu	• Killingsworth, N., Nguyen, T. M., Brown, C., Kukkadapu, G. & Manin, J. "The role of chemical mechanism in simulations of high-pressure n-dodecane spray pyrolysis",12th U. S. National Combustion Meeting, May 2021 (Virtual) • Nguyen, T. M., Manin, J., Tagliante, F., Killingsworth, N., Kukkadapu, G., Demsey, A. "Assessment of chemical kinetics for soot model development using Zero D simulations", AEC Program Review Meeting, Feb. 2021 • Kukkadapu, G. "Surrogate Formulations, Soot modeling and Reduced Mechanisms for Modeling Oxidation and Pyrolysis of Transportation Fuels", AEC Program Review Meeting, Feb. 2021 • Kukkadapu, G. "A new PAH mechanism for modeling pyrolysis of Gasoline and Diesel fuels", AEC Program Review Meeting, Aug., 2020
S.M.02.03 Hansen	• This work is very recent and has not been published yet
L.M.01 Pitz	• Killingsworth, N., Nguyen, T. M., Brown, C., Kukkadapu, G. & Manin, J. "The role of chemical mechanism in simulations of high-pressure n-dodecane spray pyrolysis",12th U. S. National Combustion Meeting, May 2021 (Virtual) • Nguyen, T. M., Manin, J., Tagliante, F., Killingsworth, N., Kukkadapu, G., Demsey, A. "Assessment of chemical kinetics for soot model development using Zero D simulations", 2021 AEC Program Review Meeting, Feb. 2021
S.M.02.02 Nguyen	• Killingsworth, N., Nguyen, T. M., Brown, C., Kukkadapu, G. & Manin, J. "The role of chemical mechanism in simulations of high-pressure n-dodecane spray pyrolysis",12th U. S. National Combustion Meeting, May 2021 (Virtual) • Nguyen, T. M., Manin, J., Tagliante, F., Killingsworth, N., Kukkadapu, G., Demsey, A. "Assessment of chemical kinetics for soot model development using Zero D simulations", 2021 AEC Program Review Meeting, Feb. 2021

Critical Assumptions & Issues

The barriers to maximum SI efficiency and power density, dilute combustion, and minimal tailpipe emissions can be overcome if the major outcomes of PACE are successful

Success in modeling formation of soot from well controlled laboratory experimental facilities (diffusion flames, spray reactors, wall film pyrolysis) would be adequate to model soot formation in cold start conditions and achieve major outcomes of PACE

S.E.07 Sjoberg	• The DISI engine hardware and operating strategies used for this research are appropriate for generating data that support the assessment of sources of soot and the development of high-fidelity CFD models, which in turn can aid in designing future engines that use different hardware and operating strategies
S.E.02 Manin	• The effects of beam steering on soot extinction are neglected for quantification • Soot optical properties vary widely in time but are considered constant in this research • They are also wavelength dependent and are known to affect measured soot mass (we present soot mass as measured via extinction at 520 nm).
L.M.01.02 Kukkadapu	• Little/No fundamental data on pyrolysis of some neat components (e.g., tetralin, trimethylbezene) needed for model validation • Need better understanding of effect or pressure, temperature and molecular size on nucleation
S.M.02.03 Hansen	• The quality (and uncertainty) of validation targets remains an issue
L.M.01 Pitz	• Validation targets related to PAH speciation under relevant conditions are rare and incomplete • Kinetic mechanism development is built on many assumptions regarding chemical kinetic pathways and reaction rates
S.M.02.02 Nguyen	• Soot modeling and evaluation of soot models assume accurate and reliable PAH kinetics