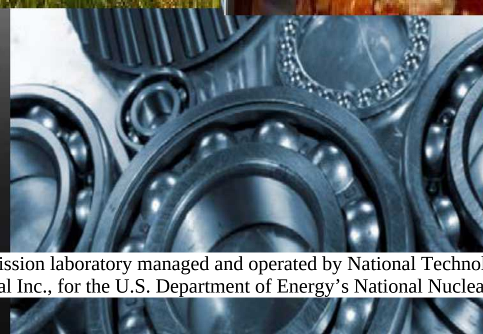
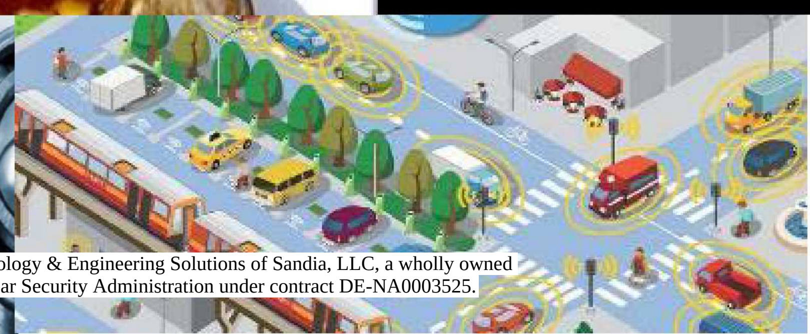
SAND2019-8505PE

An Overview of the US DOE-Sponsored Light-Duty Combustion Consortium

Key Barriers, Recent Progress, & Research Plans at the US National Laboratories





Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Objectives of this presentation

- Describe US Department of Energy efforts to speed research progress supporting the development of clean, efficient, IC engines through formation of a national laboratory research consortium

  Solicit feedback while this program is still in its design phase

- Seek to identify collaborative opportunities with the Japanese research community

  Progress will be faster with coordination (cf. the ECN)

  ENGINE COMBUSTION NETWORK

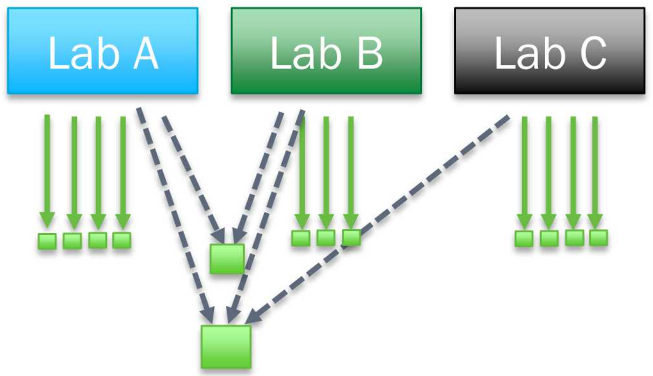
- Diesel compression ignition research is not represented here – but is an important part of DOE's MD/HD research portfolio

- Many complementary projects with a focus on fuel effects are not represented here, but are incorporated in the Co-Optima initiative

  See https://www.energy.gov/sites/prod/files/2019/06/f64/Co-Optima_YIR2018_FINAL_LOWRES%20190619_0.pdf

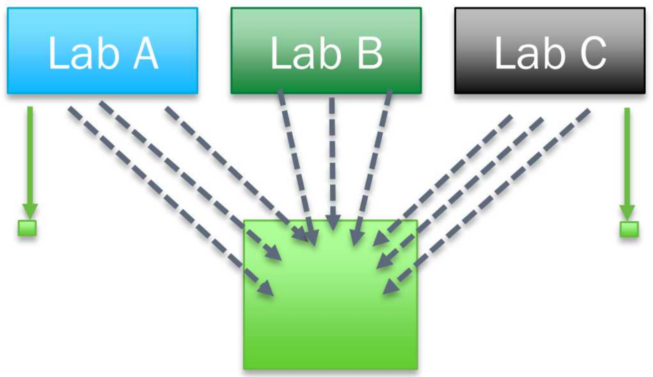
Consortium rationale

Today



- Majority of lab projects proceed independently

Opportunity

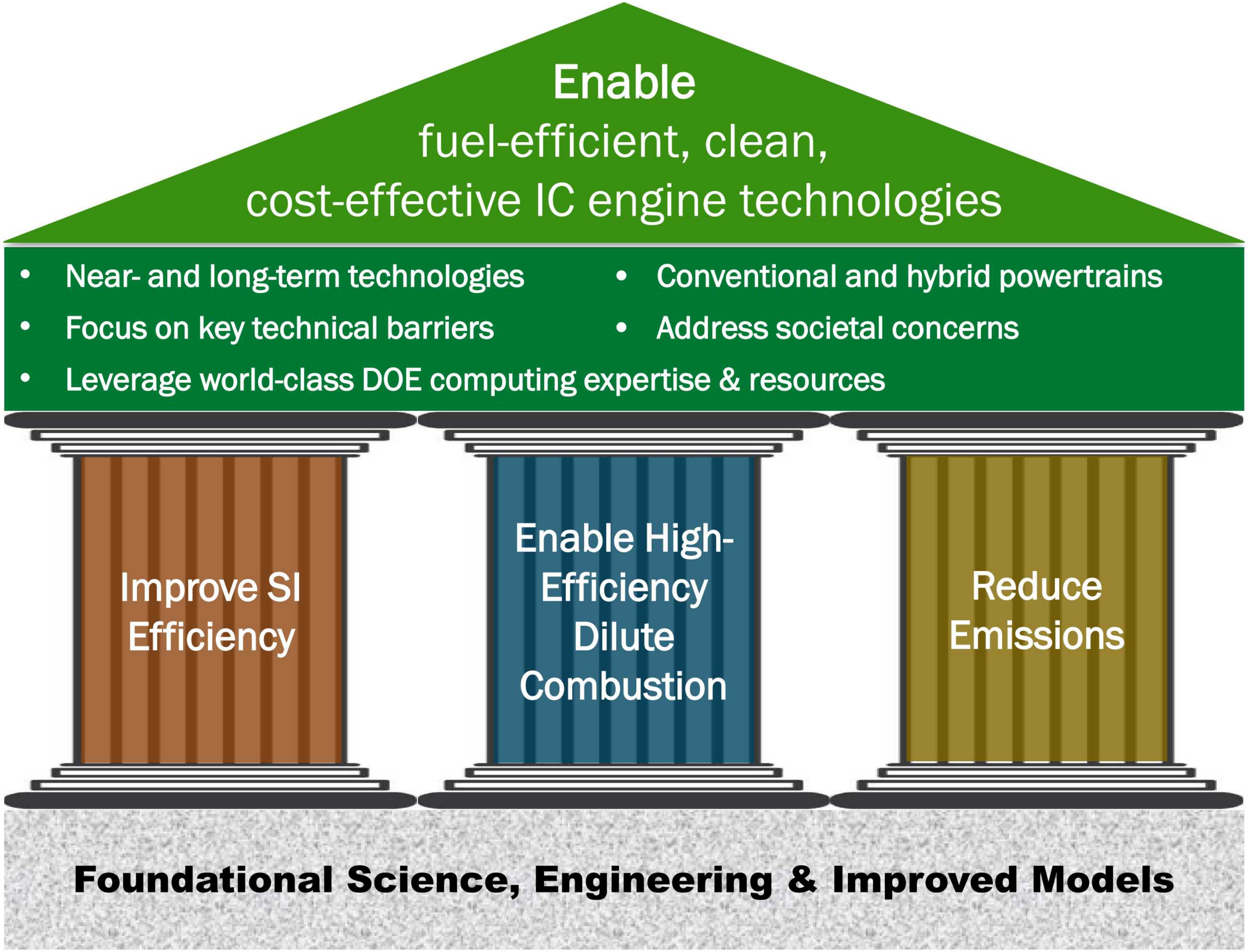


- Majority of lab projects are concentrated on a few core problems

Consortium Approach Advantages:

