Fuel Properties to Enable Lifted Flame Combustion

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FT017

Overview

Timeline

- Start Date - October 2011
- End Date - December 2014
- Percent complete – 80%

Barriers

- Understand fuel impact on combustion & emissions
- Improve predictive tools
- Enable advanced combustion regimes - LLFC

Budget

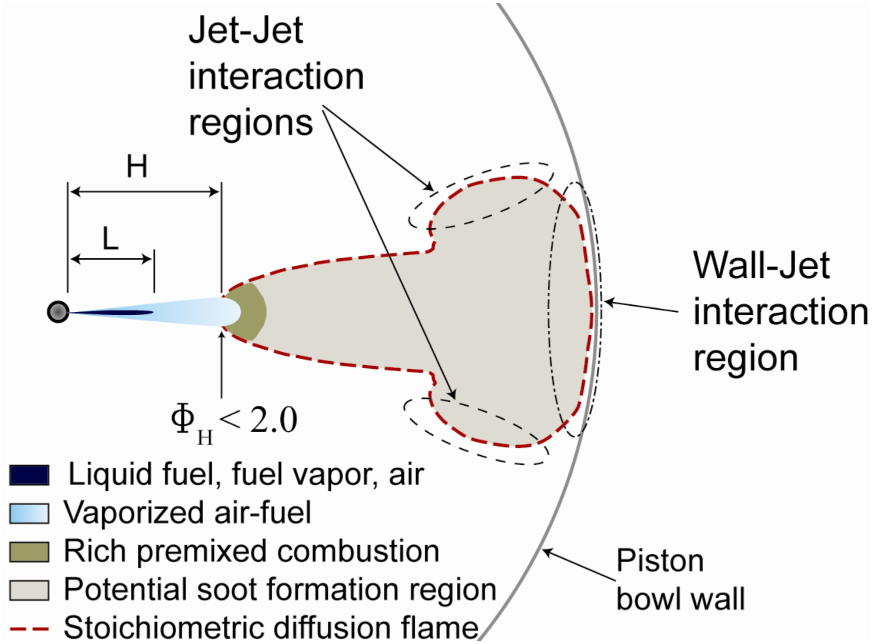
- $1.875M
  - DOE Share: $1.5M
  - Ford Share: $375k
- $406k in FY2013
- $694k in FY2014

Partners

- Interactions/collaborations
  - Sandia National Labs: sprays, optical engine
  - University of Wisconsin-Madison: Advanced model development
  - Lawrence Livermore National Labs: Kinetics model development
- Project lead: Ford

Relevance: Objective

Project objective: Identify fuel properties that can be used to enable controllable, non-sooting Leaner Lifted Flame Combustion (LLFC)

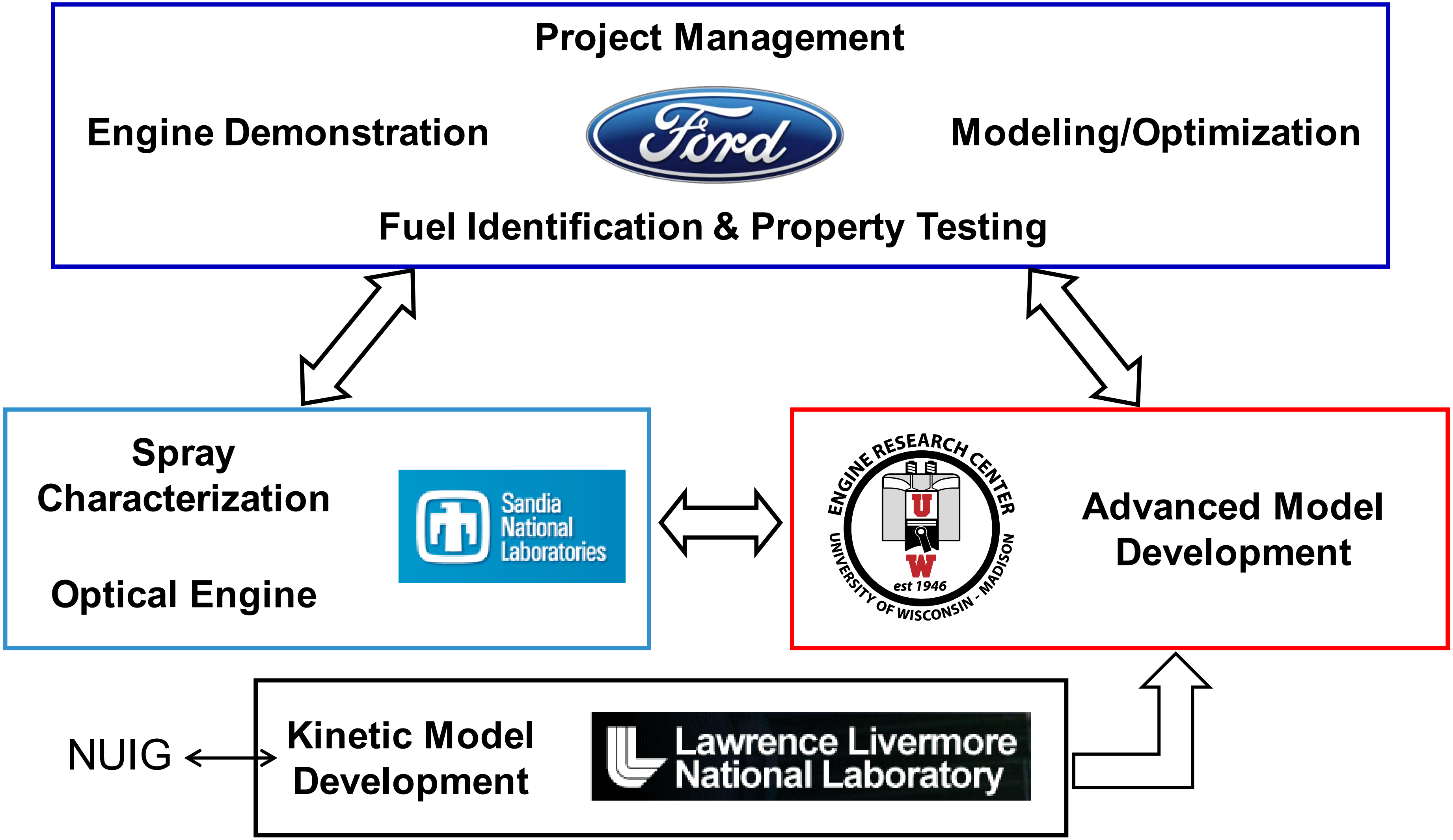


- LLFC benefit: non-sooting diffusion flame
- Requirements:
  - Short liquid penetration
  - Lean mixture ($\Phi < 2$) where the flame starts
- Methods:
  - Increase lift-off length
  - Increase air entrainment
  - Increase fuel oxygen

