Lagrangian Soot Model Considering Gas Kinetics and Surface Chemistry

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Engine **R**esearch **C**enter

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Project ID #: ACS111

Overview

Timeline

- Project Start: January 2017
- Project End: December, 2018
- Percent complete: 40%

Budget

- Total project funding
  - DOE share: $441,727
  - Contractor share: $60,192
- Funding received in FY 2016
  - $103,178
- Funding for FY 2017
  - $163,957

Barriers

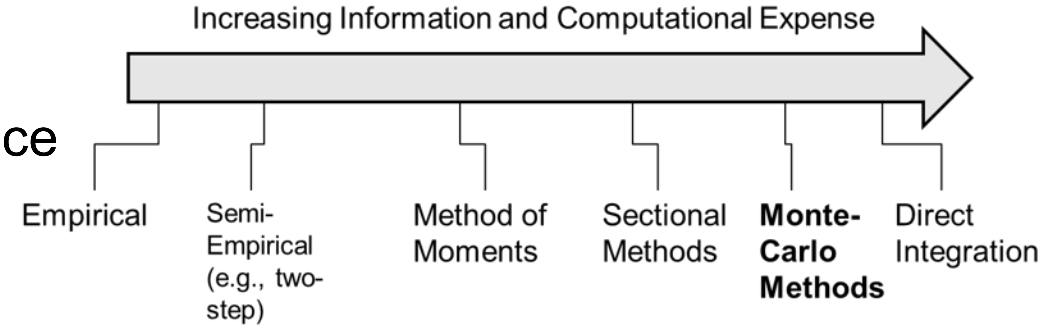
- Barriers addressed
  - Lack of fundamental knowledge of advanced engine combustion regimes
  - Lack of modeling capability for combustion and emission control

Partners

- Sandia National Labs
- Convergent Science Inc.
- University of Wisconsin – Madison Engine Research Center (Direct injection Engine Research Consortium ~ 35 member companies)

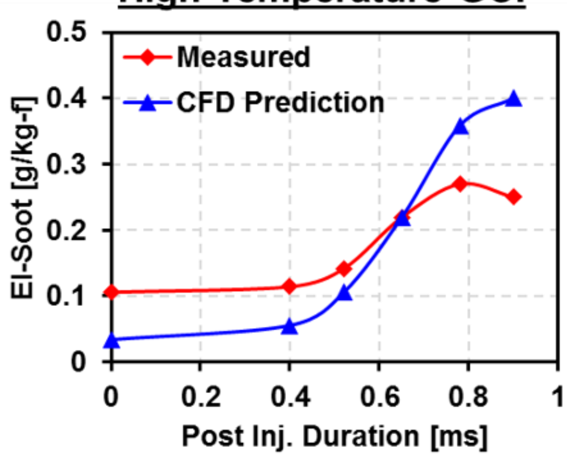
Relevance

- Current soot models range from empirical to detailed solutions of population balance equations → tradeoff in information and cost.

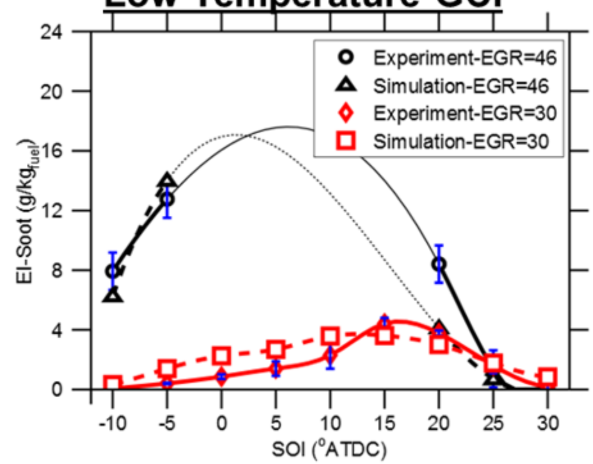


- Simple models can be "tuned" to capture soot trends and magnitudes → model coefficients vary by orders of magnitude as conditions change
- Overall project goals are to improve soot modeling capabilities and understanding of tradeoffs between computational cost and accuracy.

High Temperature GCI



Low Temperature GCI



$$\dot{M}_{sf} = A_{sf} M_{A4} P^{0.5} e^{\frac{-E_{sf}}{RT}},$$

	HTC	LTC
Asf	700	500
Esf	12,500	1,250

Objectives

Overall Objectives

- Develop high fidelity soot modeling capabilities that can be integrated into CFD codes to develop advanced combustion engines.
- Improve understanding of PAH and soot growth under engine relevant conditions using a combination of CFD simulations and optical engine experiments

Objectives Over the Past Year

- Define and validate PAH mechanism/multi-fuel chemistry model
- Develop Lagrangian based structure for soot particle storage
- Perform baseline validation experiments

Impact

- Improved soot modeling capabilities through detailed validation effort and implementation of detailed soot model that can either be used for direct simulation or "a priori" testing of simplified models
- Direct transfer to industry through collaboration with commercial code vendor (CONVERGE)

PAH: Polycyclic Aromatic Hydrocarbon
CFD: Computational Fluid Dynamics

Milestones

Budget Period	Milestone	Type	Description	Task #	Quarter	Status
1	Define PAH Mechanism	Technical	PAH mechanism is defined	1	1	Complete
	Implement PAH Mechanism	Technical	Reduced PAH mechanism is complete and implemented into the multi-fuel mechanism.	1	2	Complete
	Complete High Speed Imaging	Technical	High speed imaging under conv. diesel conditions is complete	2	3	Complete
	Complete Lagrangian Soot Framework	Technical	Coding is complete for Lagrangian soot framework in KIVA	2	4	Complete
	Validation of PAH mechanism	Go/No Go	Validation of the PAH mechanism using flame experiments from the literature.	1	4	Complete
2	Complete Coding	Technical	Coding is complete for Lagrangian soot framework	1	5	Complete
	Models Reproduce Fuel Distribution	Technical	CFD models reproduce measured fuel distribution	3	6	On Track
	Complete Metal Engine Experiments	Technical	Metal engine experiments are complete (including particle size distributions) at conv. diesel conditions	2	7	On Track
	CFD Models Reproduce Measured Parameters	Technical	CFD models accurately reproduce measured cylinder pressure, heat release rate, and combustion locations	3	8	On Track
	Soot model development completed	Go/No-Go	New soot model development completed	1	8	On Track
3	Complete Engine Experiments	Technical	Metal engine experiments are complete (including particle size distributions) at diesel LTC conditions	2	9	On Track
	CFD Models Accurately Capture PAH Growth	Technical	CFD models accurately capture PAH growth under engine conditions	3	10	On Track
	CFD Models Reproduce Measured Data	Technical	CFD models reproduce the measured soot mass, number density, and particle size distributions	3	11	On Track
	Compare New Soot Model to Existing Models	Technical	Results of the new soot model are compared to existing soot models and benefits and drawbacks documented	3	12	On Track

Methods and Approach

Simulation Approach

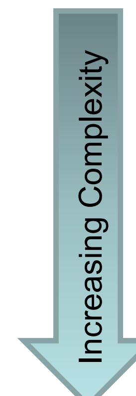
- Two CFD codes are used to ensure wide suitability of project findings: Open source: ERC KIVA (RANS) and Commercial: Converge (RANS/LES)

Experimental Approach

- Metal engine experiments (UW-Madison, C15 single cylinder research engine) – cylinder pressure, heat release, gaseous emissions/FSN, particle size distributions
- Optical engine experiments (Sandia CRF Heavy-duty Optical Engine) – cylinder pressure, heat release, limited gaseous emissions, FSN, combustion luminosity, PAH distribution and soot LII