- Increase research impact & efficiency by coordinating efforts
- Highly visible 'flagship' effort
- Leverage lab R&D management capabilities

Consortium Structure



KNOWLEDGE ⇔ DATA ⇔ PREDICTIVE TOOLS

Data

- APS, SNS
- Optical Engines
- Metal Engines

Knowledge

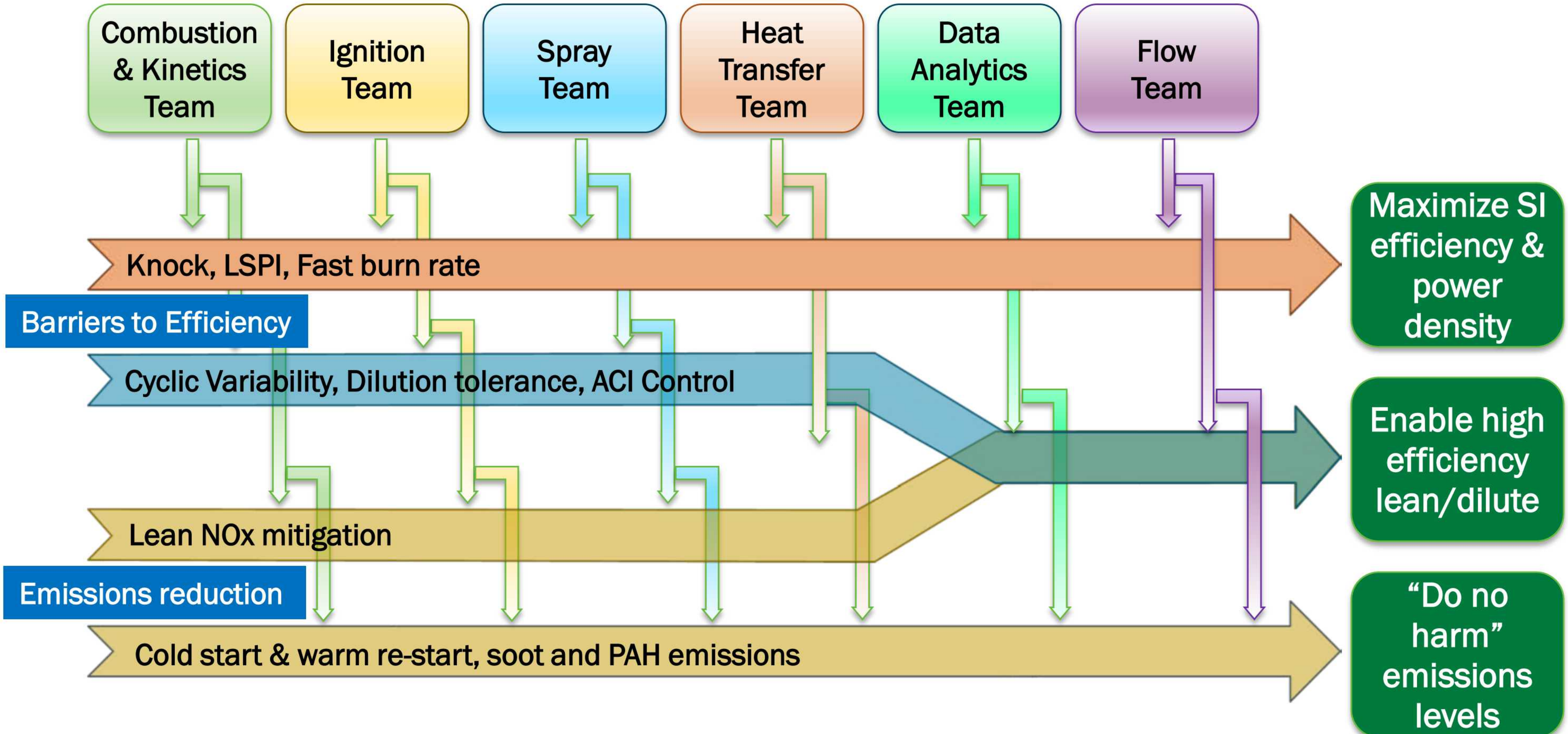
1. Turbulence chemistry interactions
2. Ignition kernel formation
3. Fuel spray injection
4. Spray Wall interaction
5. Cold start emissions

Tools

Super-computing resources
ML workflows

Research	Commercial
• Nek5000, Pele	• CONVERGE
• OpenFOAM	• ANSYS

Cross-cutting teams are guided by our main Purposes



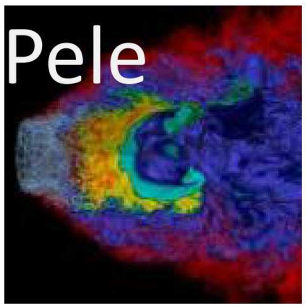
Our challenges:

- Focus the fundamental work on concrete barriers that have a clear, direct, and quantifiable connection to the goal
- Link projects through common hardware platforms

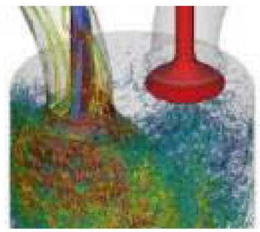
High Performance Computing & Machine Learning

