FUEL EFFECTS ON COMPRESSION IGNITION

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Topic Motivation and Objectives

- Motivation
  - ✓ Understand the fuel effects on spray at CI conditions as an additional dimension for model development and validation
- Objective
  - ✓ Summarize and understand the available experimental and computational fuel effect studies
  - ✓ Relevant studies on spray fuel effect
  - ✓ Define a “Fuel” of interest for the ECN community
- Assumption:
  - ✓ Variations of combustion chambers, boundary conditions, optical diagnostic techniques, definitions were not considered

Experimental Investigation of Spray Fuel Effects

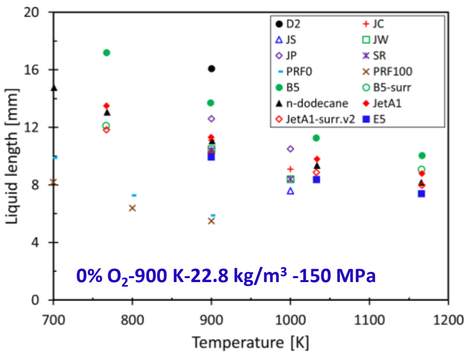
Literature Referred

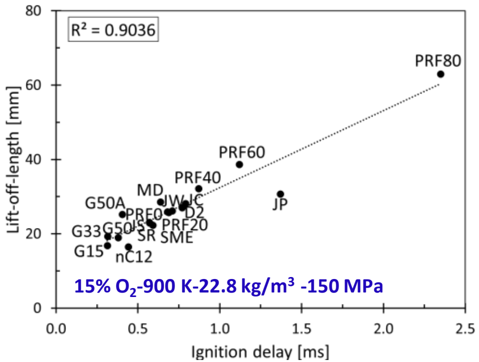
- ✓ Kook, S., Pickett, L.M., "Soot volume fraction and morphology of conventional, fischer-tropsch, coal-derived, and surrogate fuel at diesel conditions." *SAE Int. J. Fuels Lubr.* 5, 2 (2012): 647-664.
- ✓ Pastor, J. V., Garcia-Oliver, J. M., Novella, R., Vera-Tudela, W., "Investigation on ignition and combustion characteristics of primary reference fuels under diesel engine conditions." In Proceedings of the 14th Working process of the Internal Combustion Engine Congress, Graz. 2013.
- ✓ Manin, J., Skeen, S., Pickett, L.M., Kurtz, E., Anderson, J.E., "Effects of oxygenated fuels on combustion and soot formation/oxidation processes." *SAE Int. J. Fuels Lubr.* 7, 3 (2014): 704-717.
- ✓ Pastor, J. V., García-Oliver, J. M., López, J., Vera-Tudela, W., "An experimental study of the effects of fuel properties on reactive spray evolution using Primary Reference Fuels." Fuel 163 (2016): 260-270.
- ✓ Bardi, M., Bruneaux, G., Nicolle, A., Colin, O., "Experimental Methodology for the Understanding of Soot-Fuel Relationship in Diesel Combustion: Fuel Characterization and Surrogate Validation", 2017-01-0721, SAE Technical Paper, 2017.

Overview of Spray Fuel Effect Characterization

Nozzle	Spray A Single-hole, 90 µm, K 1.5 / 0.86
Ambient temperature	700 – 1200 K
Ambient density	15.2, 22.8, 45.6 kg/m^3
Ambient oxygen	0%, 15%, 18%, 21%
Injection pressure	50, 100, 150 MPa
Institutions	CMT, SNL, IFPEN

Fuels	Density [kg/m^3]	CN
D2 (No. 2 diesel)	843	46
JC (JP-8)	812	38
JW (World Average Jet A Blend)	806	46
JS (Fischer-Tropsch Fuel)	755.9	62
JP (Coal-Derived Fuel)	870.2	34
SR (Surrogate Fuel)	778.9	70
SME (soy ethyl ester)	877	51
nC12	750	80
PRF0	-	-
PRF20	-	-
PRF40	-	-
PRF60	-	-
PRF80	-	-
PRF100	-	-
B5 (5% esters)	833	53.1
JetA1	812	45.6
JetA1-surr.v1	-	-
JetA1-surr.v2	-	-
E5 (5% ethanol)	746	17
n-dodecane	745	73
G15	800	108
G33	835	110
G50	869	112
G50A	859	88
MD (Methyl decanoate)	871	48