Model Validation/Assessment Approach

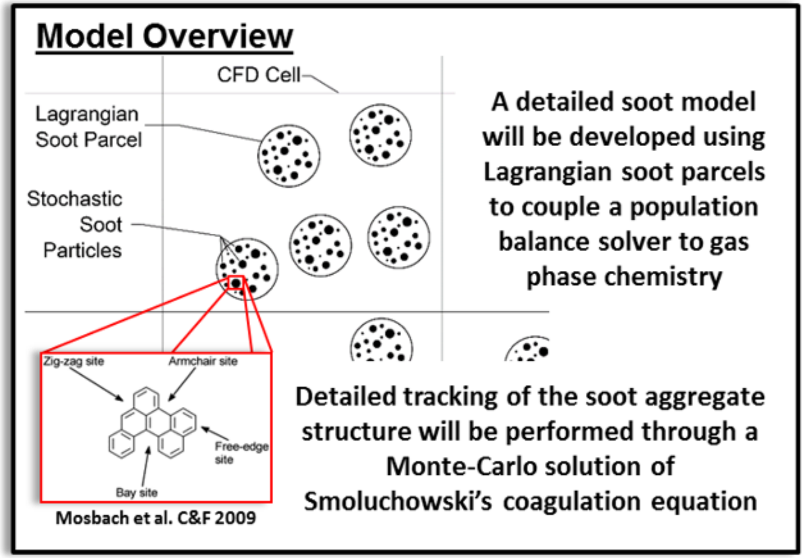
- Soot is sensitive to all upstream processes → Targeted validation effort is underway to validate sub-models important for soot prediction
  - Spray and mixing → TPLIF images from the literature
  - Chemical kinetics → ignition delay and laminar flame speeds
  - PAH growth → Flame species profiles and in-cylinder PAH PLIF (future work)
  - Spray, mixing, and ignition (engine combustion)
  - Soot mass and number → Flame PSD from literature and engine experiments (future work)



Soot Modeling Approach

Approach

- SWEEP population balance solver → Smoluchowski population balance equation solved using a Monte-Carlo particle technique
  - Balance of accuracy and computational cost between moment methods and direct integration
  - Enables prediction of soot makeup (C/H ratio, size, # density, etc…)
  - Arbitrarily precise solutions are possible → results converge with increasing number of stochastic particles (~512 – see backup slides).



- **Particle inception:** Two body collisions using transition kernel taken as harmonic mean of free molecular regime and slip flow regime
- **Surface reactions:** Arrhenius type equation considering effects of particle volume, mass, collision diameter, surface area, and active surface area
- **Condensation:** Collision between PAH and soot particle

Celnik, M.S. and Patterson, R.I.A., "Sweep – The Cambridge Soot Simulator", Cambridge, 2006.

Technical Accomplishments

- **UW – ERC:** Developed and validated multi-fuel chemistry/PAH mechanism. Performed detailed validation of upstream processes and engine combustion.

Spray and mixing (TPLIF from Literature) → Chemical Kinetics (ign. delay and flame speed from literature) → PAH growth (Flame species profiles from literature) → Engine Combustion

- **UW – ERC/CSI:** Developed Lagrangian particle storage framework to enable implementation of stochastic solution to population balance equations
- **Sandia CRF:** Performed baseline validation experiments

Multi-fuel/PAH Model Development

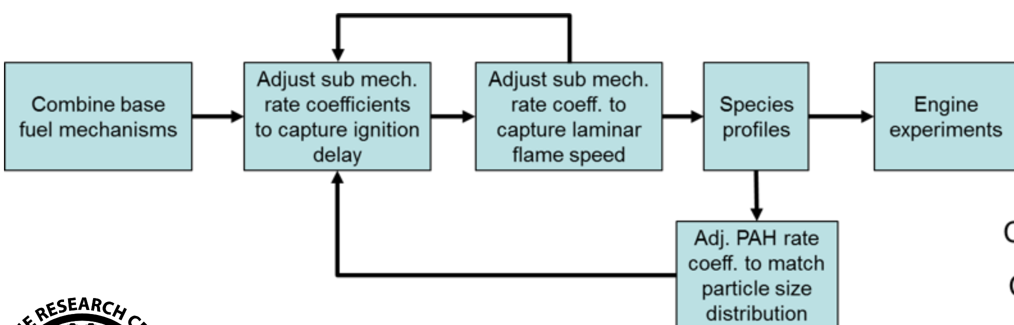
Accomplishments

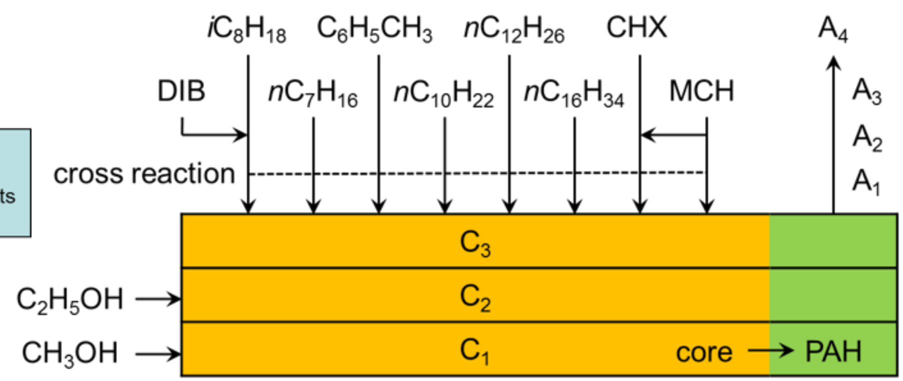
Approach

- Select well-validated sub-mechanisms from the literature and combine to a multi-fuel chemical kinetics mechanism
- Rate constants of sub-mechanisms adjusted using sensitivity analysis on ignition delay, laminar flame speed, and particle size distribution

Results

- 11-component chemical kinetic mechanism containing species capable of representing gasoline, kerosene and diesel fuel
- 178 species and 758 reactions. Co-oxidation reactions included.
- PAH to pyrene (A4) (included up to Benzo[A]pyrene, but little advantage was found)





Base Mechanism from Wang et al. Comb. Flame 2015 (http://dx.doi.org/10.1016/j.combustflame.2015.02.005)