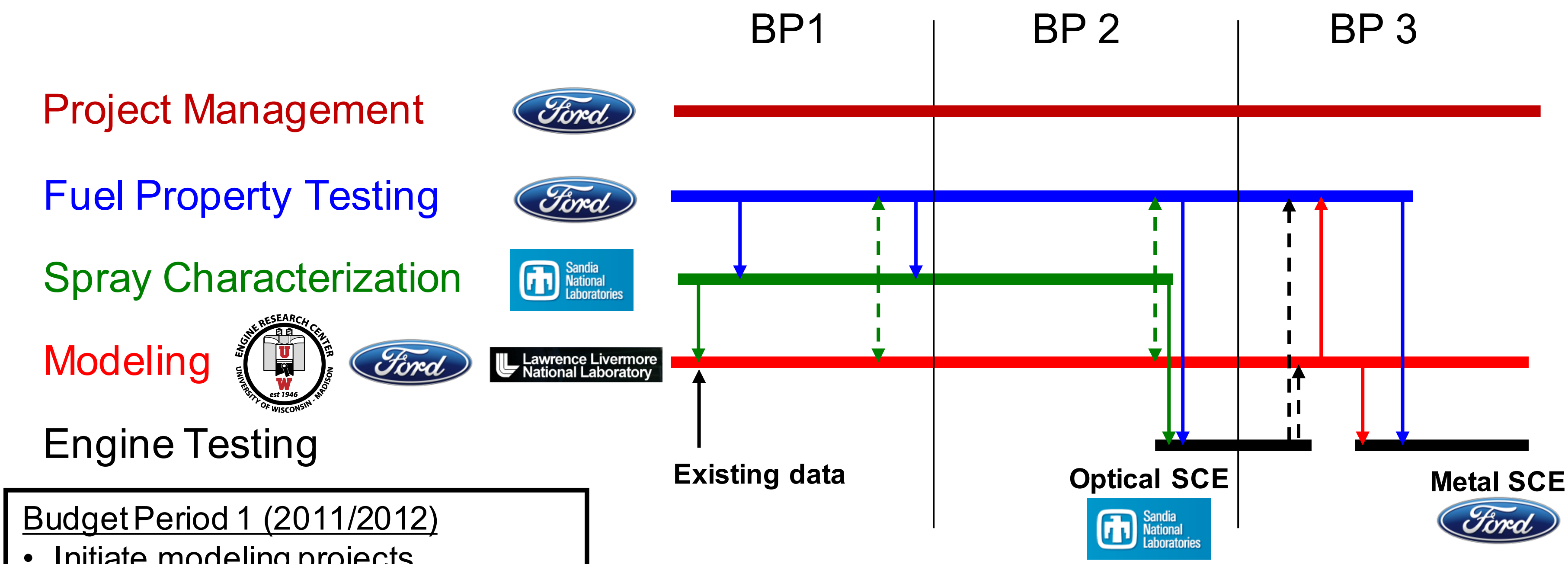
Investigate fuel effects on the ability to achieve LLFC

- Improve fundamental understanding – relatively new combustion mode
- Enhance predictive tools – develop models to capture observed fuel effects
- Improve efficiency – potential to eliminate the DPF
- Reduce petroleum consumption – application for renewable fuels

Collaboration: Roles & Responsibilities



Approach: Timeline



Budget Period 1 (2011/2012)
- Initiate modeling projects
- Identify, select & test fuels
- Initiate spray characterization

Budget Period 2 (2013)
- Complete spray characterization
- Initiate optical engine studies
- Models ready for used in BP3

Budget Period 3 (2014)
- Explore fuel effects with models
- Optimize SCE for LLFC
- Complete optical engine studies
- Demonstrate LLFC on SCE

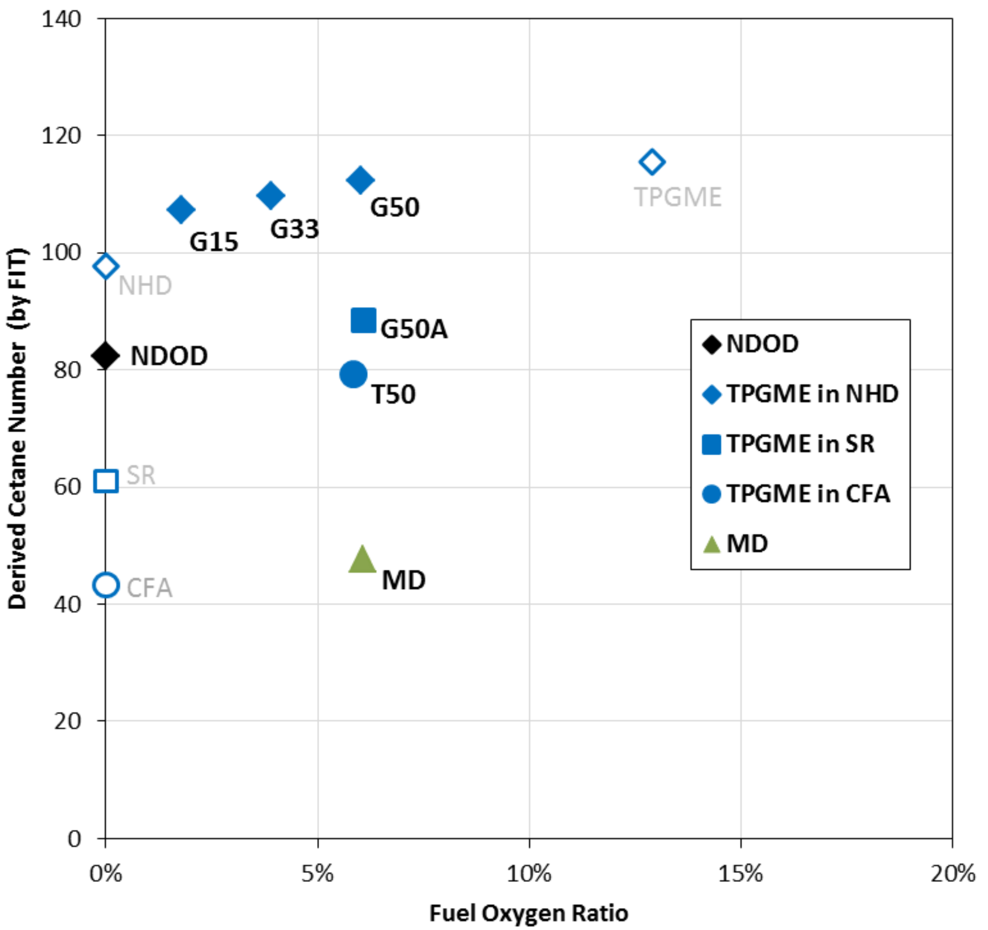
The project is structured to progress from fundamental investigations to more applied studies over the duration of the project.