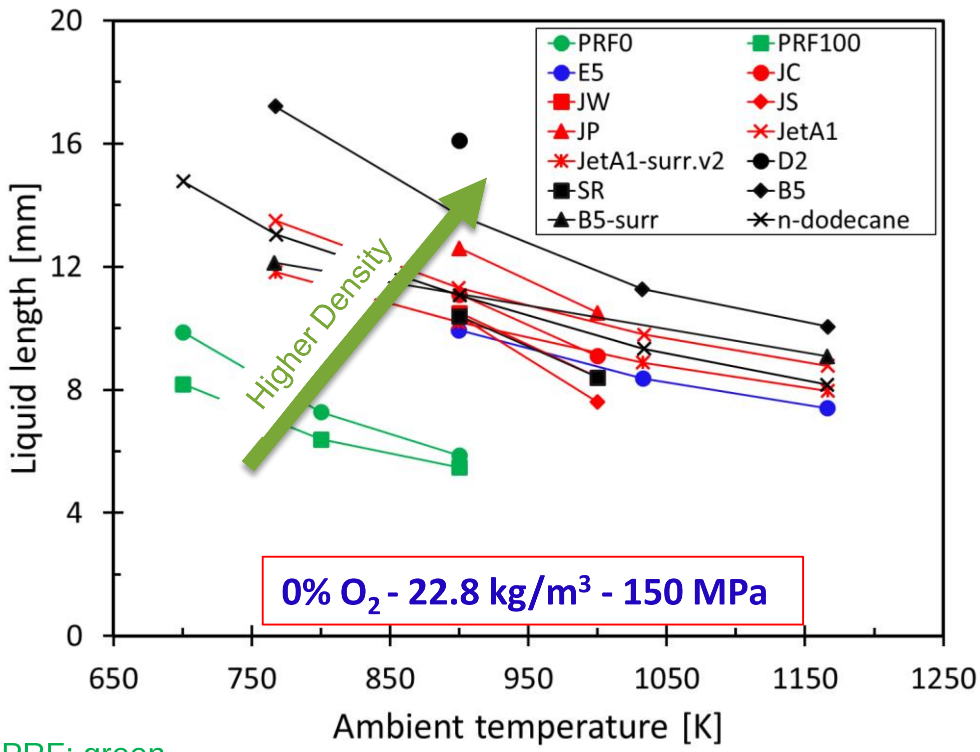




Fuel type	Fuels	Fuel details	Density [kg/m³]	CN/DCN	LHV [MJ/kg]	C/H mass ratio	Aromatics volume %	Boiling temp. [ºC]	Kinematic viscosity (40ºC)
PRF fuel	PRF0	100% n-heptane, 0% iso-octane	684	55	44.6	5.25	0	98	0.51
	PRF20	80% n-heptane, 20% iso-octane	685	46	44.5	5.27	0	99	0.54
	PRF40	60% n-heptane, 40% iso-octane	686	38	44.5	5.29	0	99	0.57
	PRF60	40% n-heptane, 60% iso-octane	688	29	44.5	5.30	0	99	0.59
	PRF80	20% n-heptane, 80% iso-octane	689	21	44.5	5.32	0	99	0.62
	PRF100	0% n-heptane, 100% iso-octane	690	13	44.4	5.33	0	99	0.65
Gasoline fuel	E5	European standard gasoline containing 5% of etha[illegible]	746	17	42.8	-	-	27-225	-
Jet fuel	JC (JP-8)	a low cetane number fuel that can also be used [illegible] assess the use of aviation fuel using diesel engine hard[illegible]at diesel engine condition	812	38	43.2	6.19	11	266	~1.4
	JW	an equal blend of five Jet-A fuel samples from different U.S. manufacturers, and with the same [illegible]e number as D2	806	46	43.2	6.19	19	274	-
	JS	a Fischer-Tropsch fuel characterized as fuel with minimal aromatics (0.4%) and high cet[illegible] number	756	62	44.1	5.49	0.4	276	-
	JP	a coal-derived fuel, a low cetane number fuel with low 1.9% aromatics but high (>90%) cyclopa[illegible]c content	870	34	42.8	6.58	1.9	270	-
	JetA1	European standard Jet fuel	812	46	43.5	-	-	187-300	-
	JetA1-surr.v1	51.3% n-decane, 19.8% iso-octane, 28.9% n-propylb[illegible]	760	48	43.4	6.10	-	99-174	0.89
	JetA1-surr.v2	47.5% n-decane, 17.6% iso-octane, 35.0% n-propylb[illegible]	770	46	43.3	6.27	-	99-174	0.89
Diesel fuel	D2 (No. 2 diesel)	an emissions-certification fuel with a cetane number of 46 and [illegible] aromatics	843	46	42.9	6.53	27	350	2.35
	SR	a surrogate fuel, a mixture of 23% m-xylene (aromatics) and 77% n-dodeca[illegible]	779	70	43.3	5.96	23	216	-
	SME	soy ethyl ester	877	51	37.4	6.48	0	-	3.98
	nC12 (SNL)	normal dodecane	752	87	44.2	5.54	0	216	1.5
	B5	European standard Diesel fuel with 5% esters composition	833	53	42.5	-	-	187-343	-
	n-dodecane (IFP)	normal dodeca[illegible]	[illegible]45	73	46.5	5.54	0	216	1.5
	G15	Three fuels were blends of tri(propyl[illegible] ether (TPGME) and n-hexadecane, id[illegible] G50 the last two digits indicating the percentage of TPGME in the blend, by volume	[illegible]00	108	41.5	5.63	-	287	3.81
	G33		[illegible]35	110	38.5	5.60	-	287	4.21
	G50		869	112	35.8	5.57	-	287	4.59
	G50A	Aromatic hydrocarbon, a 50/50 volume percent blend of TPGME and a diesel surrogate fuel, the latter composed of 77 % n-dodecane and 23 % m-xylene by volume.	859	88	35.5	6.25	-	287	3.43
	MD (Methyl decanoate)	A different oxygenate chemical structure and was a surrogate for traditional biodiesel fuel	871	48	37.5	-	-	224	-