Multi-fuel/PAH Model Validation

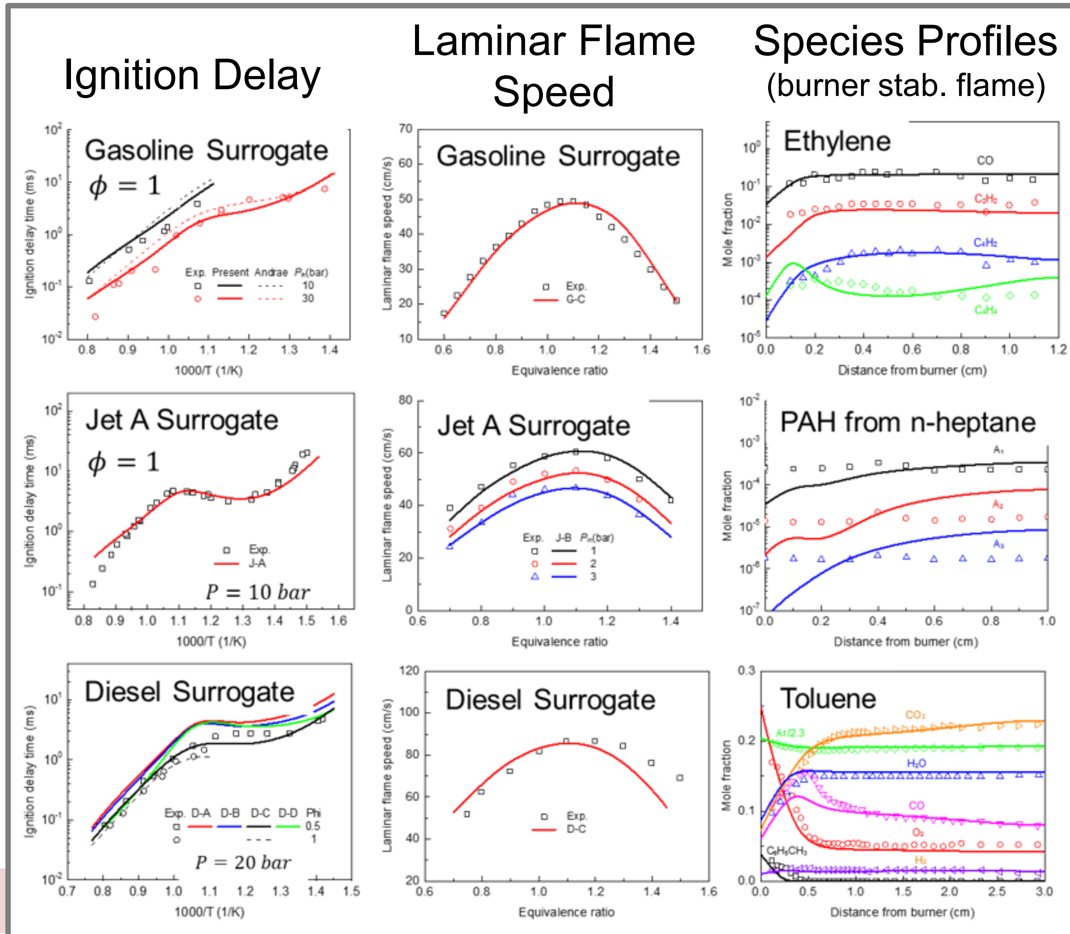
Approach

- Compare simulation results to ignition delay (ID), laminar flame speed (LFS), and species profiles (SP) for a range of single components, mixtures and surrogates from literature

Fuel	Single Comp.	Mixture
nC_7H_{16}	ID / LFS / SP	ID / LFS
iC_8H_{18}	ID / LFS / SP	ID / LFS
$C_6H_5CH_3$	ID / LFS / SP	ID / LFS
C_2H_5OH	ID / LFS / SP	ID / LFS
CH_3OH	ID / LFS / SP	ID / LFS
$nC_{10}H_{22}$	ID / LFS / SP	ID / LFS
$nC_{12}H_{26}$	ID / LFS / SP	ID / LFS
$nC_{16}H_{34}$	ID / LFS / SP	ID / LFS
DIB	ID / LFS / SP	ID / LFS
CHX	ID / LFS / SP	ID / LFS
MCH	ID / LFS / SP	ID / LFS
C_2H_4	SP	
Gasoline		ID / LFS
Jet A		ID / LFS
Diesel Fuel		ID / LFS

Results

- Mechanism accurately captures trends and magnitudes of ID, LFS, and SP for real fuels



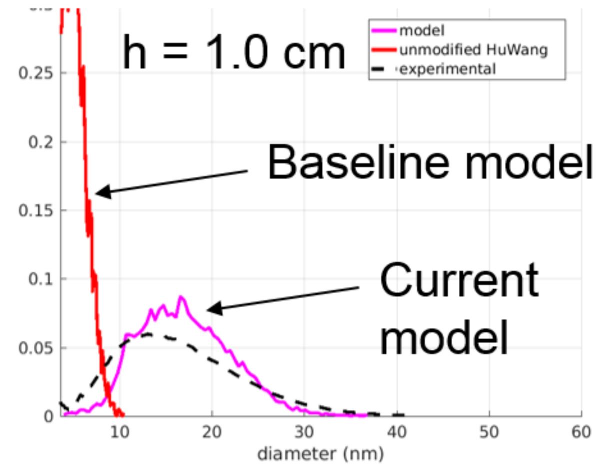
Additional validation in technical backup slides

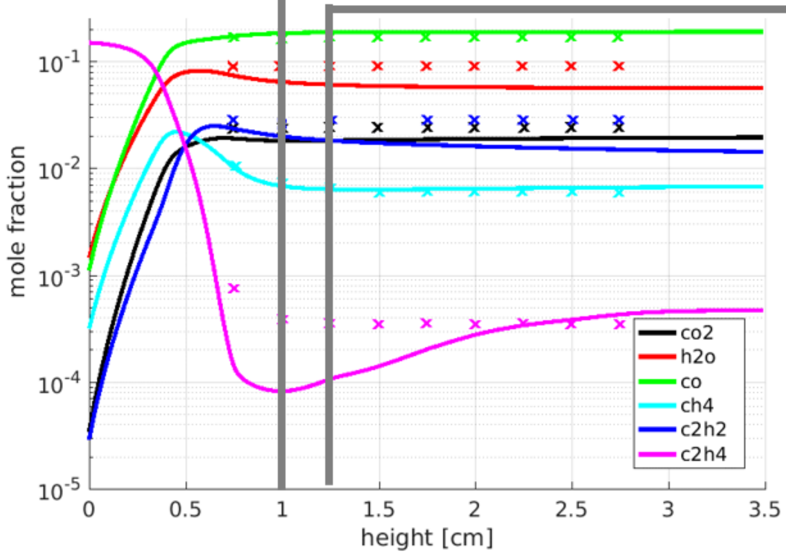
Particle Size Distribution Validation

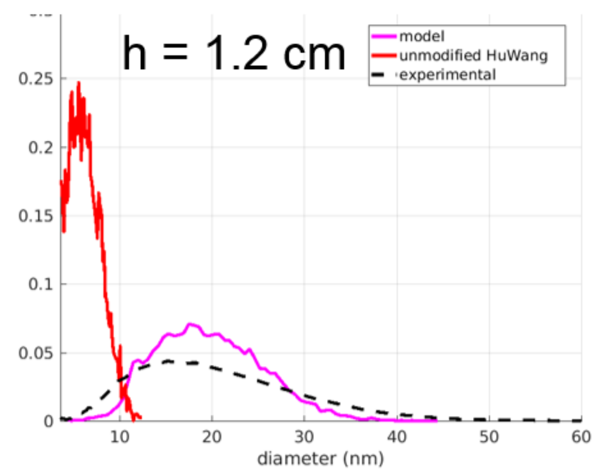
Accomplishments

Baseline model from Wang et al. Comb. Flame 2015

- **Approach:** Model burner stabilized premixed flame and post-process results with detailed soot model
- **Results:** Combined multi-fuel mechanism and detailed soot model accurately reproduces particle size distribution