Approach: Milestones

Year	Milestone	Status
2011/2012	Develop a list of potential oxygenated fuels to use in the study	Complete ✓
	Select fuels for spray studies	Complete ✓
	Initiate modeling studies	Complete ✓
2013	Complete spray characterization of different fuels identifying BCs for LLFC	Complete ✓
	Select fuels for optical engine studies	Complete ✓
	Validate CFD models based on engine and spray studies	Complete ✓
	Improve TPGME kinetic mechanism	Complete ✓
2014	Complete optical engine study	Ongoing
	Optimize SCE combustion system for LLFC demonstration	Ongoing
	Select fuels for SCE demonstration	Q3
	Demonstrate LLFC on SCE	Q3/Q4

Accomplishments: Test Fuels

Presumed desired fuel: sufficient oxygen content (clean) and quick transition to diffusion burn (controllable)



- Line of similar cetane rating
- Line of similar oxygen content
- Two hydrocarbon base fuels
  - Aromatics vs. aromatic free
- Two oxygenate types
  - Ether vs. ester

NDOD = n-dodecane
G15 = 15%v TPGME in NHD
G33 = 33%v TPGME in NHD
G50 = 50%v TPGME in NHD
G50A = 50%v TPGME in SR
MD = methyl decanoate
T50 = 50%v TPGME in CFA

TPGME = tri(propylene glycol) methyl ether
NHD = n-hexadecane
SR = 23%v m-xylene in n-dodecane
CFA = No. 2 diesel certification fuel

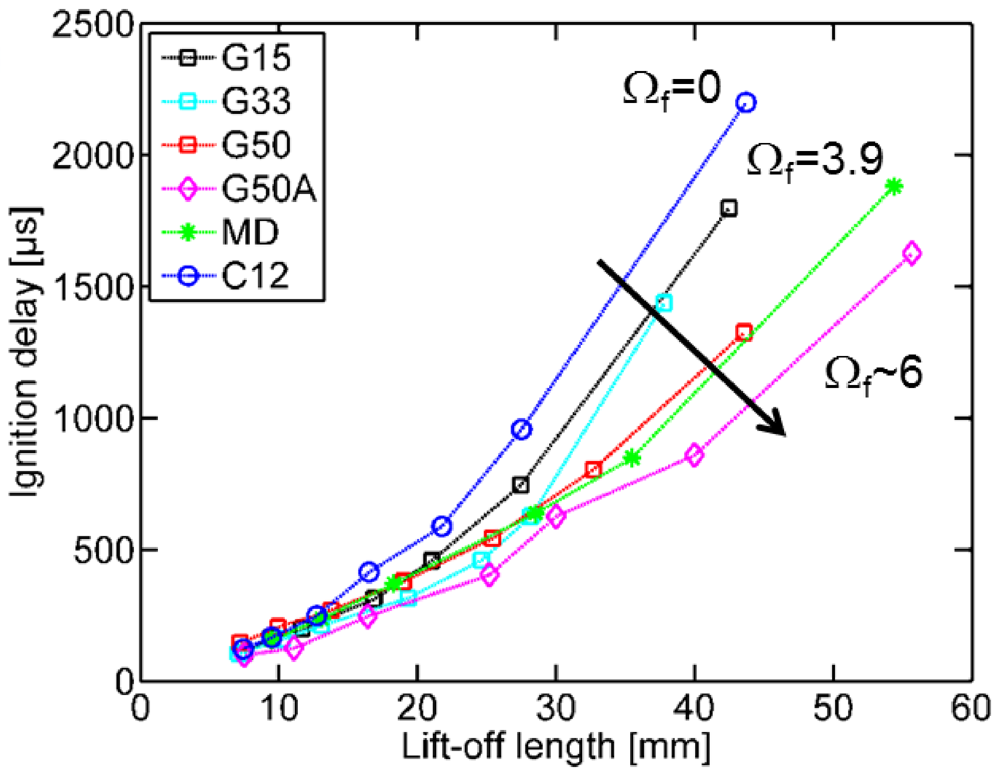
Accomplishments: Transient luminosity and lift-off imaging for hydrocarbon vs. oxygenated fuels

n-dodecane
22.8 kg/m^3 – 850 K

G50
22.8 kg/m^3 – 850 K

New method developed allows the ability to generate quantitative, high-speed, soot measurements with dual wavelength diffused back-illumination extinction imaging