- Leverage significant DOE investment in high-performance computing

ECP
EXASCALE COMPUTING PROJECT



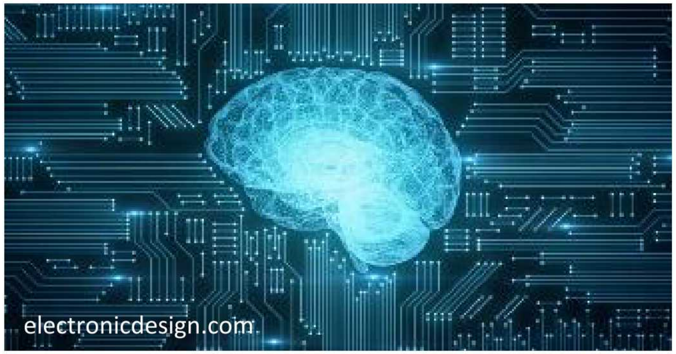
NEK5000



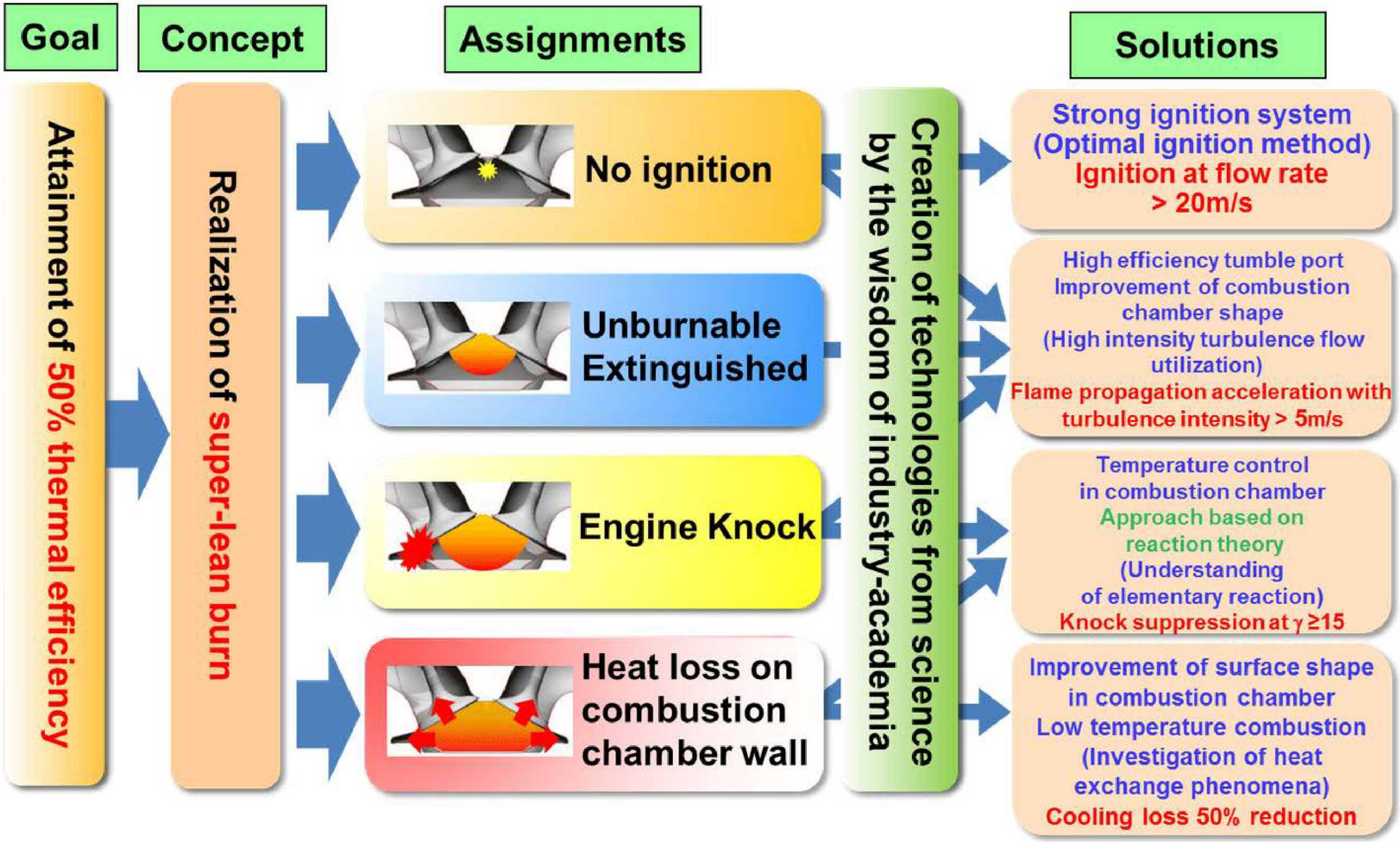
FEARCE
Fast, Easy, Accurate & Robust Continuum Engineering

- Adapt and use high-accuracy codes on the latest supercomputers to solve problems needed for better engineering models

- Exploit DOE expertise in artificial intelligence and machine learning to discover hidden relationships or create better models



The Japanese SIP project had very similar objectives



http://sip.st.keio.ac.jp/en/reserch-overviews/

Key barriers facing the Combustion and Kinetics team

Validated reduced kinetic mechanisms with accurate autoignition characteristics are needed for realistic surrogate fuels

- Accurately knock predictions
- Uncertainties with EGR
- Light species for cold-start mixtures

Current Status:

- Reduced mechanisms exist for commercial fuel surrogates that match experimental autoignition behavior over a wide range of pressure & temperature

Planned work:

- Additional tuning/validation needed when EGR is used
- Impact of trace species needs further investigation (e.g. NO, peroxides…)
- Hybrid approaches to mitigate error as the number of species grows
- Better mechanisms for PAH / soot precursors
- Validation of surrogates

	Test Fuel	Surrogate	
Hydrocarbon class	*Molar fraction*	*Molar fraction*	*Species*
N-alkanes	16.3%	9%	N-heptane
		9%	N-pentane
Iso-alkanes	23.6%	29%	Iso-octane
Cyclo-alkanes	12.2%	7%	Cyclo-pentane
Aromatics	21.1%	20%	Toluene
Olefins	5.8%	6%	1-Hexene
Oxygenated	19.9%	20%	Ethanol
RON	92.1	91.6*	
MON	84.8	83.8*	
Sensitivity	7.3	7.8	
Formula	$C_{6.03}H_{12.21}O_{0.20}$	$C_{5.91}H_{11.96}O_{0.20}$	
H/C ratio	2.025	2.024	
A/F_{stoich} ratio	14.084	14.098	

Key barriers facing the Combustion and Kinetics team

Improved numerics are needed to speed computation, even with reduced kinetics and high-performance computing resources

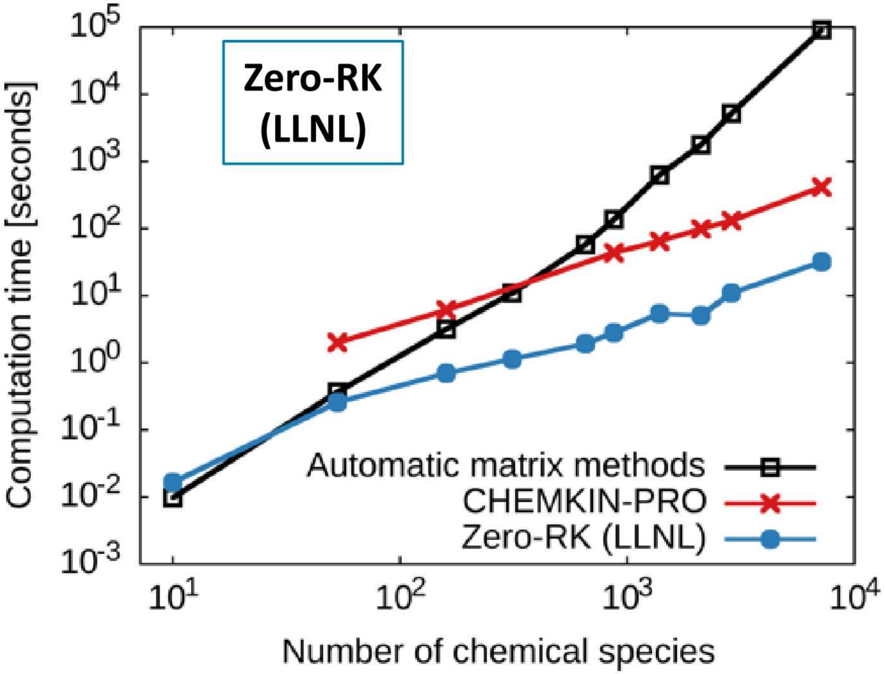
- Autoignition & flame propagation
- Lean & dilute ignition simulation
- Precursors for soot formation

Current Status:

- Fast chemistry solvers have reduced computation time by orders of magnitude

Planned work:

- Continued speed-up of chemistry solvers
- Reduction of computational cost of species transport in CFD
- Made available through codes like CONVERGE, Nek5000, etc.