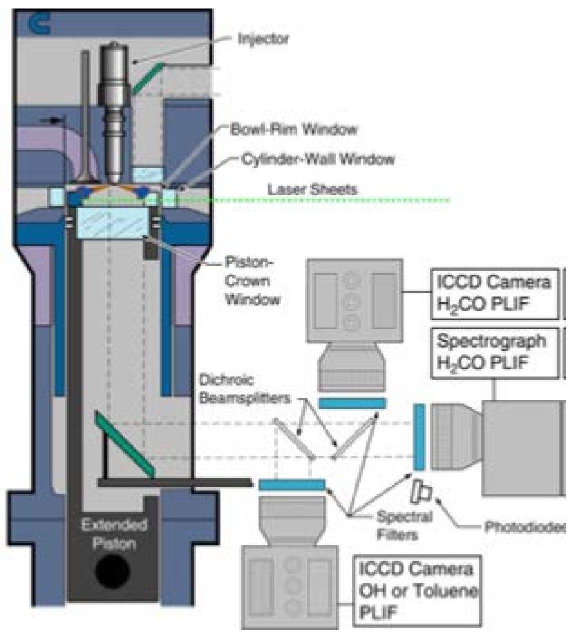




Spray Model Validation

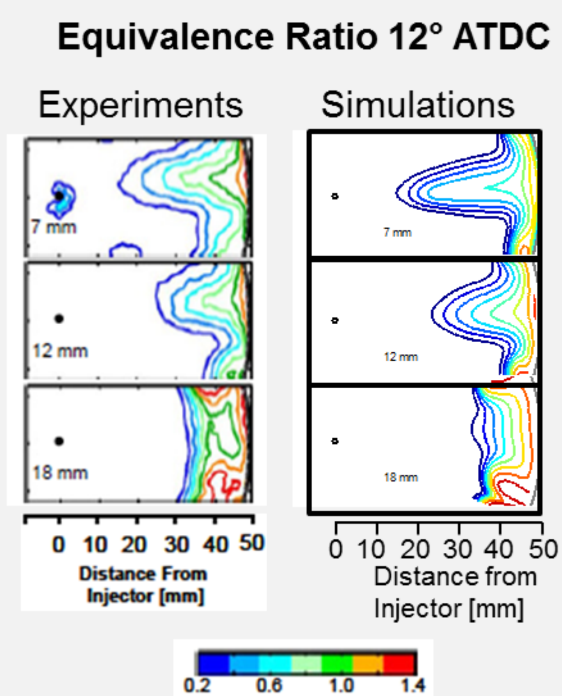
Accomplishments

- **Approach:** Spray model predictions compared to data from the literature
- **Results:** CFD simulations accurately capture vapor penetration and fuel distributions under diesel LTC conditions and dual-fuel RCCI conditions

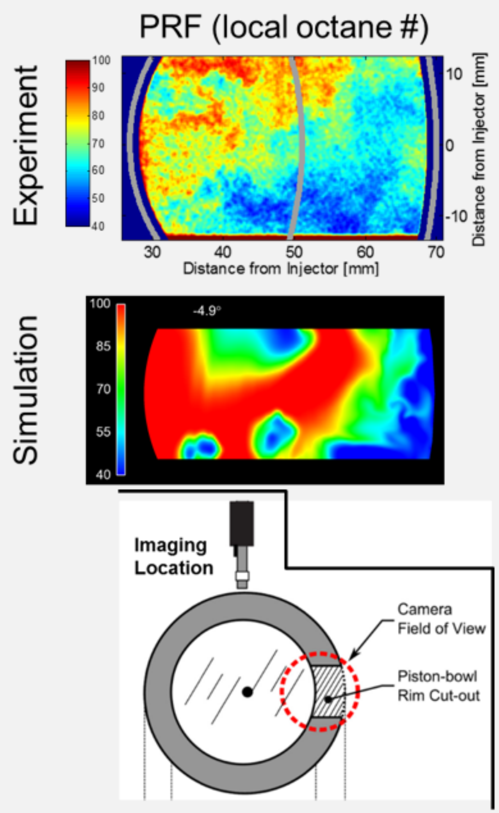


Toluene Fuel Tracer PLIF
(Genzale et al. SAE 2009, Kokjohn et al. Comb. Flame 2015)

RANS ERC KIVA
Diesel LTC



LES CONVERGE
RCCI

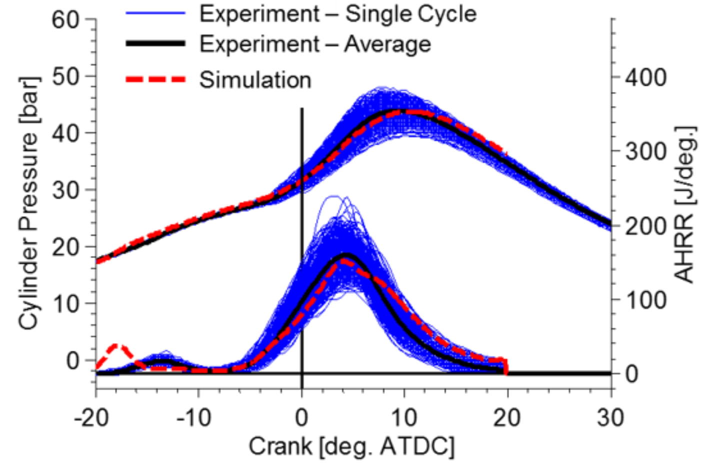


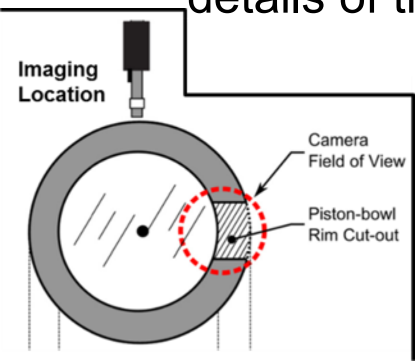
Combustion Model Validation

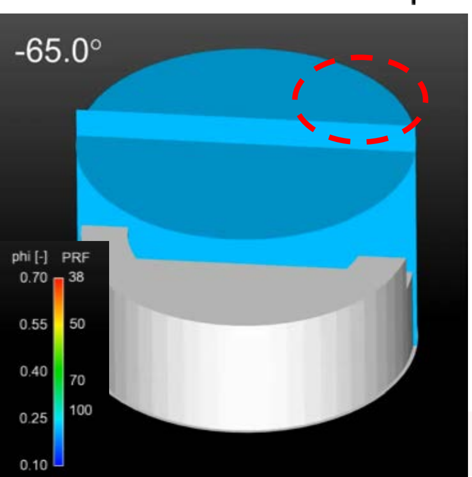
Accomplishments

- **Approach:** Combustion model validation under engine conditions through comparison with conventional and dual-fuel RCCI experiments
- **Results:** CFD approach reproduces the bulk combustion characteristics and details of the reaction zone growth