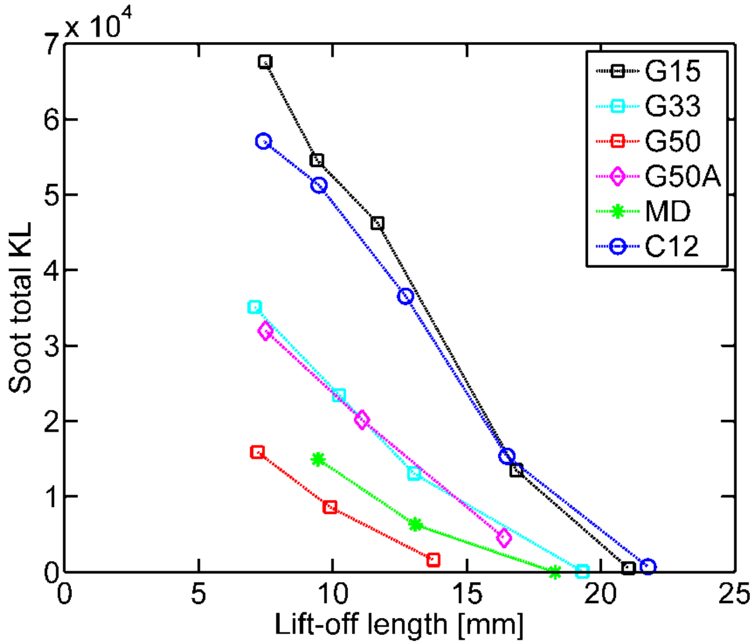
Accomplishments: Ignition delay as a function of lift-off length



- N-dodecane (pure alkane) shows the shortest lift-off lengths of all fuels at a specific ignition delay time
- Increasing the amount of oxygen in the fuel produces longer lifted flames for a given ignition delay (only noticeable at lower ambient temperatures)
- The mixture of m-xylene (aromatic), n-dodecane and TPGME provides the longest lift-off length for a given ignition delay, despite a cetane number that is higher than methyl decanoate

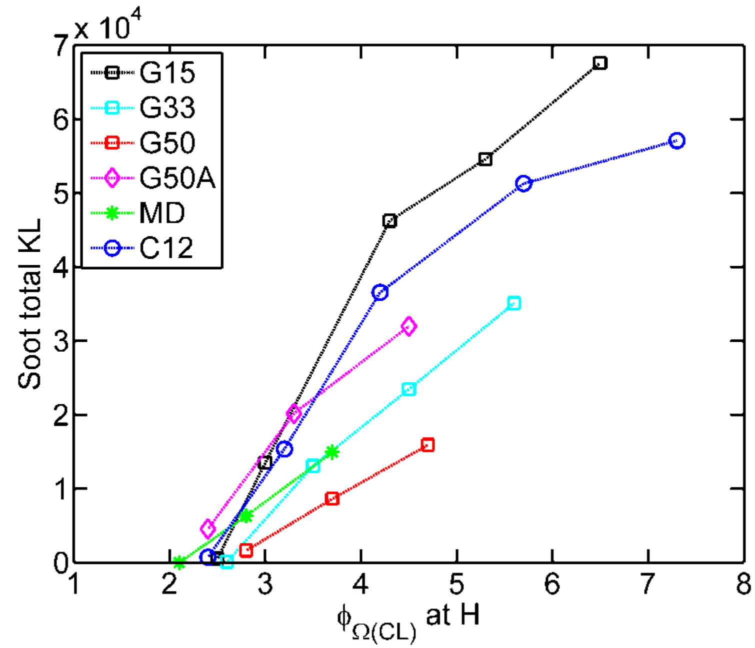
Oxygenated fuels appear to be naturally well suited for LLFC – lower air entrainment requirement & longer flame lift-off for a given ignition delay

Accomplishments: Flame lift-off and soot



- Fuels producing lower amount of soot at short lift-off distances offer clear advantages
  - Low soot production while good engine/combustion control

- Normalizing the fuel to an oxygen adjusted equivalence ratio at lift-off length highlights the benefit of highly oxygenated fuels



- G50 appears to enable non-sooting combustion at richer mixtures.
- Aromatics may lead to a leaner equivalence ratio requirement for LLFC.

Accomplishments: Modeling Fuel Effects

- Two primary fuel properties of interest in LLFC: CN, Ω_f
- Single-component fuel models cannot capture CN range

THREE FUELS TESTED

- High-CN: 57 CN, Aromatics ~2%
- Mid-CN: 44 CN, Aromatics ~29%
- Low-CN: 41 CN, Aromatics ~32%

Hydrocarbon Class

- lower MW normal paraffins
- higher MW normal paraffins
- naphthenes
- aromatics

Experimental Fuel

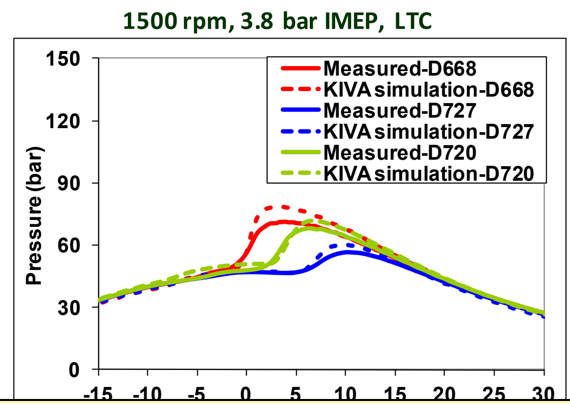
Hydrocarbon Species

Physical Surrogate

Hydrocarbon species	Mass fractions		
	High-CN	Mid-CN	Low-CN
n-decane	0.110	0.160	0.110
n-dodecane	0.092	0.000	0.000
n-tridecane	0.090	0.000	0.000
n-tetradecane	0.273	0.179	0.171
n-hexadecane	0.081	0.171	0.170
n-octadecane	0.171	0.081	0.041
n-heneicosane	0.090	0.090	0.094
Decalin	0.070	0.020	0.070
Naphthalene	0.005	0.017	0.000
Phenanthrene	0.000	0.049	0.048
m-xylene	0.013	0.050	0.041
n-pentylbenzene	0.000	0.040	0.010
Tetralin	0.000	0.052	0.122
n-heptylbenzene	0.000	0.078	0.104

Chemistry Surrogate (GCR)

Hydrocarbon species	Mass fractions		
	High-CN	Mid-CN	Low-CN
n-heptane	0.1150	0.1730	0.1290
n-tetradecane	0.7970	0.5210	0.4764
cyclohexane	0.0700	0.0200	0.0700
n-pentylbenzene	0.0180	0.2860	0.3246



Fuel effects on combustion and emissions were well captured over a wide range of operating conditions & parametric studies.