Higher Density

Experimental Results - Liquid Length vs. Temp

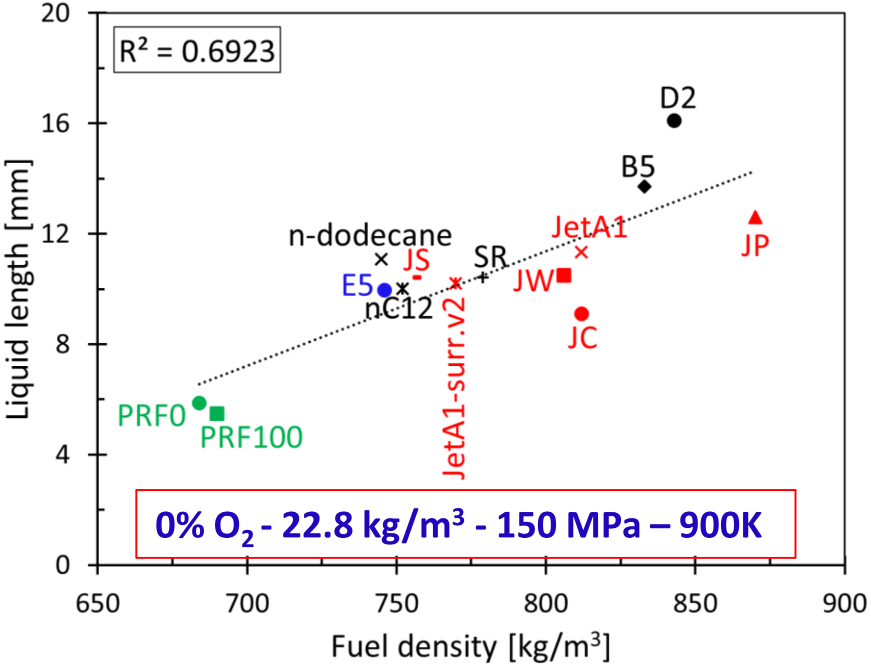


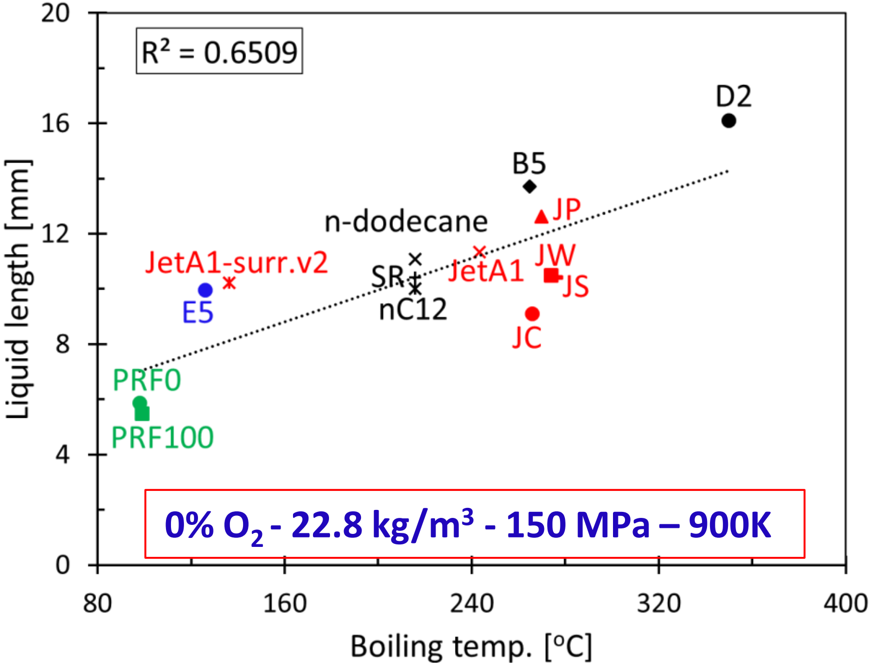
PRF: green
Gasoline: blue
Jet: red
Diesel: black

Higher density generally leads to longer liquid length:

- ✓ PRF < Gasoline < Jet < Diesel
- ✓ PRFs show shorter LL, while D2 and B5 have a longer LL