RANS results and NOx comparison in technical backup slides

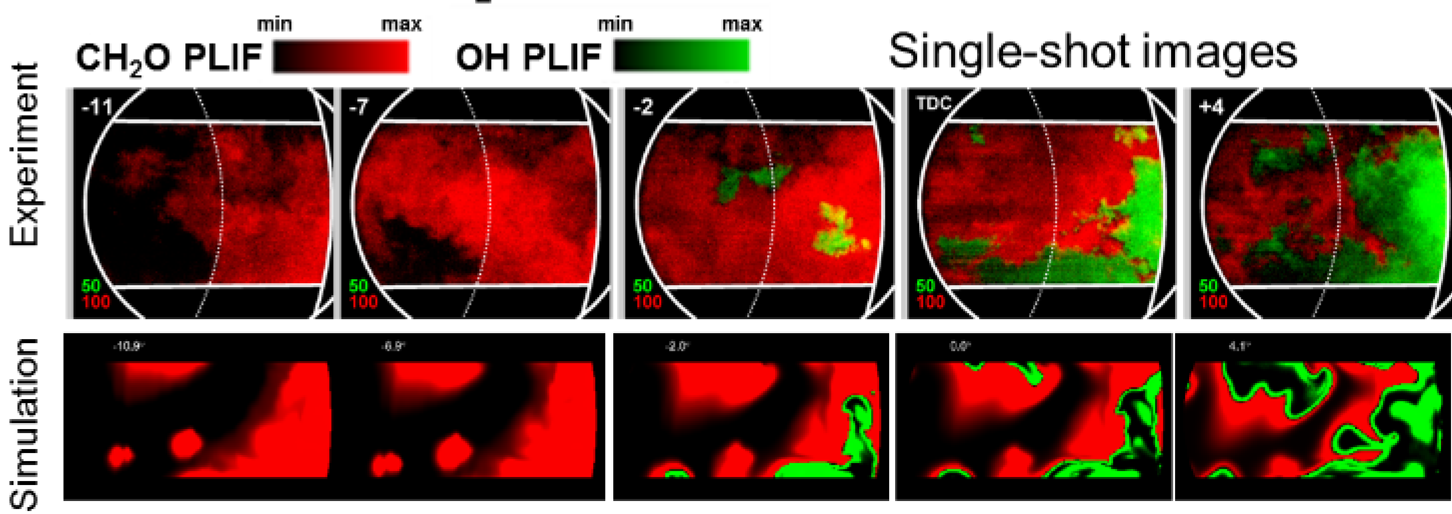






LES using CONVERGE with dynamic structure model and validated reaction mechanism

OH/CH_2O



Optical Engine Experiments

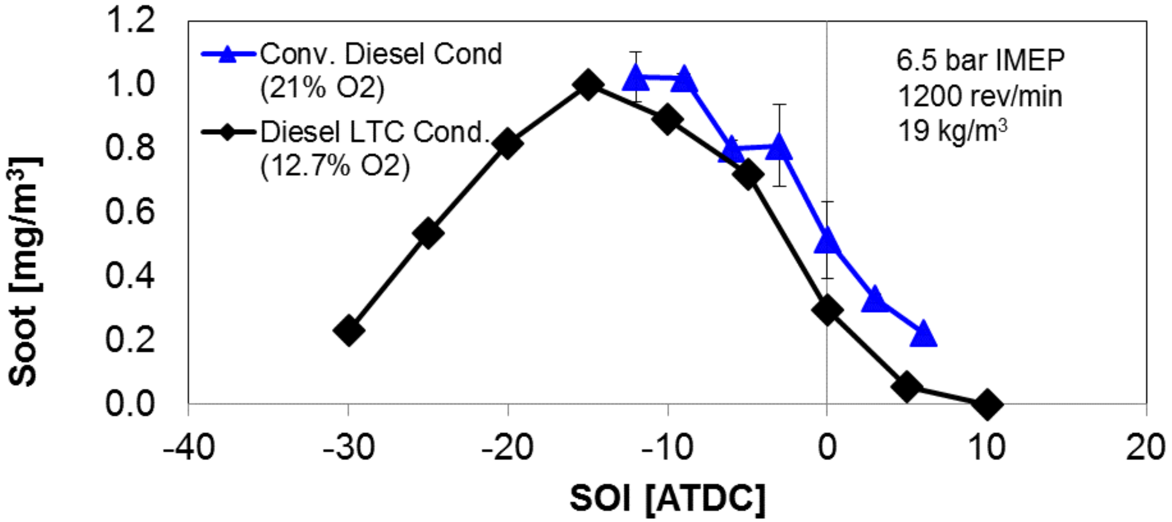
Accomplishments

Approach

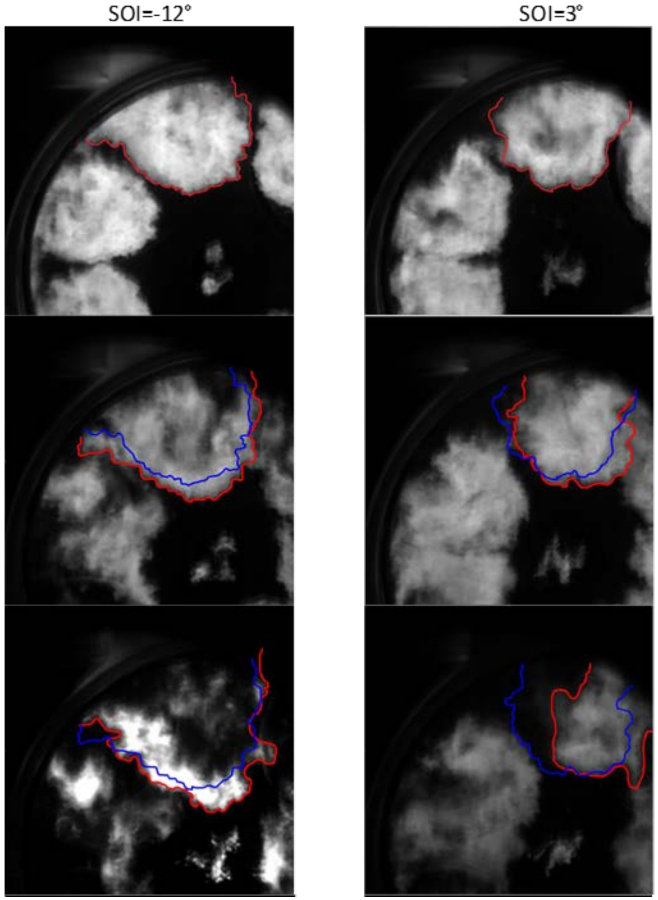
- High speed imaging and FSN measurements used to identify conditions of interest for future PAH LIF experiments

Results

- Completed high speed imaging and FSN measurements over a range of injection pressures and intake oxygen concentrations to ensure relevance for current and future engines (conventional diesel and diesel LTC conditions)



Combustion Luminosity
Conv. Diesel Conditions



Lagrangian Soot Tracking

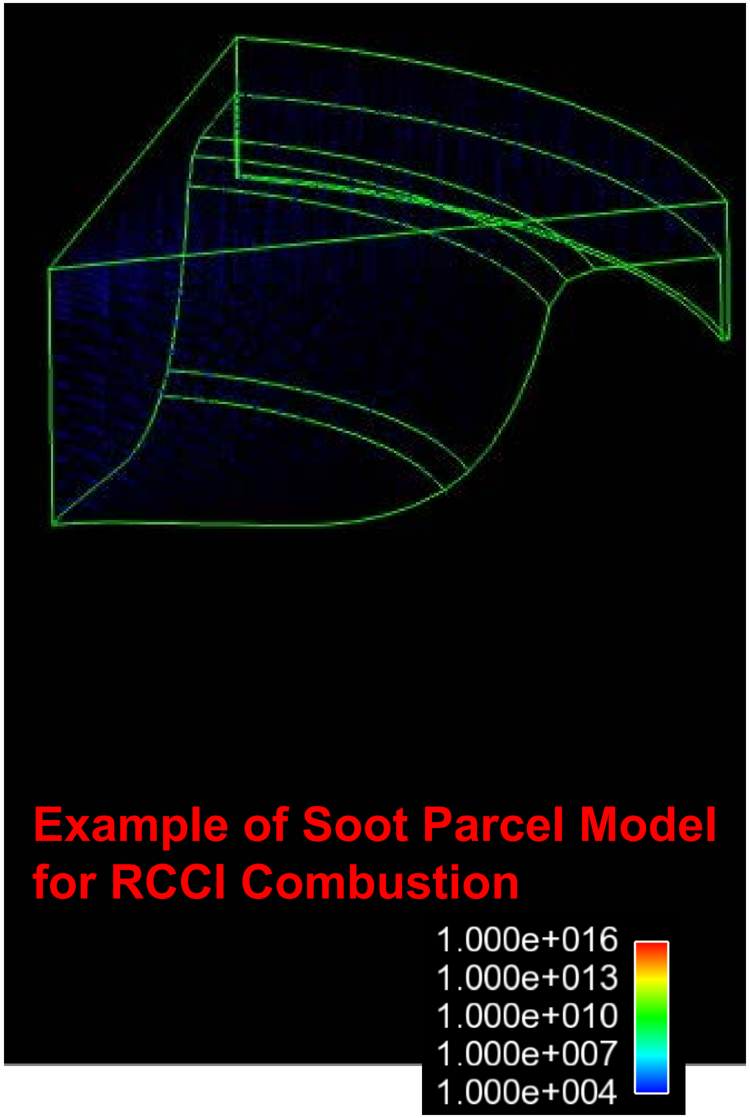
Accomplishments

Approach

- Expand KIVA / CONVERGE Lagrangian parcel model to include storage for soot population data