Accomplishment: Oxygenate Modeling

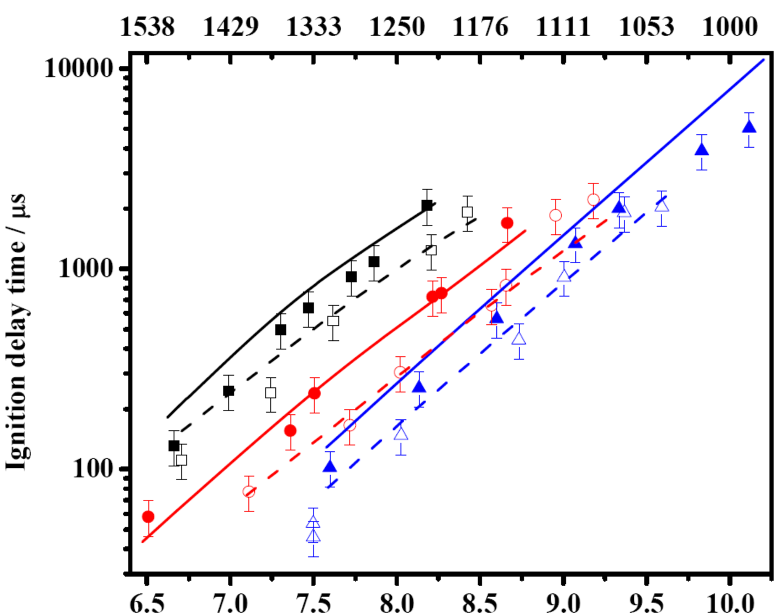
TPGME is the primary fuel being used in spray and engine testing in this project

Issue: increased ignition delay predicted with TPGME, misfire @ <1000 K (CN_{TPGME} > 60!)

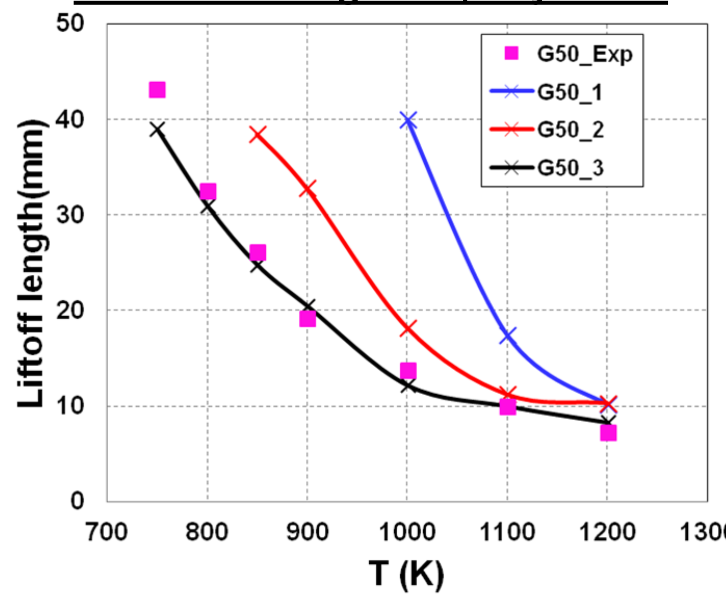
Conclusion: low temperature chemistry not well developed

Solution: engage Bill Pitz at LLNL to improve detailed TPGME kinetics model

Shock-tube ignition of T PGME/O2/Ar mixtures:



UW Modeling of Spray Data



- New full kinetic model shows reasonable agreement with shock tube data
- UW has reduced and refined this model – excellent agreement with Sandia spray data (ignition delay and lift-off length)

Remaining Challenges and Barriers

- Spray studies provided a good foundation to understand the effect of fuel properties on the ability to achieve non-sooting conditions in a well controlled environment.
- Additional work is needed to understand how the complexity of the engine environment alters this picture.

Planned Future Work

- Conduct optical engine studies to understand LLFC in an engine using T50.
- Leverage models to further understand the results of the spray studies.
- Improve combustion system to facilitate LLFC - implement changes on the Ford metal single-cylinder engine.
- Demonstrate LLFC on the Ford single-cylinder engine evaluating several different fuel blends with varying fuel oxygen ratio.
- Project is planned to be completed by December 2014.

Summary

Relevance: Project is aimed at understand the role fuels can play to enable LLFC.

Approach: Through collaboration with Sandia & UW, use a suite of tools including spray vessel, optical engine, metal engine and CFD to improve fundamental understanding and model capability.

Technical Accomplishments:

- Found increasing flame lift-off length with fuel oxygenation – new finding.
- Demonstrated LLFC over a wide set of conditions with Ω_f~6.
- Demonstrated CFD models that are able to capture the effect of CN.
- Validated CFD model for TPGME blends – ready to use.

Collaboration: Core team includes researchers from Ford, Sandia National Labs, UW-Madison and LLNL with support from NIUG.

Future Work:

- Use CFD models to help better explain spray results.
- Complete optical and metal single-cylinder experiments to demonstrate LLFC.

QUESTIONS?

Note: This project was not reviewed at the 2013 AMR.

Technical Back-Up Slides

(Note: please include this “separator” slide if you are including back-up technical slides (maximum of five technical back-up slides). These back-up technical slides will be available for your presentation and will be included in the DVD and Web PDF files released to the public.)