Experimental Results - Liquid Length Correlation

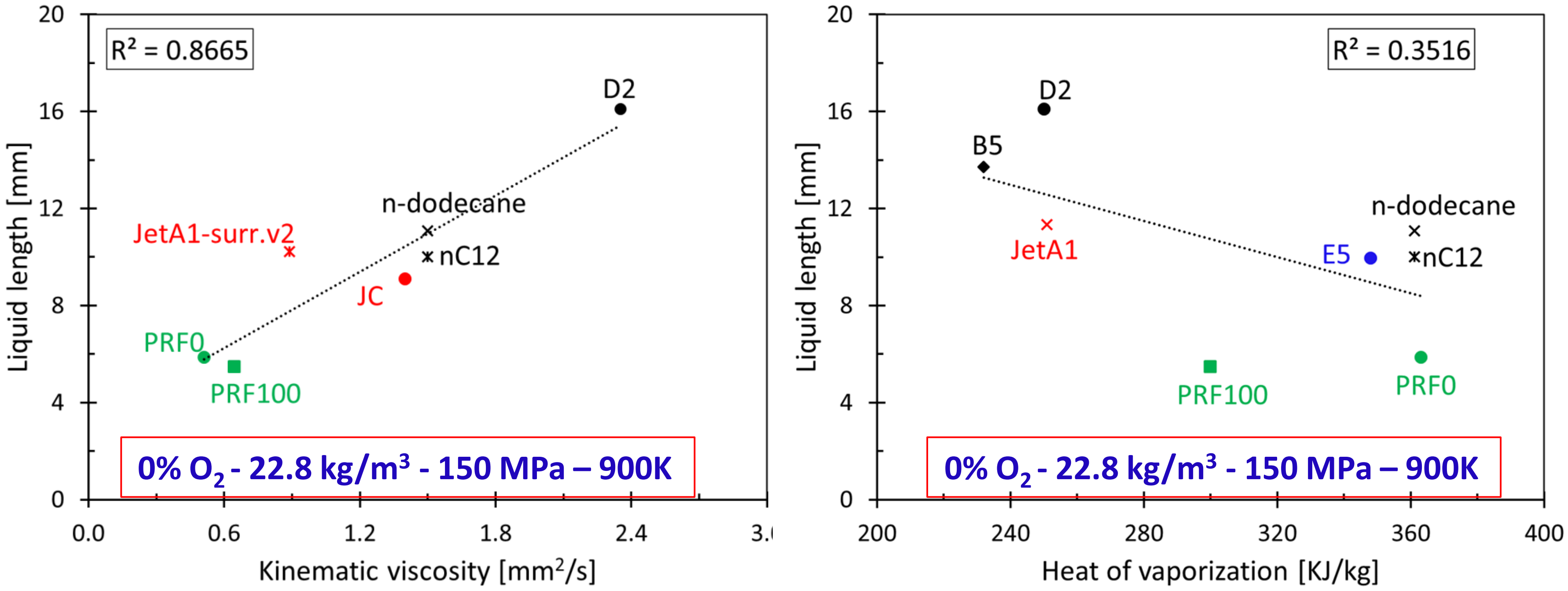




PRF: green
Gasoline: blue
Jet: red
Diesel: black

- A strong correlation is observed between:
  - ✓ LL and fuel density
  - ✓ LL and boiling temperature

Experimental Results - Liquid Length Correlation



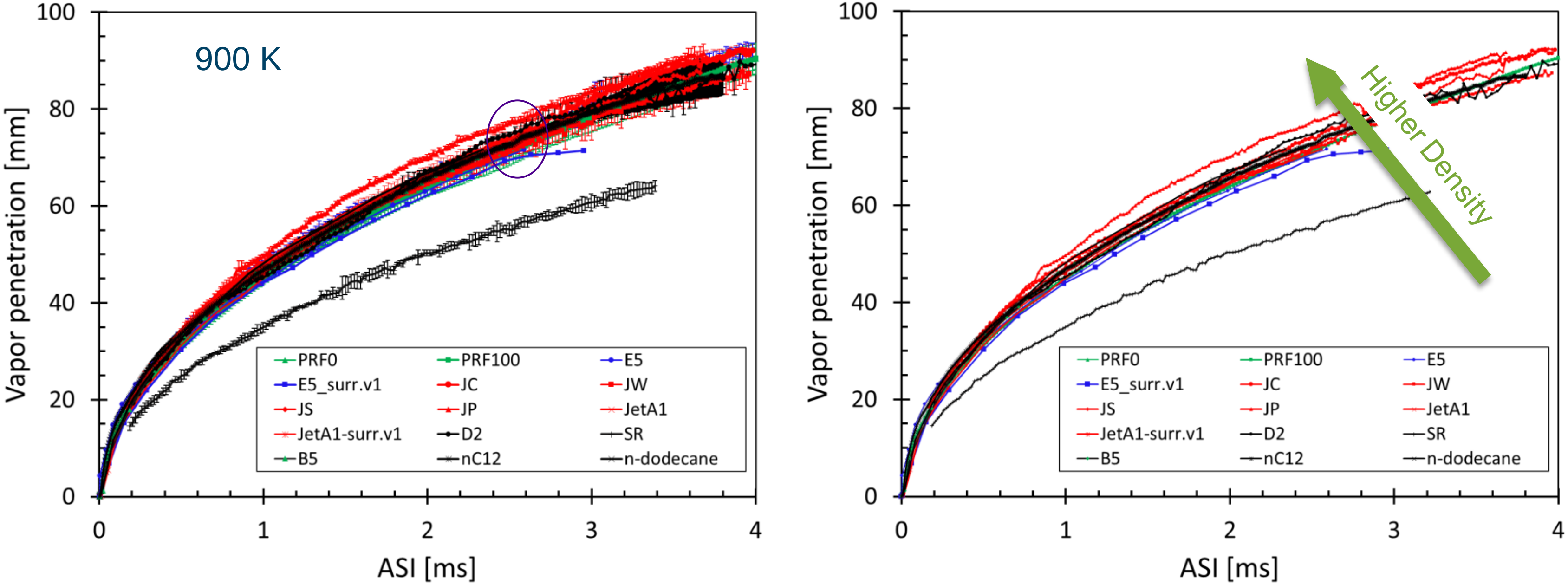
- Viscosity seems to correlate with LL well
- Heat of vaporization correlation is not expected
- A sensitivity analysis would be useful to differentiate the relevant importance of all fuel properties