Results

- Lagrangian framework is functional to track soot
- Soot mass, diameter, and number is solved in each parcel using method of moments
- Soot formed is transferred out of gas phase and handled by soot model
- Ongoing work will extend to stochastic solution to population balance equations (FY17 effort)



Number of Particles

Responses to Previous Year Reviewers' Comments

This project is a new start and was not reviewed last year

Collaboration and Coordination

Combustion Research Facility	**Sandia National Labs Combustion Research Facility**	Perform optical engine experiments and supply data for computational model validation
Convergent Science	**Convergent Science Inc.**	Provide CONVERGE CFD code and incorporate project results into commercial CFD code for dissemination to industry
Engine Research Center, University of Wisconsin - Madison, est 1946	**UW Madison – Direct injection Engine Research Consortium (DERC)**	Disseminate project findings to consortium's 35+ member companies

Remaining Challenges and Barriers

- Coupling of detailed soot model and lagrangian parcel model (addressed in FY17)
- Understanding of balance between required fidelity in spray, chemical kinetics, and soot models and computational cost (addressed in FY17/18)
- Availability of PAH data under engine relevant conditions (addressed in FY17)
- Availability of particle size distribution data in advanced combustion conditions (addressed in FY17/18)

Proposed Future Research

Future Work

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

Model Development

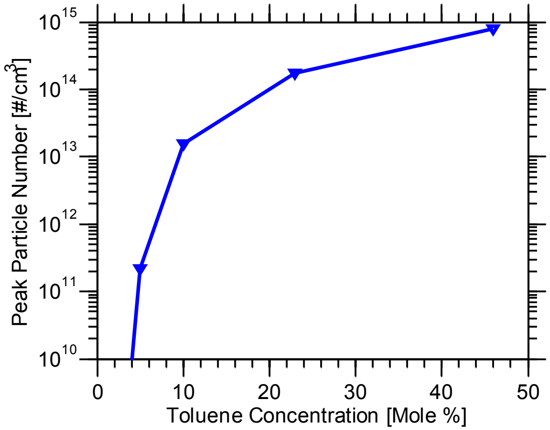
- FY17 - Complete coupling of lagrangian particle structure with stochastic soot model
- FY17/FY18 – Complete validation effort through detailed comparisons with literature and compare to PAH and particle size distributions from present experimental effort

Experimental Effort

- FY17 – Perform PAH LIF experiments to identify growth of PAH and transition to soot in-cylinder to supply validation data to computational effort and improve fundamental understanding of soot formation under engine conditions
- FY17/FY18 – Perform diesel and low temperature combustion experiments with particle size distribution measurements to enable evaluation of soot model prediction under engine relevant conditions

Application

- FY18 - Evaluate impact of soot inception species on soot mass and particle size/number predictions
- FY17 - Exercise detailed soot model to identify the impact of fuel properties on particle count and morphology



Summary

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

Relevance

- Simplified soot models do not have enough fidelity to enable predictive design space exploration for advanced combustion conditions

Approach

- Develop and validate a detailed PAH/soot model that enables prediction of particle formation events
- Perform optical and metal engine experiments to validate model predictions
- Couple experimental effort and computational effort to improve the understanding of soot formation under engine relevant conditions.

Collaborations

- Project includes close collaboration between industry, academia, and government labs

Technical Accomplishments

- Multi-fuel/PAH chemical kinetics model is capable of reproducing ignition delays, laminar flame speeds, and species profiles for a range of components relevant to real fuels.
- Detailed soot model shows acceptable agreement with particle size distribution
- Lagrangian framework completed to enable detailed tracking of soot aggregate structure
- Initial optical engine experiments completed to identify relevant conditions for PAH LIF

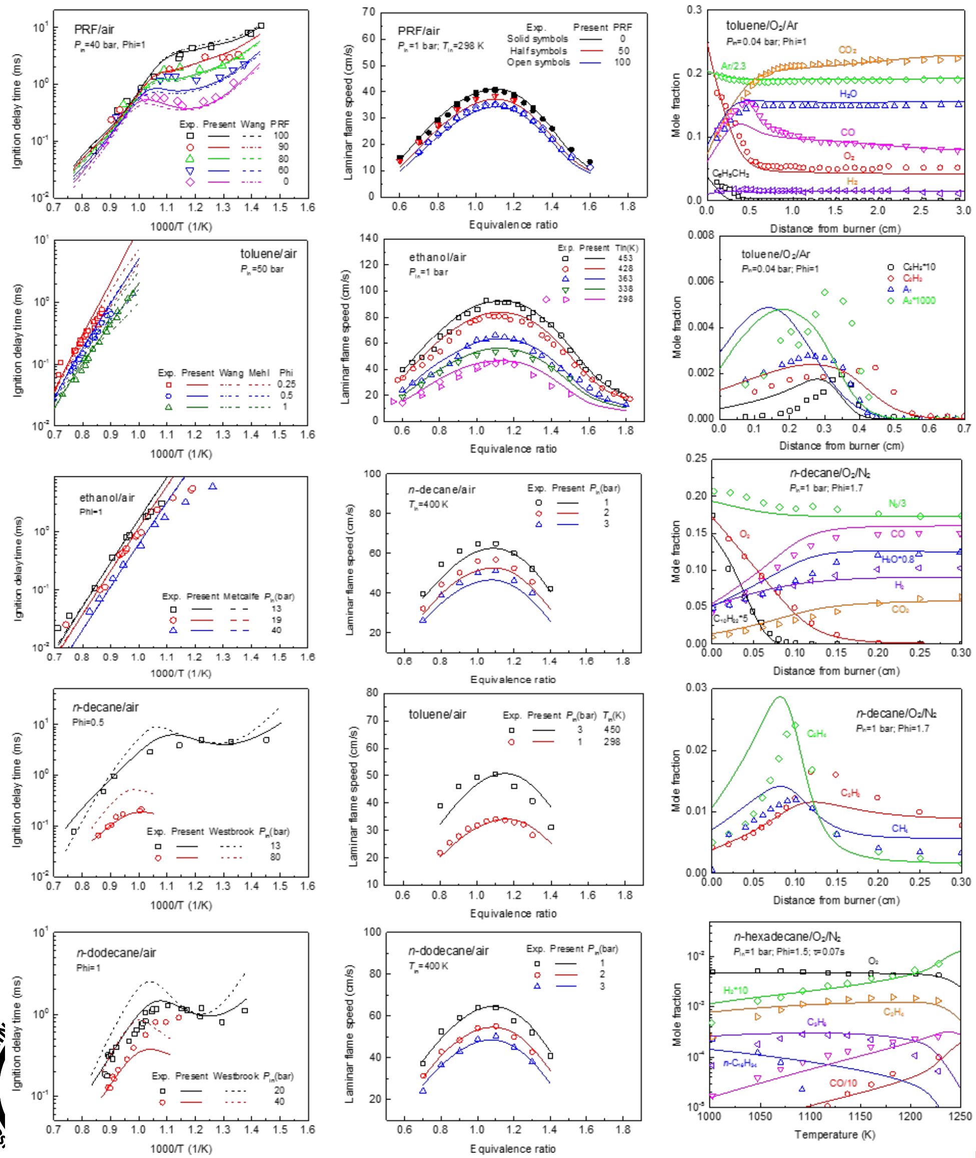
Proposed Future Research

- Complete coupling of detailed soot model and lagrangian framework in CFD code
- Complete engine experiments and perform final model validation
- Exercise model to improve understanding of key physics required for accurate soot prediction