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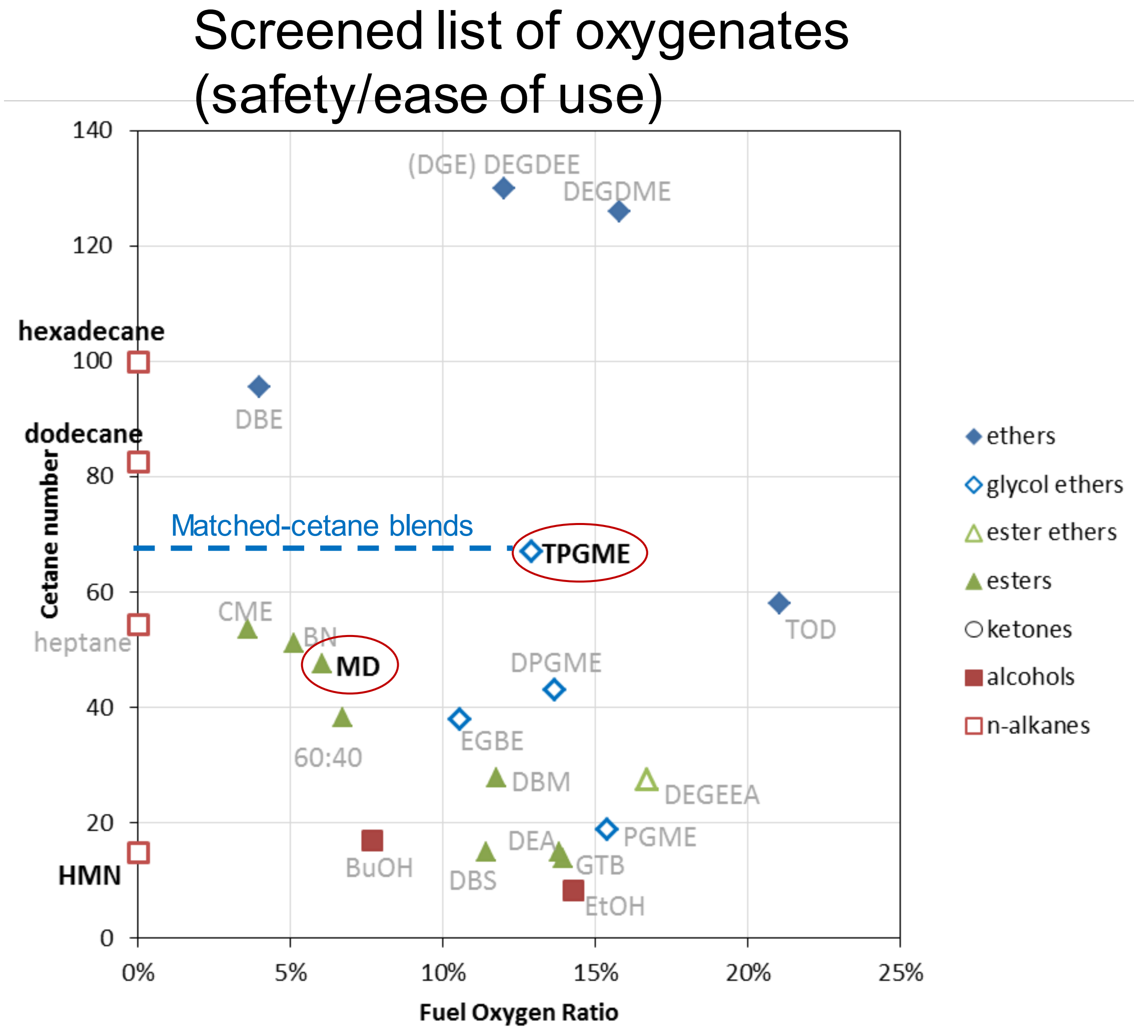
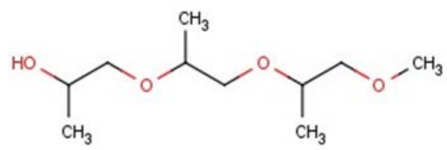
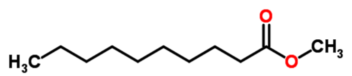
Oxygenates Considered



- Tri(propylene glycol) methyl ether (TPGME, 8 isomers, $C_{10}H_{22}O_4$)



- Methyl decanoate ($C_{11}H_{22}O_2$)



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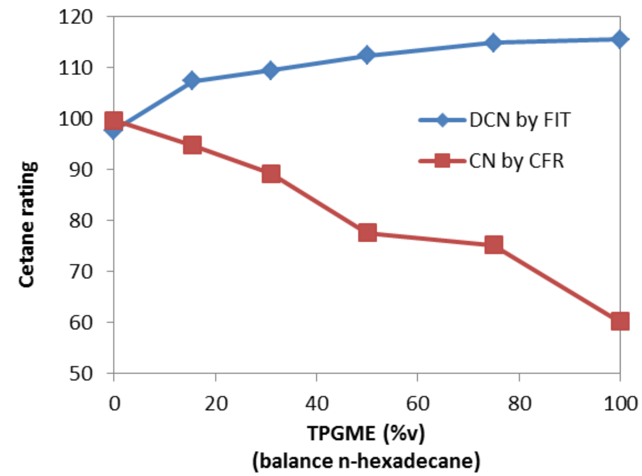
Cetane Rating Measurements

- Attempted to create "matched-cetane" blends of TPGME in PRF
  - PRFs are blends of NHD (n-hexadecane) and HMN (2,2,4,4,6,8,8-heptamethylnonane)
  - PRFs have method-defined CNs on CFR engine
- Different TPGME cetane ratings by CFR engine, FIT, and IQT

	Meas.	Literature
CFR (CN)	64 ± 4	63 (blend)
FIT (DCN)	108 ± 8	n/a
IQT (DCN)	79	74 (neat)

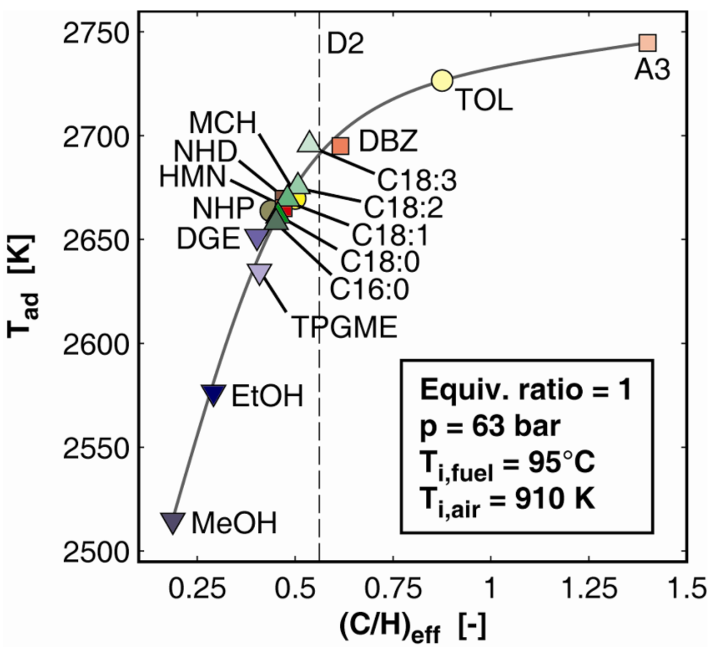


- NHD selected as base fuel (DCN=CN=100)
  - Matched DCN of TPGME (by FIT)
  - Simple composition
- Similar behavior in blends with NHD and a surrogate reference fuel.
- *Cetane rating methods give substantially different results for these fuels. Explanations being investigated.*
- *Sandia spray lab testing later indicated ignition delays for TPGME-NHD blends were similar.*