PRF: green
Gasoline: blue
Jet: red
Diesel: black

ENGINE COMBUSTION NETWORK

Experimental Results – Vapor Penetration Length

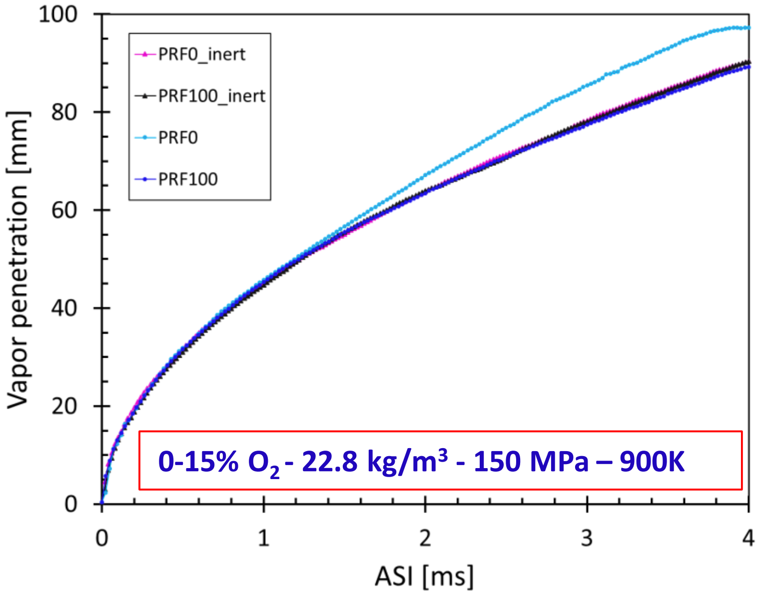
0% O_2 - 22.8 kg/m^3 - 150 MPa – 900K

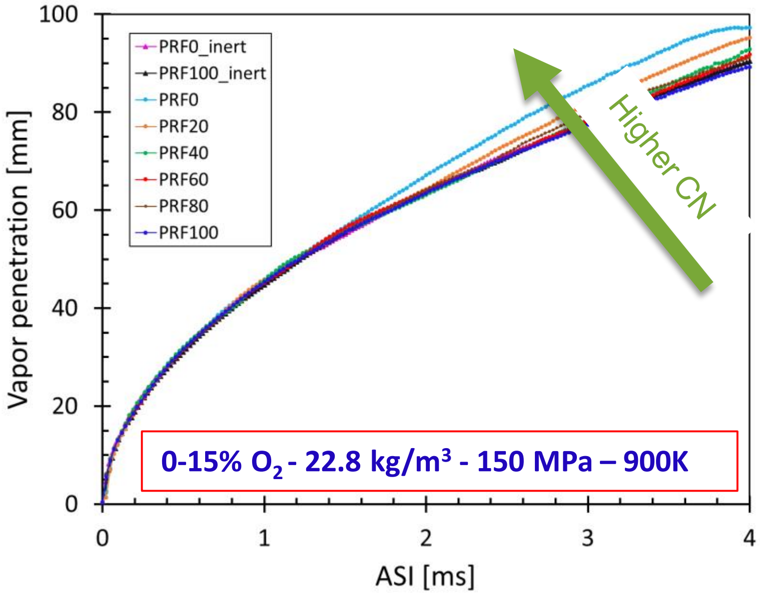


PRF: green
Gasoline: blue
Jet: red
Diesel: black

- Higher density generally leads to longer vapor penetration
  - ✓ SR is an outlier

Experimental Results – Reacting Spray Penetration Length





- Viscosity effect on liquid length doesn't reflect on vapor penetration length
- Faster penetration of PRF0 due to higher CN – dilatation effect at reacting conditions
    - ✓ Higher CN leads to longer penetration

Fuel type	Fuels	Fuel details	Density [kg/m³]	CN/DCN	LHV [MJ/kg]	C/H mass ratio	Aromatics volume %	Boiling temp. [°C]	Kinematic viscosity (40°C)
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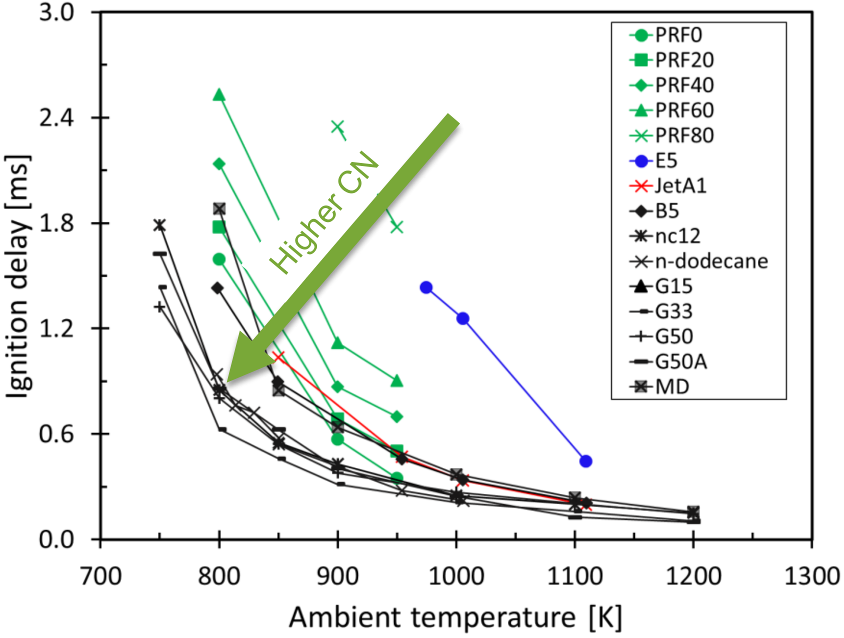
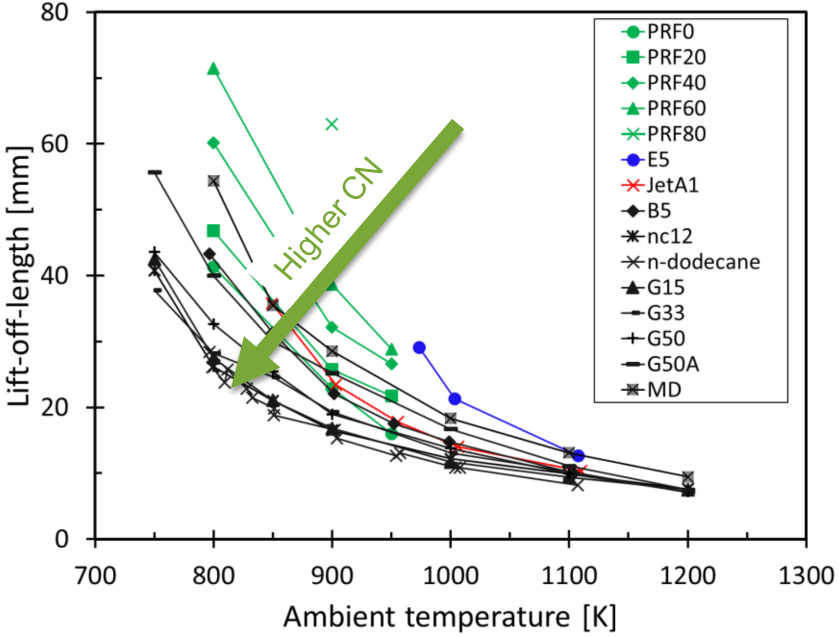
	PRF100	0% n-heptane, 100% iso-octane	690	13	44.4	5.33	0	99	0.65