Key barriers facing the Combustion and Kinetics team

Efficient flame propagation models coupled to end-gas autoignition, with realistic near-wall behavior are needed

- Accurate SI knock/HRR predictions
- Simulation of SPCCI/SACI strategies
- Cold-wall/film quenching behavior

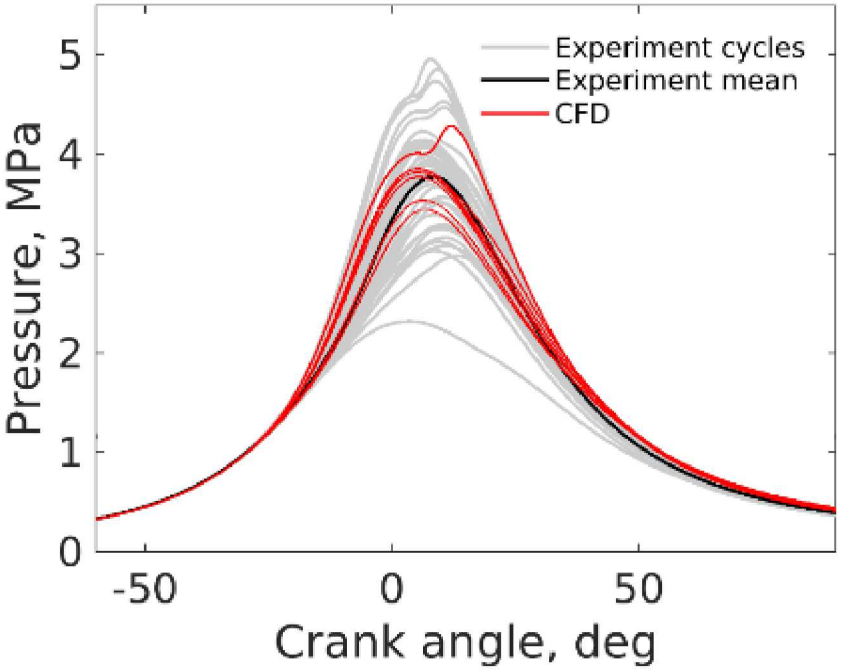
Status:

- Simulations can qualitatively reproduce experiments, but model tuning is required
- Few studies of near wall behavior

Planned work:

- Better understanding of the impact of low temperature chemistry on burning velocities (tabulated methods)
- Higher-fidelity turbulence chemistry interactions
- Improved model behavior near walls; interactions with fuel wall films – key to particulate formation
- Near-wall behavior likely to require DNS simulations to resolve

Source: Simulations – ANL; Experiments – SNL



Key barriers facing the Combustion and Kinetics team

Accurate soot models for particulate mass, number, and size – with accounting for pyrolysis processes

- GDI bulk gas & film pyrolysis
- PM from stratified-lean strategies
- Cold-start dominates soot emissions

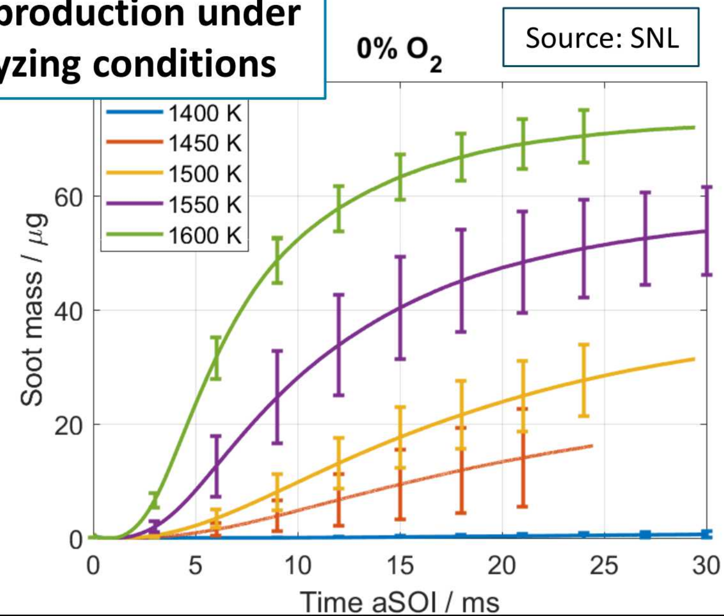
Status:

- Models are currently interpolative and highly dependent on calibration
- Sectional- and moments-based methods can lead to improved soot predictions, but modeled terms need further improvement

Planned work:

- Kinetic mechanisms for soot precursors
- Data characterizing impact of multiple injections and wall interactions
- Improved models for particle inception, incorporating new understanding of the role of aliphatically-bridged PAHs
- Quantitative evaluation of the importance of various sources of GDI particulates

Soot production under pyrolyzing conditions



Key barriers facing the Ignition team

Modeling improvement needed for:

- **Thermal & non-thermal plasma development**
- **Plasma-to-flame kernel transition**
- **Kernel-to-turbulent flame transition**

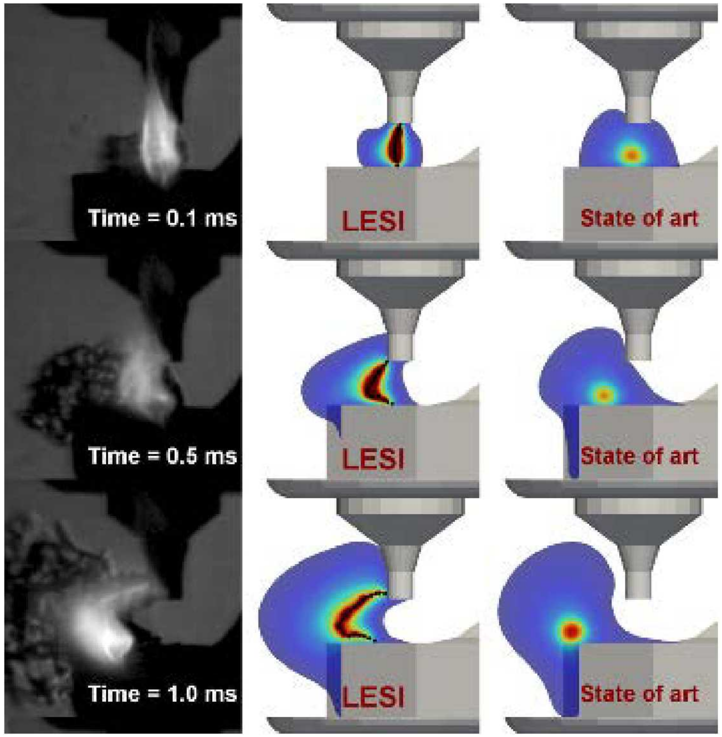
Current Status:

- *Ad hoc* energy deposition and re-strike modeling
- Plasma kinetics not well understood – impact on kernel inception and growth is unknown
- Curvature effects on kernel growth simplistic or absent

Planned work:

- High cross-flow spark channel measurements
- Characterization & modeling of thermal & non-thermal plasmas and kernel initiation
- DNS and experiments of kernel growth to support improved modeling (may be different under cold-start conditions)

- High-tumble extinction/re-strike
- Lean and dilute ignition
- Cold, low-Re ignition



Experimental Images: Prof. Lee (MTU)
LESI: Lagrangian Eulerian Spark Ignition @ ANL
State of the art: Current model in CONVERGE

Key barriers facing the Ignition team

Need for robust, low-temperature plasma (LTP) igniters

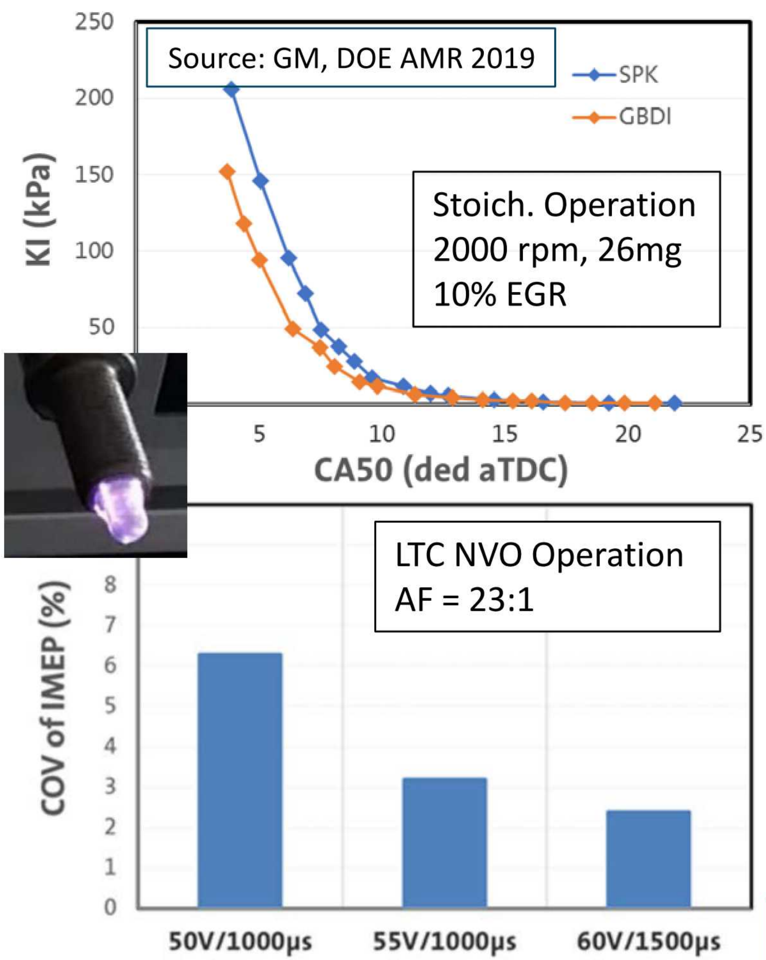
- Faster burning dilute SI
- Extended dilution limits
- More robust cold-start ignition

Current Status:

- LTP igniters have demonstrated benefits for high-load SI and low-load, low-temperature combustion
- Variability/robustness issues need to be overcome

Planned work:

- Modeling and experiments clarifying impacts of igniter design on field strength, plasma generation & robustness
- Evaluation of excitation variants (e.g. ns-pulsed DC vs. RF)
- Development and testing of “viable” prototypes (collaboration with Tier 1 suppliers)



Key barriers facing the Ignition team

Lack of understanding of how LTP igniters can assist HCCI/SPCCI-like combustion strategies through O_3 creation

- Extended dilution limits
- More robust cold-start ignition

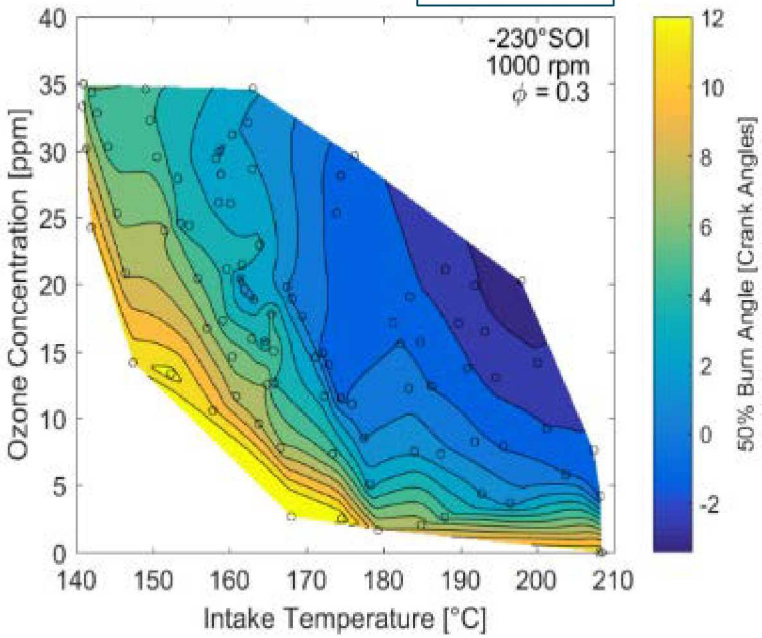
Current Status:

- O_3 addition has been shown to benefit both emissions and efficiency of HCCI/SACI/SPCCI combustion, but our quantitative understanding of its creation, in-cylinder evolution, and impact on combustion is limited

Planned work:

- Quantify efficacy of various igniter operation strategies for in-cylinder O_3
- Clarify mechanism whereby O_3 enhances auto-ignition and evaluate impact on homogeneous & stratified SACI/SPCCI combustion
- Improve kinetic mechanisms for O_3 oxidation

Source: SNL



Combustion phasing control and intake temperature requirements can be significantly impacted by O_3

Key barriers facing the Ignition team

Overcoming barriers to commercialization of pre-chamber (PC) igniters and assessing their impact on various operating modes

- Faster burning dilute SI
- Extended dilution limits
- More robust cold-start ignition