Technical Back-Up Slides

Combustion Model Validation

Ignition Delay | Laminar Flame Speed | Species Profiles



ID = Ignition Delay
LFS = Laminar Flame Speed
SP = Species Profiles

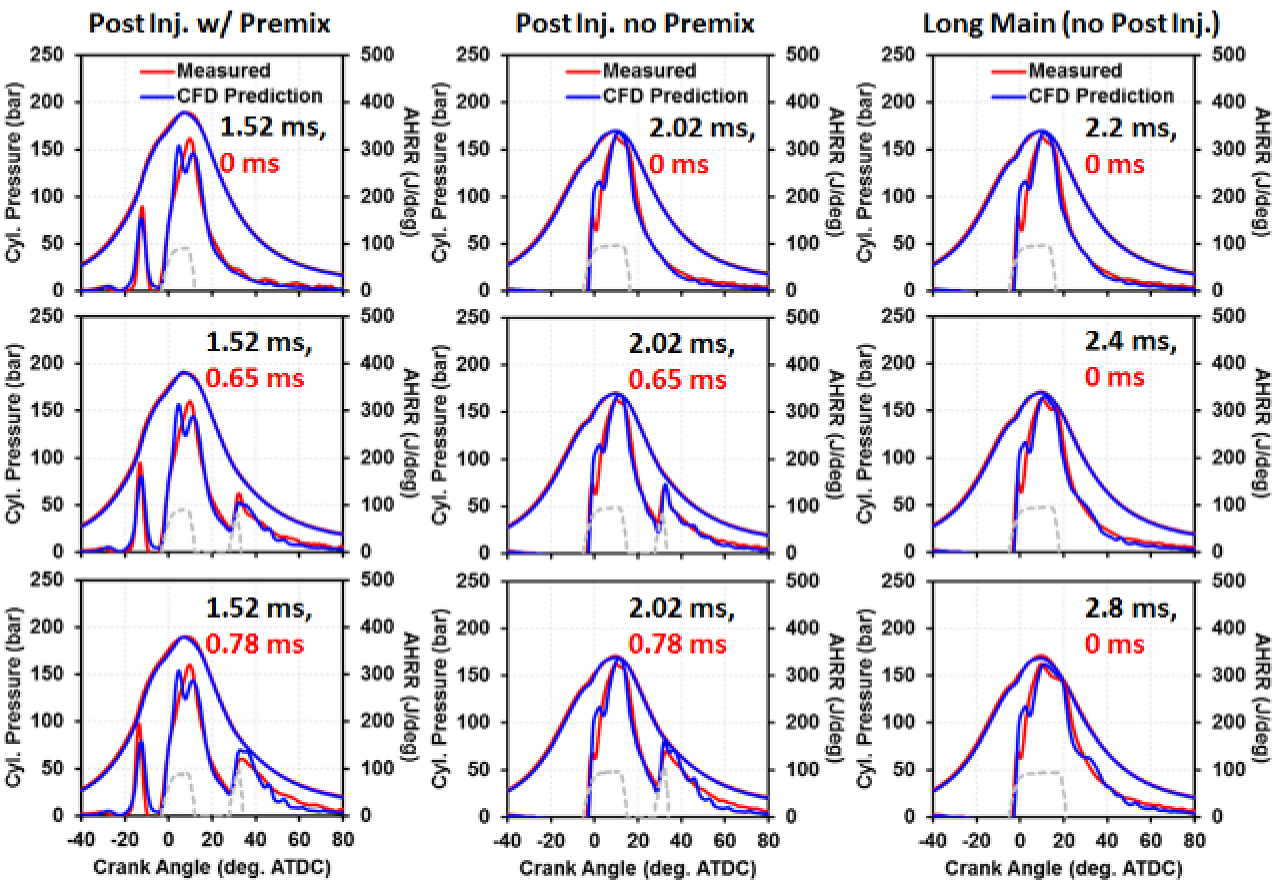
Fuel	Single Comp.	Mixture
nC_7H_{16}	ID / LFS / SP	ID / LFS
iC_8H_{18}	ID / LFS / SP	ID / LFS
$C_6H_5CH_3$	ID / LFS / SP	ID / LFS
C_2H_5OH	ID / LFS / SP	ID / LFS
CH_3OH	ID / LFS / SP	ID / LFS
$nC_{10}H_{22}$	ID / LFS / SP	ID / LFS
$nC_{12}H_{26}$	ID / LFS / SP	ID / LFS
$nC_{16}H_{34}$	ID / LFS / SP	ID / LFS
DIB	ID / LFS / SP	ID / LFS
CHX	ID / LFS / SP	ID / LFS
MCH	ID / LFS / SP	ID / LFS
C_2H_4	SP	
Gasoline		ID / LFS
Jet A		ID / LFS
Diesel Fuel		ID / LFS

Multi-fuel model validated through comparisons with a wide range of single components, mixtures, and surrogates (figure shows example comparisons showing typical level of agreement)

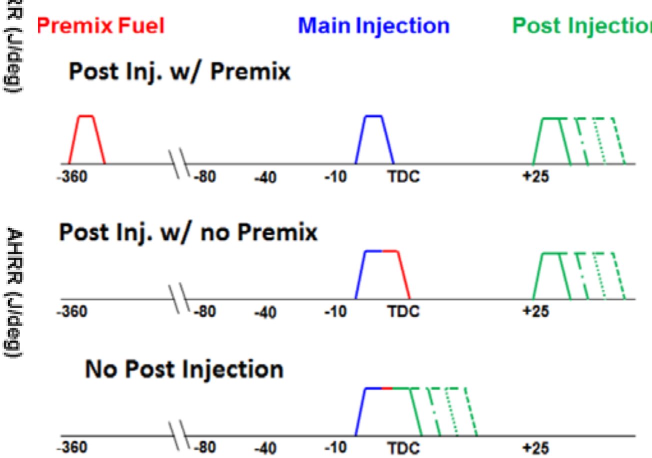
Source for experimental data shown in Ren and Kokjohn Fuel 2017

RANS Comb. Model Validation (1/2)