Experimental Results – ID/LOL vs. Temp

15% O_2 - 22.8 kg/m^3 - 150 MPa



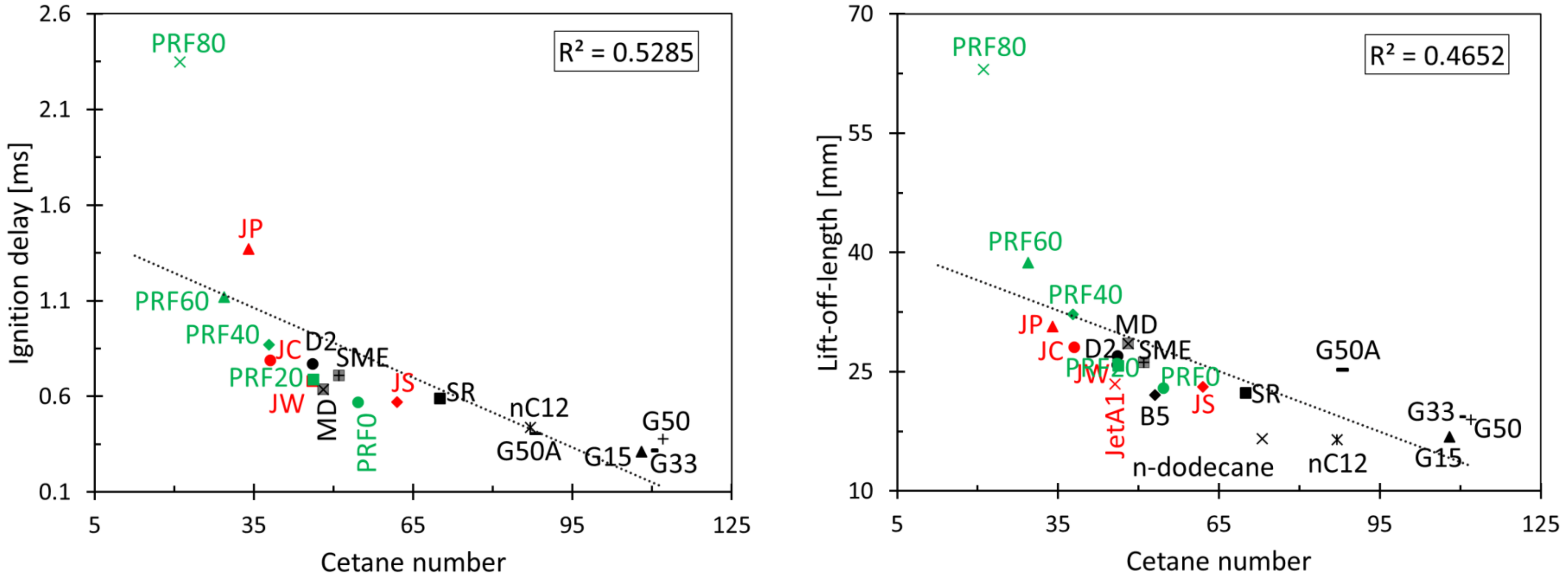


- Higher CN generally results in shorter ID and LOL

PRF: green
Gasoline: blue
Jet: red
Diesel: black

Experimental Results – ID/LOL vs. CN

15% O_2 - 22.8 kg/m^3 - 150 MPa – 900 K

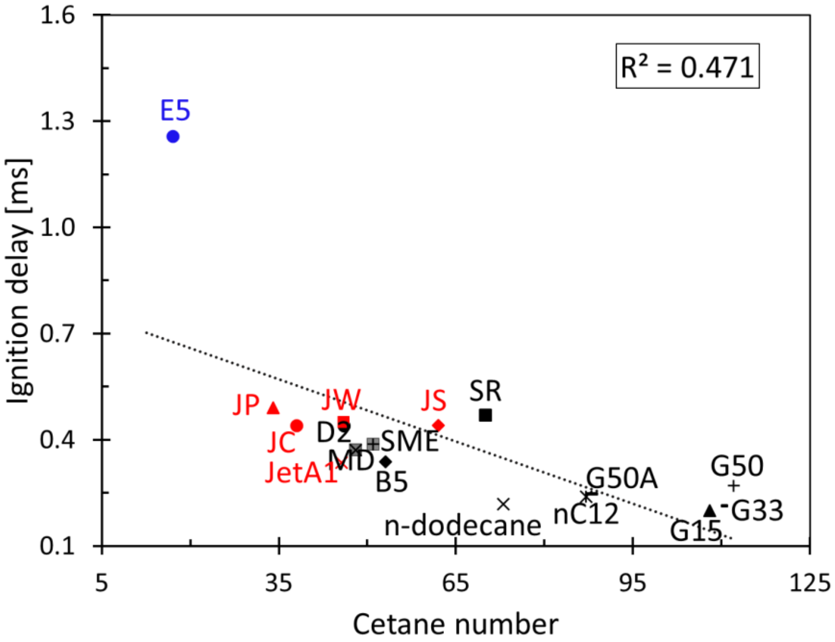


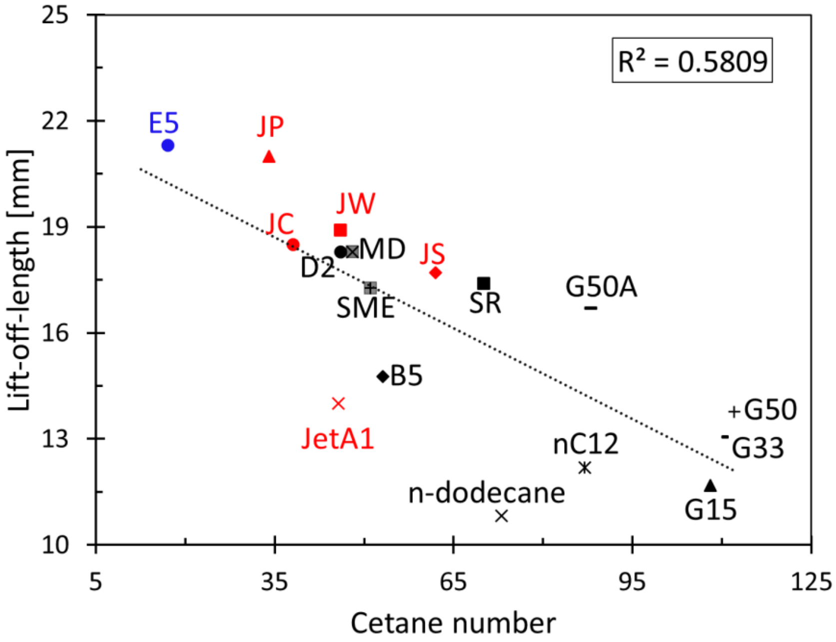
PRF: green