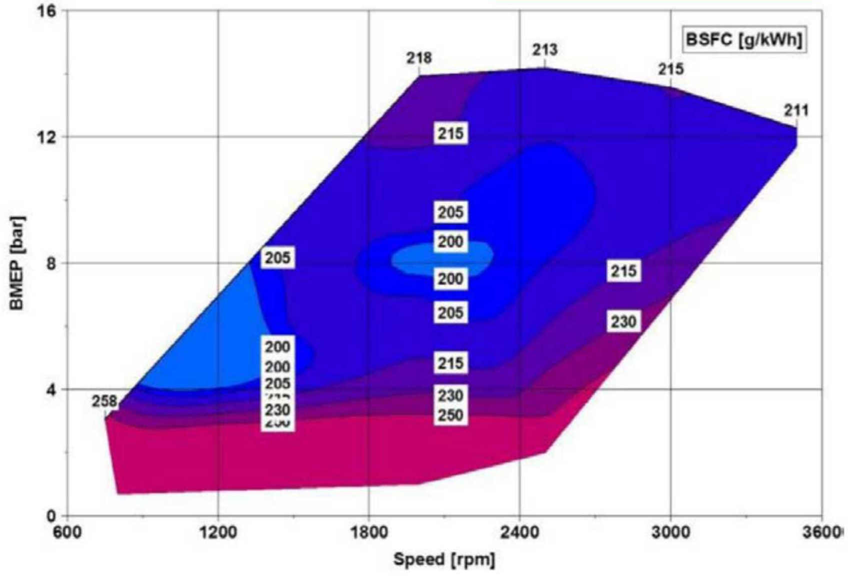
Current Status:

- Pre-chambers can significantly extend dilution limits and speed combustion yielding high η
- Drawbacks include COV/NOx trade-offs, cold-start, noise, PM emissions (active PCs)…
- Mechanisms of main charge ignition and best modeling approaches are not well understood

Planned work:

- Assess potential of LTP igniters to overcome PC drawbacks
- Assess potential to alleviate cold-start emissions
- Investigate synergies between PC igniters and SPCCI/SACI combustion
- Develop appropriate modeling approaches

Source: 2016-01-0709



Above 4 bar BMEP the BSFC is typically < 215 g/kWh

Key barriers facing the Spray team

Free spray models are not predictive

Current Status:

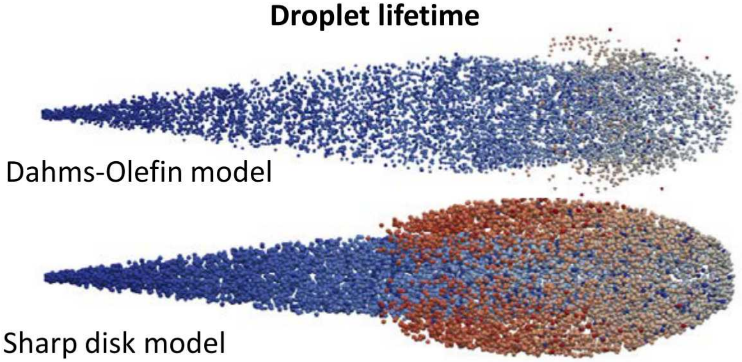
- Free spray models require tuning for ambient P/T, FIE, & fuel – heavily dependent on experiment
- Little validation data is available for transient sprays (multiple injections)
- Dribble and nozzle film formation not predicted
- Spray cyclic variability largely unassessed

Planned work:

- Develop quantitative free spray mixture formation data base, supported by near-nozzle BCs
- Liquid volume fraction and drop-size measurements to support wall-wetting work
- Measurements and simulations of nozzle films
- Work closely with code developers to enhance transfer of results to OEM workflows

- Mixture impacts SI knock & emissions
- Stratified mixture design difficult
- Liquid penetration during cold-start

Source: Imaging and Simulations from ANL



Key barriers facing the Spray team

Existing spray-wall interaction models are inadequate

Current Status:

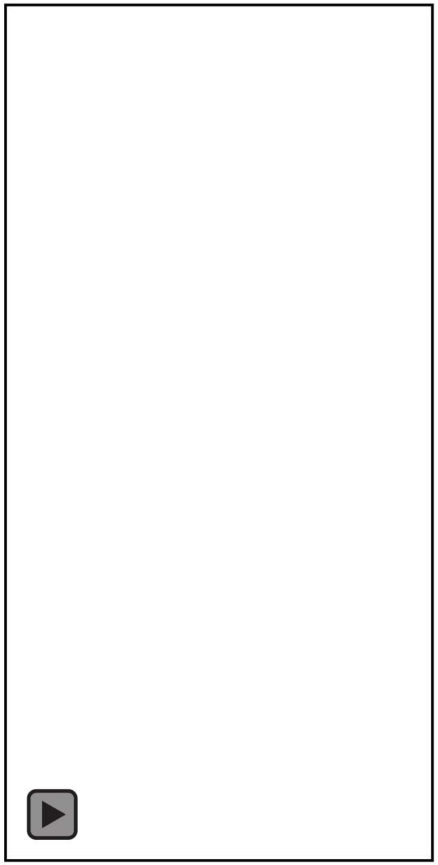
- Wall jet penetration, vortex, rebound height and film formation processes have poor or uncertain performance
- Subsequent splash & vaporization process modeling requires improvement – improved surface temperature modeling will help

Planned work:

- Well-characterized, quantitative wall impingement experiments with controlled wall temperature and heat flux measurement
- Development and validation of multi-component vaporization models applicable to films and poly-disperse sprays
- Concurrent CFD simulations and model improvement

- Impact on LSPI

- Cold-start fuel film formation



Fuel mixture fraction (and soot volume fraction) can be quantitatively measured in an axisymmetric configuration using absorption diagnostics

Film thickness on the surface can likewise be obtained with optical or x-ray absorption techniques

Key barriers facing the Spray team

Key processes impacting spray collapse are poorly understood, and model predictions require significant tuning

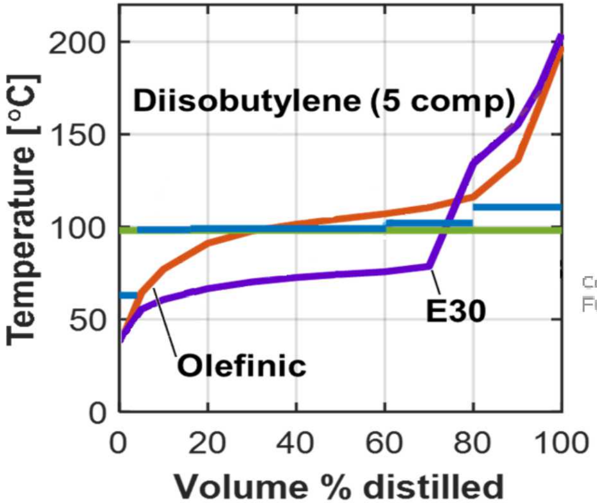
- Homogeneous mixture preparation
- Stratified mixture formation
- Cold-start spray penetration

Current Status:

- Collapsed sprays mix poorly and likely cause impingement on surfaces
- Spray collapse depends on FIE geometry, ambient conditions, and fuel properties

Planned work:

- Work will continue on quantifying the impact of properties, geometry and ambient conditions, with emphasis on understanding aerodynamics and plume-to-plume interactions
- Surrogate fuels will be developed that provide adequate spray as well as ignition and combustion behavior