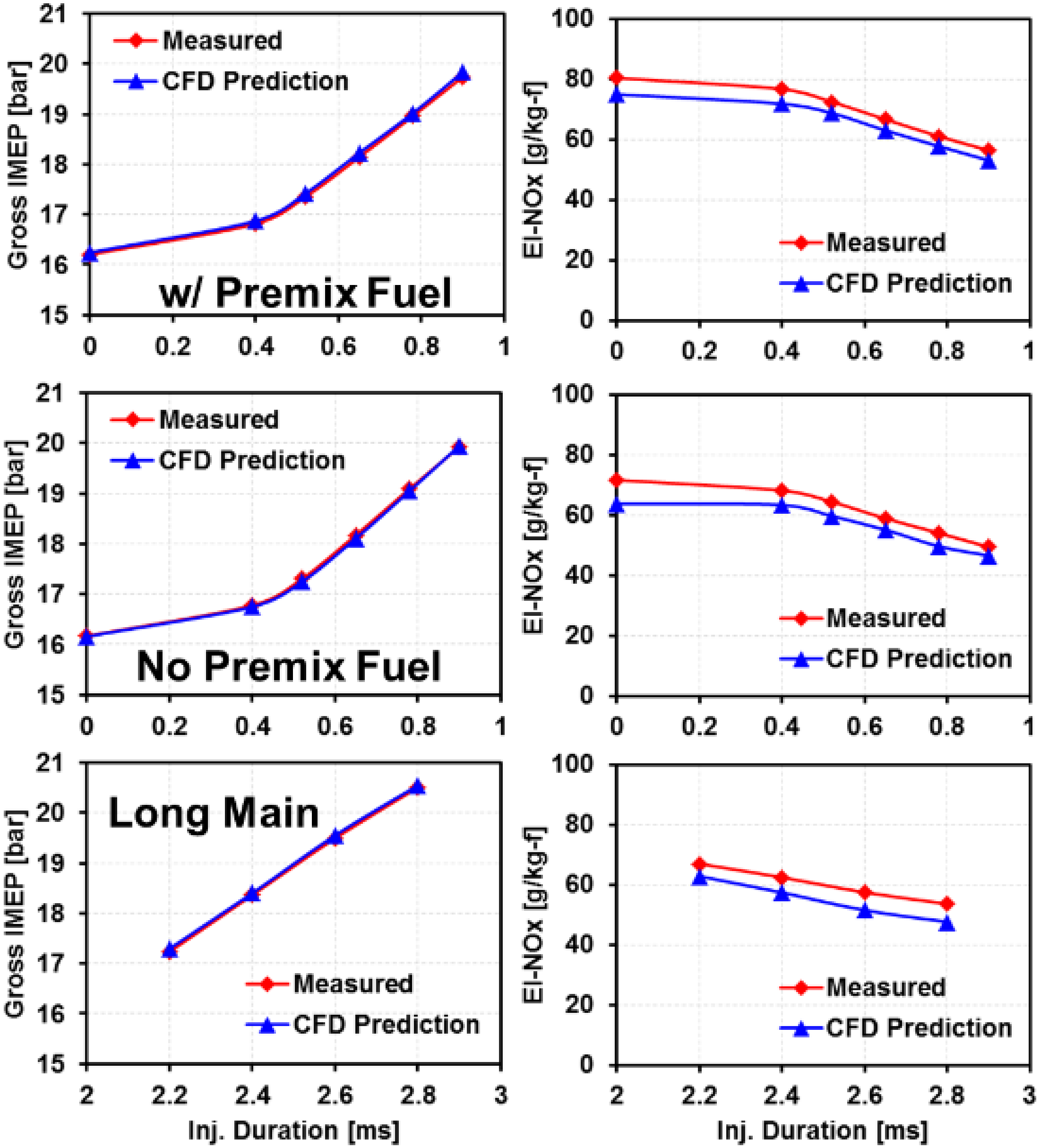
- **Approach:** Model predictions compared to high-load gasoline compression ignition data with several injection strategies
- **Results:** KIVA RANS Simulations accurately reproduce changing combustion characteristics



Operating Condition	No Premix Fuel	With Premix Fuel	Long Main
Fuel	91E10	91E10	91E10
IMEP (bar)	~ 16 to 20	~ 16 to 20	~ 16 to 20
Total Fuel Mass (mg)	~ 215 to 290	~ 215 to 290	~ 238 to 292
Premixed Mass (mg)	0	68	0
Main Inj. Mass (mg)	215	147	~238 to 292
Main Inj. SOI Timing (°ATDC)	-8	-8	-8
Post Inj. Mass (mg)	0 to 75	0 to 75	0
Post Inj. SOI Timing (°ATDC)	16, 25, 40	12, 25, 40	-
Inj. Pressure (bar)	1358	1358	1358
Intake Pressure (bar)	2.96	2.96	2.96
EGR (%)	0	0	0



RANS Comb. Model Validation (2/2)



Operating Condition	No Premix Fuel	With Premix Fuel	Long Main
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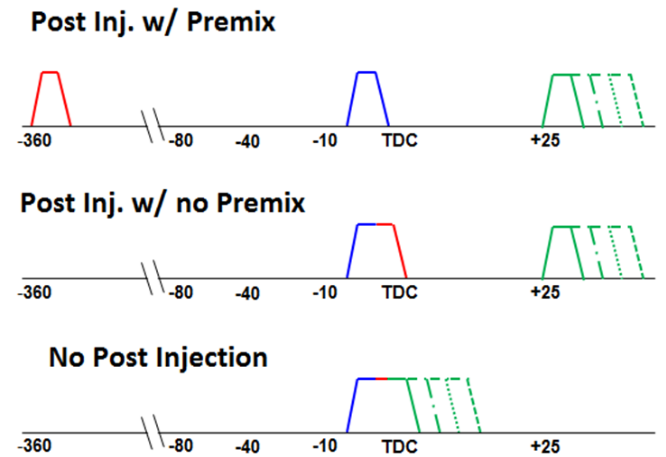
Post Inj. Mass (mg)	0 to 75	0 to 75	0
Post Inj. SOI Timing (°ATDC)	16, 25, 40	12, 25, 40	-
Inj. Pressure (bar)	1358	1358	1358
Intake Pressure (bar)	2.96	2.96	2.96
EGR (%)	0	0	0

Premix Fuel   Main Injection   Post Injection



Improving Understanding of Soot Formation

Approach

- MZ results post-processed with population balance solver
  - 2048 stochastic particles used for each zone

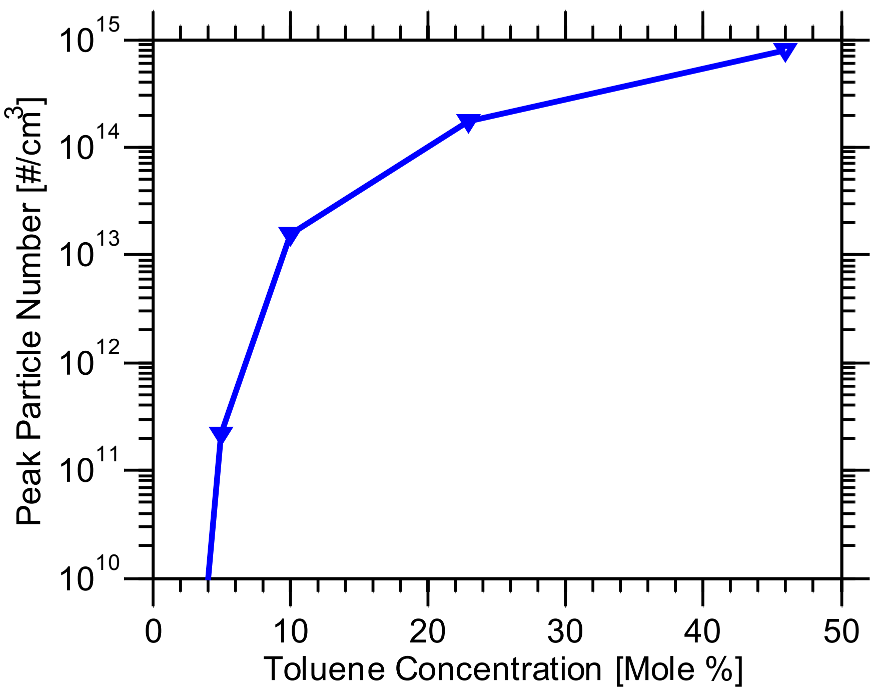
Results

- The peak particle count increases by five orders of magnitude from 5% toluene to 46% toluene
- Model predicts sensitivity to aromatic content that is qualitatively consistent with experiments→ validation experiments needed to quantify predictive ability

Premixed Fuels Considered

	iso-octane	5% toluene	10% toluene	23% toluene	46% toluene
iso-octane	100	81	76	63	40
n-heptane	0	14	14	14	14
toluene	0	5	10	23	46

Direct Injected fuel was n-heptane for all cases



Population Balance Solver Performance

Approach

- Evaluate convergence and run-time of population balance solver

Results

- Population balance solver converges around 512 stochastic particles
- Computational cost is comparable to chemistry under LTC conditions and increases linearly with number of stochastic particles