Gasoline: blue
Jet: red
Diesel: black

- A strong negative correlation is observed between ID/LOL and CN
- PRF80 seems an outlier

Experimental Results – ID/LOL vs. CN

15% O_2 - 22.8 kg/m³ - 150 MPa – 1000 K

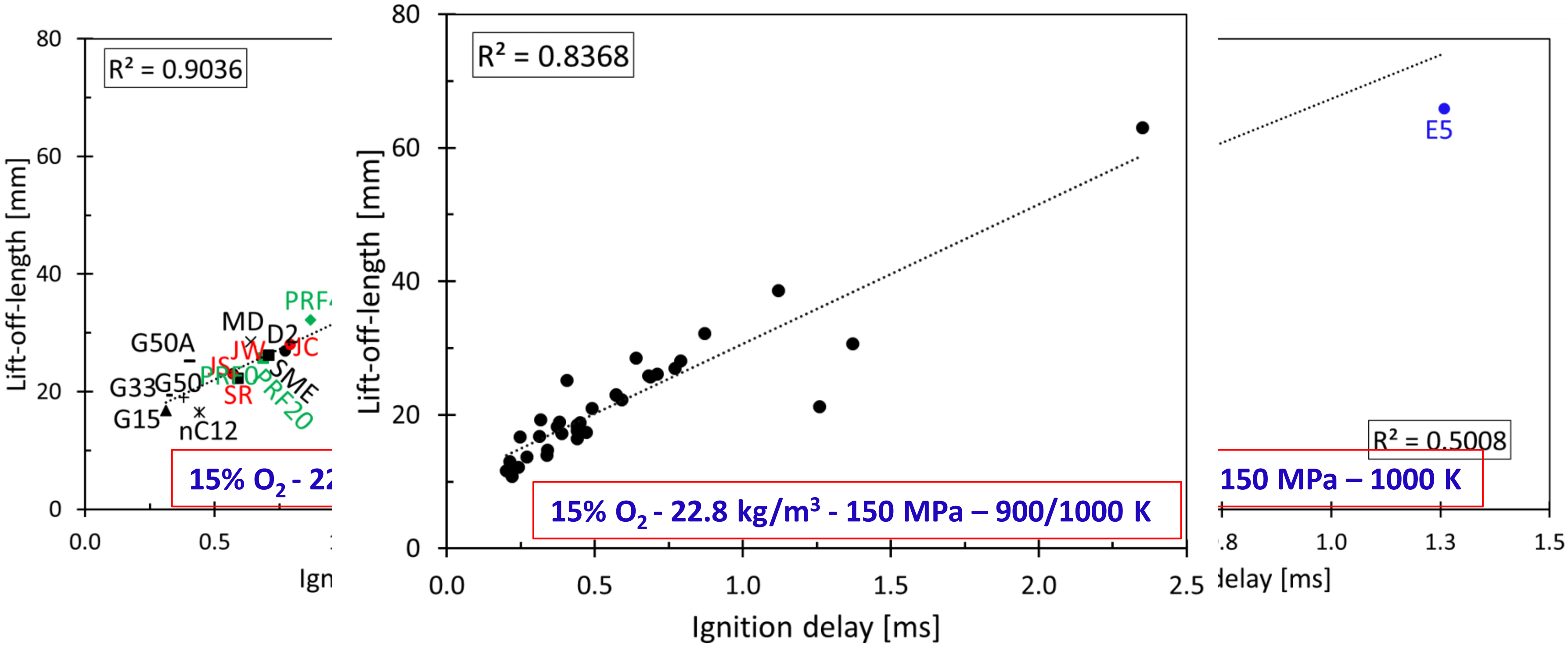




PRF: green
Gasoline: blue
Jet: red
Diesel: black

- A negative correlation is observed between LOL / ID and CN
- E5 is an outlier on ID