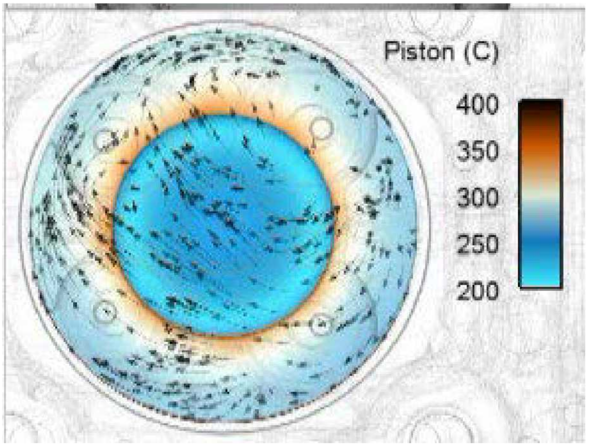


Co-Optimization of Fuels & Engines

Key barriers facing the Heat Transfer team

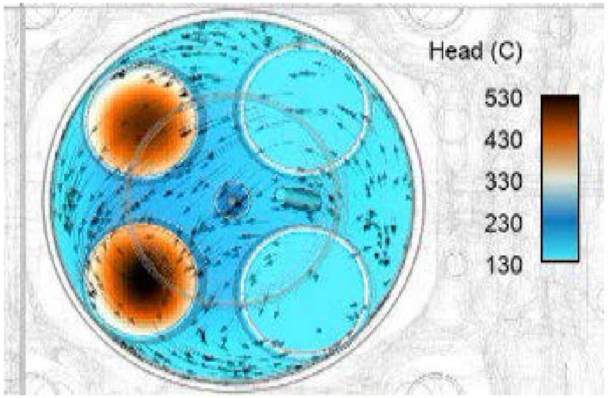
- **Improved boundary conditions and validation data are needed**
- **CHT workflows need improvement**
- **Boundary layer modeling suspect**

- Knock initiation at surfaces
- Heat loss to igniter electrodes
- Cold-start ignition & film evaporation



Current Status:

- In-cylinder surface temperature measurements in engines with a well characterized flow field do not exist
- Accuracy loss incurred with super-cycling approaches are not well quantified



Planned work:

- Develop and incorporate new, transient boundary layer models
- Investigate heat flux predictions for impinging sprays
- Provide validated, needed surface temperature BCs to combustion modeling team
- Support cold-start work with full engine modeling – including exhaust system

Source: ORNL

Key barriers facing the Data Analytics team

Methods to predict knock, LSPI, and instabilities in HCCI-like combustion are undeveloped and untested

- Knock/LSPI Mitigation
- Alleviate combustion instabilities
- Identify future misfires/partial burns

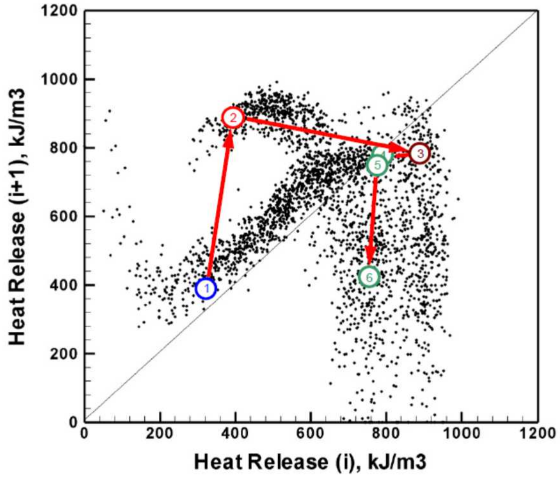
Current Status:

- Short-term predictable patterns in combustion behavior provide potential for development of mitigation strategies

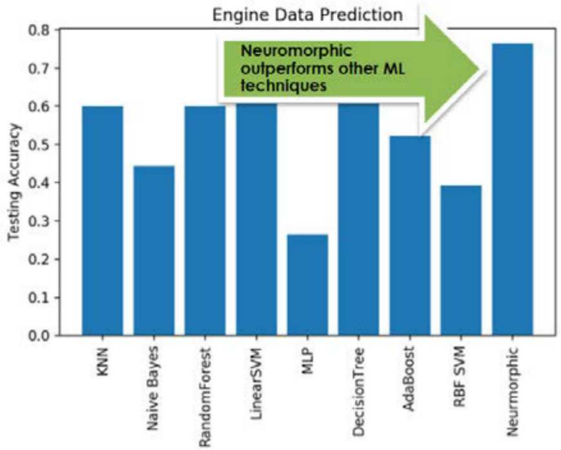
Planned work:

- Acquire extensive data sets at borderline knocking conditions, unstable SACI conditions, and near mis-fire cold-start conditions
- Use classic statistical, nonlinear dynamics, and machine learning analysis techniques to identify prior- or same cycle indicators for abnormal combustion
- Identify and evaluate mitigation strategies

Example of complex but short-term predictable patterns in spark assisted HCCI combustion



Neuromorphic systems are promising candidates for engine predictions



Key barriers facing the Flow team

- **Adequate flow data in an accessible, representative engine do not exist**

- Accurate flow predictions are foundational to the prediction of combustion, sprays and mixture formation, ignition, and heat transfer

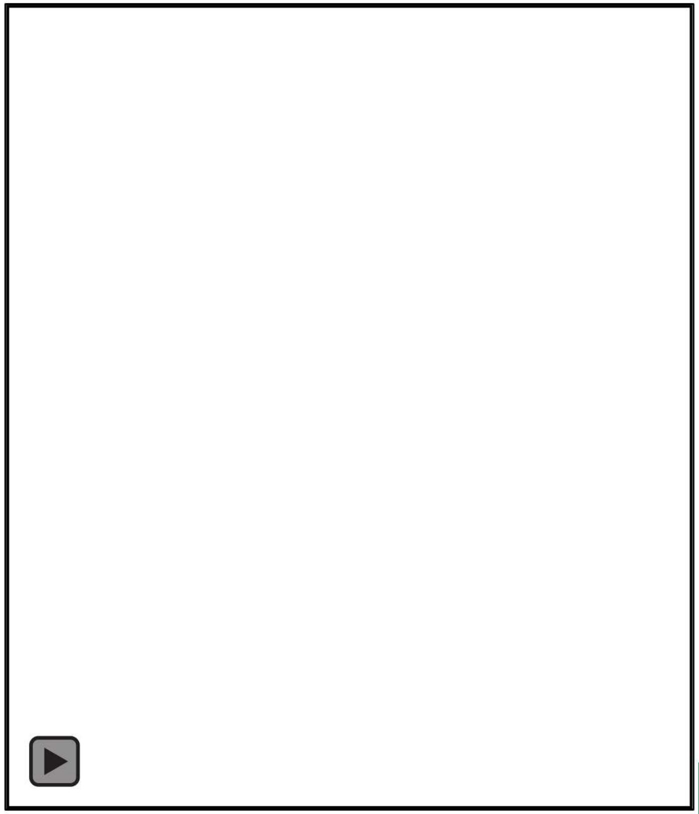
Current Status:

- Velocity measurements exist (Darmstadt, SJTU, etc.) but are not comprehensive enough for systematic evaluation of flow, sprays and combustion, heat transfer, and ultimately predictive simulations of knock and cold-start

Planned work:

- Install a high-tumble, down-sized-boosted engine (US OEM macro-trend) in optical, single, and multi-cylinder configurations at all of the laboratories
- Perform flow measurements and simulations under high-load and low-load conditions to:
  - Allow detailed evaluation of root causes and potential mitigation strategies for cyclic variability