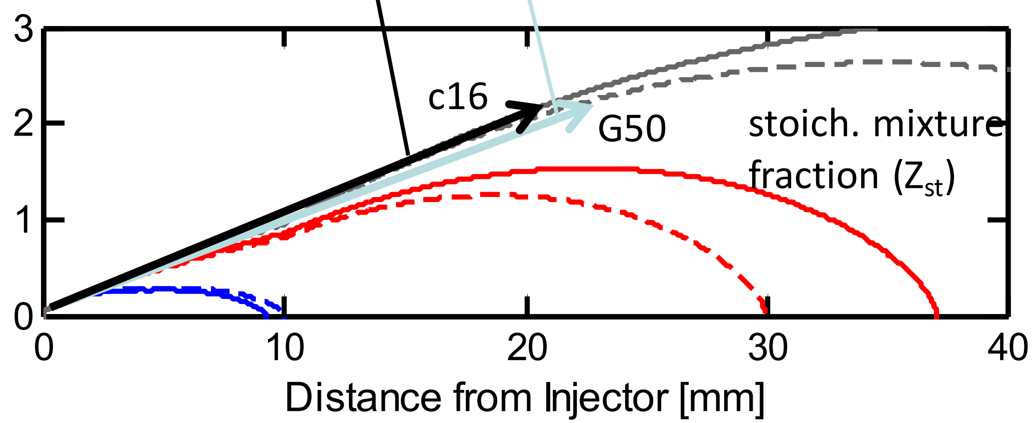
Lift-off length: Equivalence ratio and flame temperature

- Due to the presence of oxygen in the fuel, oxygenated fuels produce igniting mixtures shifted toward the center of the jet
  - Because of the different stoichiometric contour locations, lift-off length is expected to be further downstream for oxygenated fuels

A fuel parcel following a stoichiometric contour mixing path, travels farther downstream for G50 compared to C16 over the same ignition delay



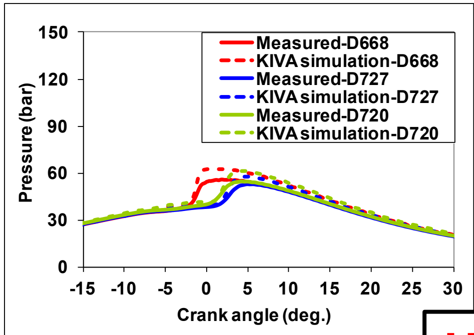
Mueller et al. SAE paper 2009-01-1792



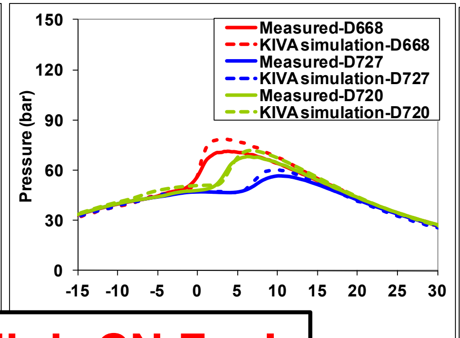
- Stoichiometric adiabatic flame temperature may also play a role in the explanation towards longer lifted flames with oxygenated blends
  - Lower adiabatic flame temperature fuels are expected to have decreased reaction rates at lift-off length which might extend lift-off length