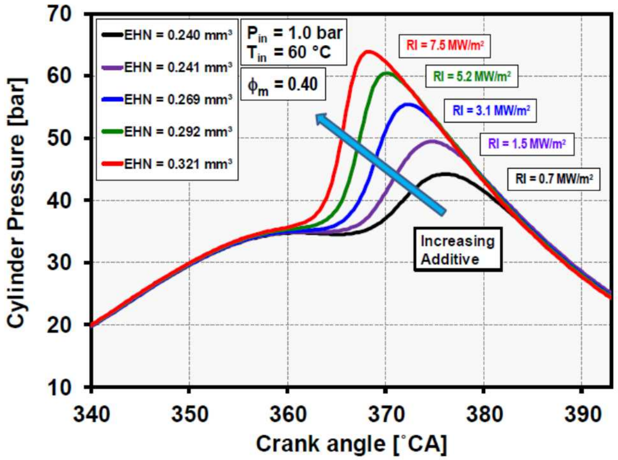
Courtesy: ANL (Scale resolved simulations with Nek5000)



"Purpose-aligned" Combustion Phasing Control task

CA50 control and low-load operation are the most significant obstacles to highly efficient HCCI-like combustion

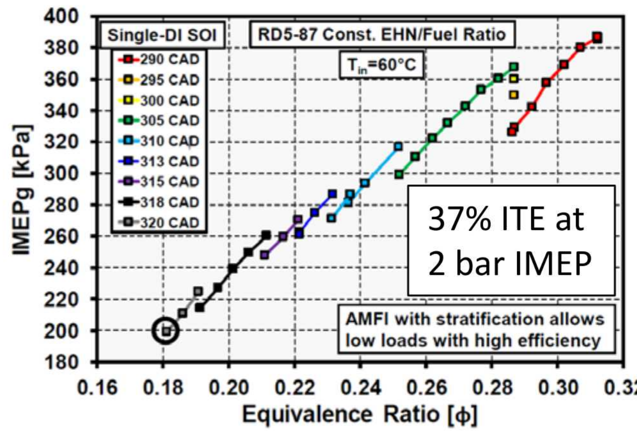
- Enables efficient, ultra-low emission comb.



Current Status:

- SACI/SPPCI techniques can provide effective phasing control, but are challenged by NOx emissions
- Autoignition-based control methods can greatly alleviate emissions difficulties and potentially provide higher efficiencies
- Low-load operation requires extensive intake heating, NVO, or retained residuals

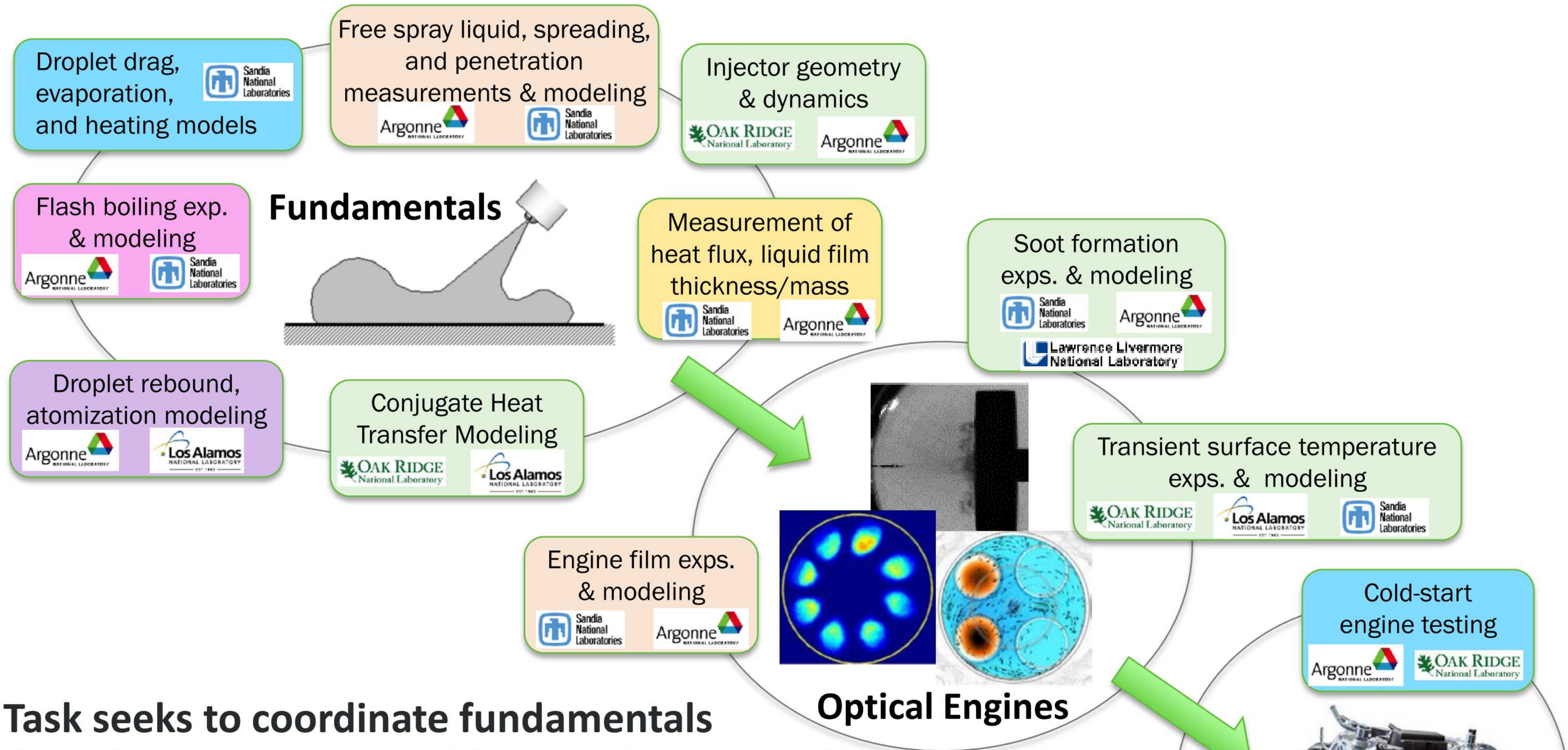
Microfluidics-based additive mixing provides rapid phasing control & high efficiency low-load operation



Planned work:

- Continued development of additive mixing injector and control strategies
- Further development of control strategies based on mixture stratification with ϕ–sensitive fuels
- Optical studies of mixture stratification supporting spray modeling

“Purpose-aligned” Cold-Start task



Task seeks to coordinate fundamentals & engine testing to provide an end-to-end solution:

- Provide data to fundamental researchers and modelers to guide their work
- Coordinate needed optical & single cylinder work
- Perform both initial and final CFD modeling to identify shortcomings and validate performance

Closing remarks

- The IC engine has significant improvement potential, but external pressures require that we make these improvements quickly
- A successful coordination effort will likely significantly improve the impact of DOE-sponsored engine research
- A top-down approach to organizing the projects has been adopted. Previous efforts with “organic” collaborations have only been partially successful in focusing and coordinating research
- Development of improved engineering models and incorporating them into commercial codes is an efficient method for both archiving knowledge and transferring it effectively to industry
- An improved predictive simulation capability will be key to both speeding progress and achieving optimal ICE performance and emissions