CN - Surrogate Model Validation

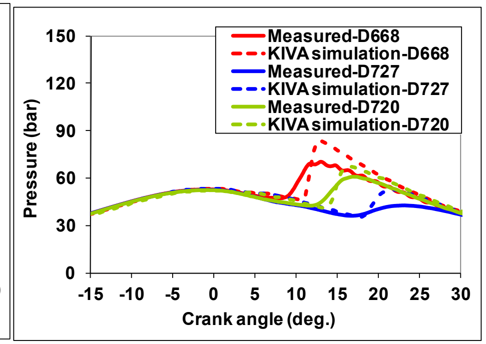
750 rpm, 2.2 bar IMEP, LTC



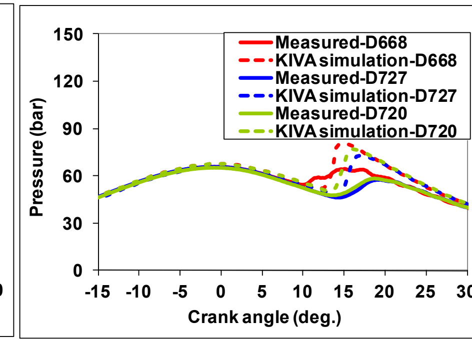
1500 rpm, 3.8 bar IMEP, LTC



1500 rpm, 6.8 bar IMEP, LTC

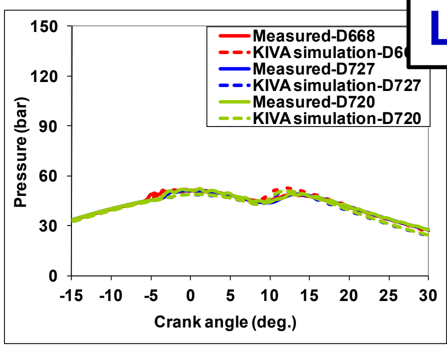


2500 rpm, 5.4 bar IMEP, LTC

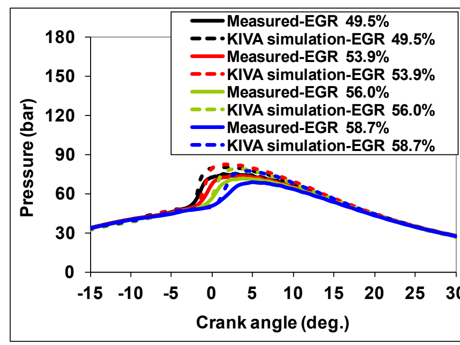


High-CN Fuel
Mid-CN Fuel
Low-CN Fuel

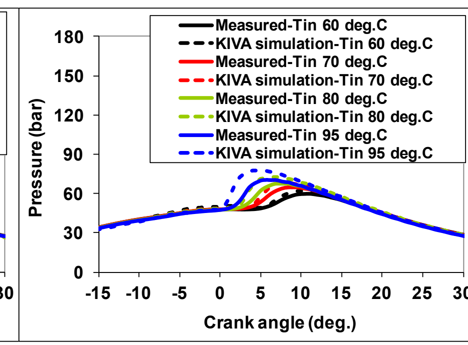
1500 rpm, 3.7 bar IMEP, convention



EGR Sweep-1500rpm, 3.7 bar IMEP



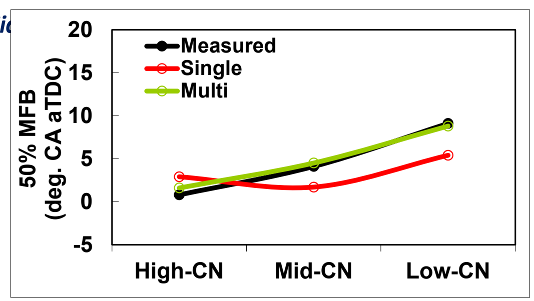
T_{intake} Sweep-1500rpm, 3.7 bar IMEP

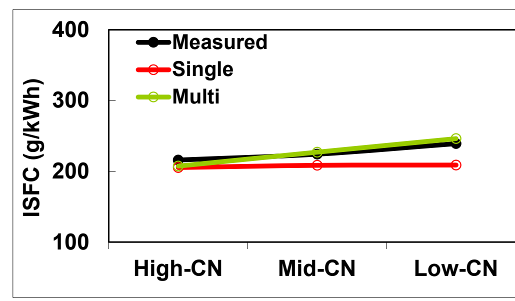


Note: D668 – High-CN Diesel Fuel, D727-Low-CN Diesel Fuel, D720-Mi

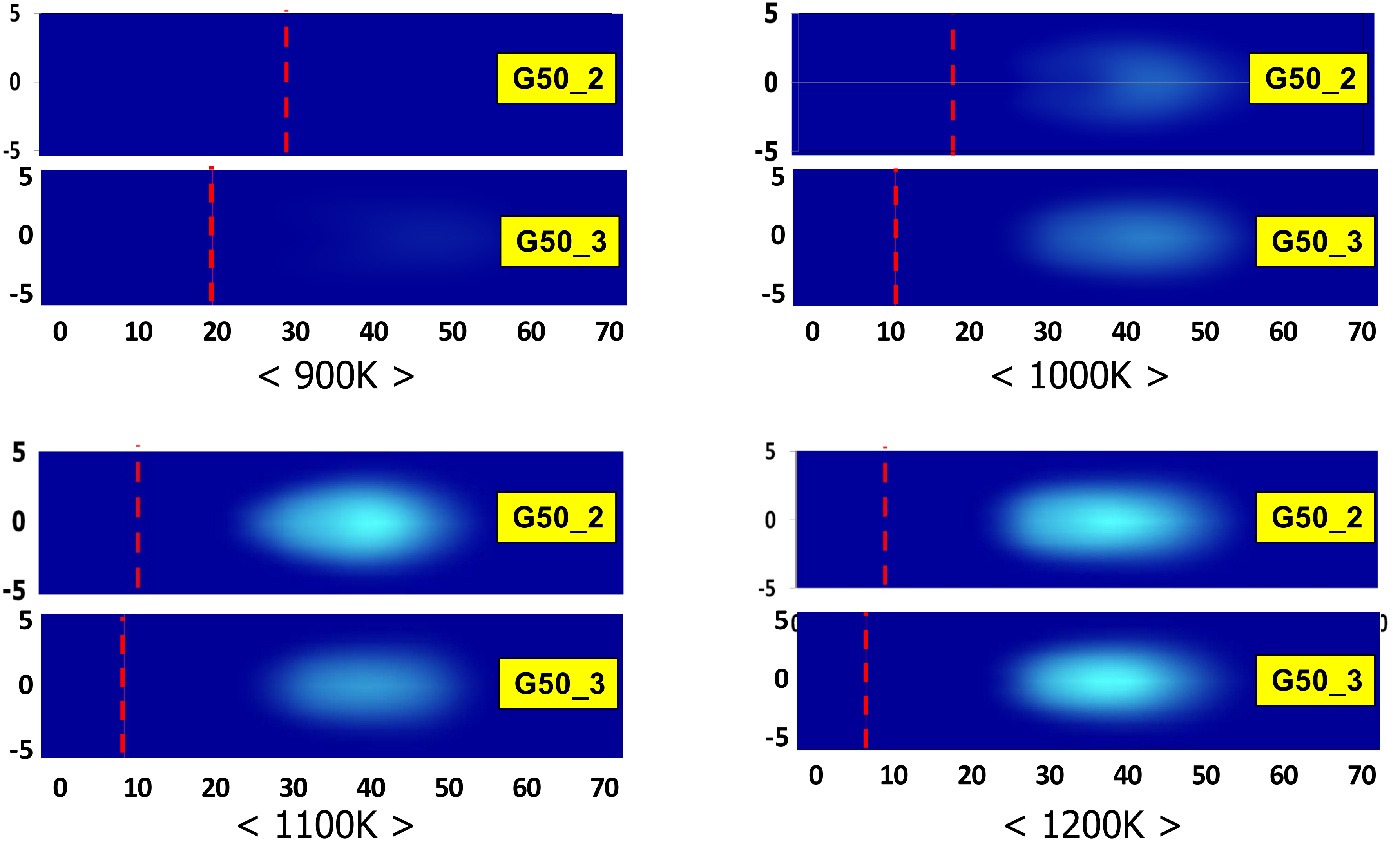
Validated model at various speed-load points, EGR, intake temperatures and combustion modes.

D720





G50_2 & G50_3 Soot Prediction Comparisons



* Red dashed line = Liftoff length

Distance from injector orifice (mm)