Experimental Results – LOL vs. ID

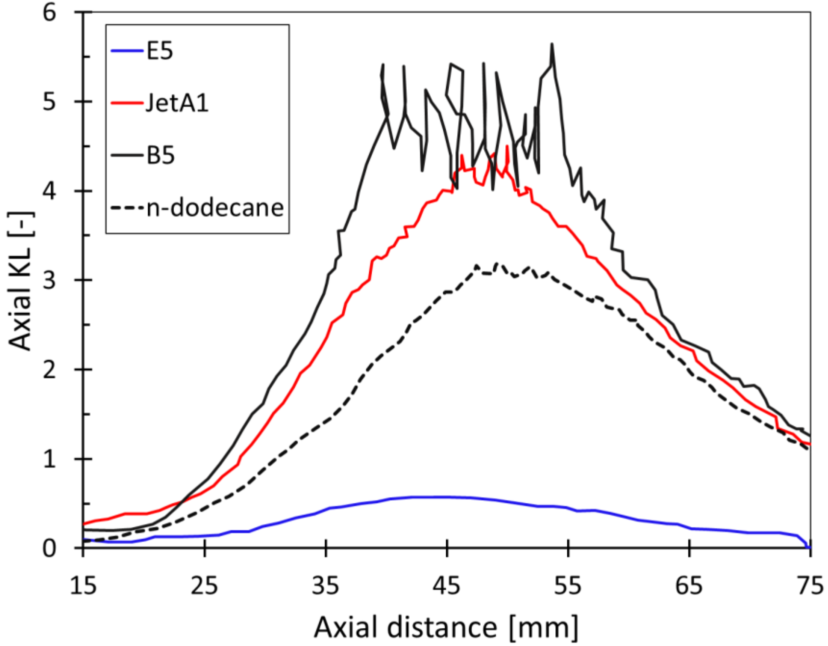


PRF: green
Gasoline: blue
Jet: red
Diesel: black

- A strong positive correlation is observed between LOL and ID with various fuels

Experimental Results – Soot

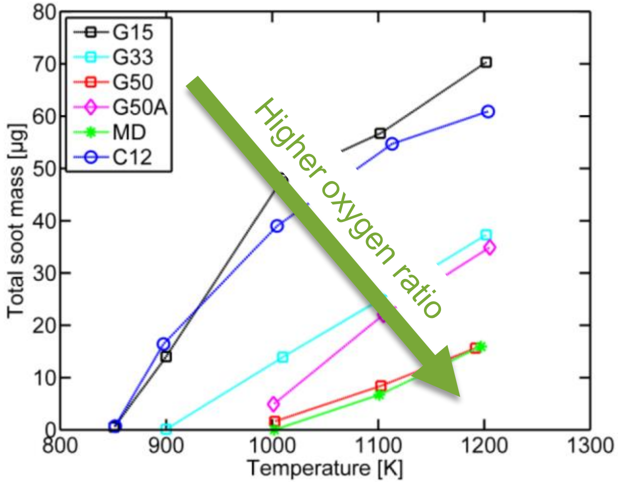
15% O_2 - 22.8 kg/m³ - 150 MPa – 1000 K



PRF: green
Gasoline: blue
Jet: red
Diesel: black

At $T_{amb.}$ = 1000 K, B5 (diesel fuel) forms more soot

- ✓ B5 (53) > JetA1 (46) > n-dodecane (73) > E5 (17)
- ✓ LOL, ID, fuel oxygen ratio, and aromatic content, affect the soot formation



Manin et al., *SAE Int. J. Fuels Lubr.* 2014.

Summary

- Liquid length:
  - ✓ Higher density, boiling temperature and viscosity generally lead to longer liquid length, but their relevant importance needs to be further investigated.
- Vapor penetration length:
  - ✓ Higher density generally leads to longer vapor penetration
  - ✓ Viscosity doesn't seem to have any effect
  - ✓ Higher CN leads to longer spray penetration at reacting conditions
- Ignition delay and lift-off length
  - ✓ Higher CN generally leads to shorter ID and LOL
  - ✓ Strong negative correlations between ID/LOL and CN – PRF80 and E5 are outliers
  - ✓ Strong positive correlation between LOL and ID was observed for a wide range of fuels
- Soot is affected by CN, fuel oxygen and aromatic contents etc.

Relevant Studies on Spray Fuel Effect

Literature Referred

- ✓ Tang, M., Pei, Y., Zhang, Y., Tzanetakis, T., Traver, M., Cleary, D.J., Quan, S., Naber, J., Lee, S.Y., "Development of a Transient Spray Cone Angle Correlation for CFD Simulations at Diesel Engine Conditions", *SAE Paper*, 2018-01-0304.

- ✓ Torelli, R., Matusik, K.E., Nelli, K.C., Kastengren, A.L., Powell, C.F., Som, S., Pei, Y., Tzanetakis, T., Zhang, Y., Traver, M., Cleary, D.J., " Evaluation of Shot-to-Shot In-Nozzle Flow Variations in a Heavy-Duty Diesel Injector Using Real Nozzle Geometry", *SAE Int. J. Fuels Lubs*, 2018.

- ✓ Torelli, R., Sforzo, B., Matusik, K.E., Kastengren, A.L., Powell, C.F., Som, S., Pei, Y., Zhang, Y., Traver, M., Cleary, D.J., "Investigation of Shot-to-Shot Variability during Short Injections", *ICLASS*, Chicago, 2018.

- ✓ Torelli, R., Matusik, K.E., Sforzo, B., Kastengren, A.L., Powell, C.F., Som, S., Pei, Y., Traver, M., " In-Nozzle Cavitation-Induced Orifice-to-Orifice Variations Using Real Injector Geometry and Gaoline-Like Fuels", International Symposium on Cavitation, 2018.

- ✓ Pei, Y., Torelli, R., Tzanetakis, T., Zhang, Y., Traver, M., Cleary, D.J., Som, S., "Modeling a Gasoline Spray under Heavy-Duty Diesel Engine Conditions", ASME *ICEF 2017-3530*, Oct. 15-18, 2017, Seattle, WA, USA.

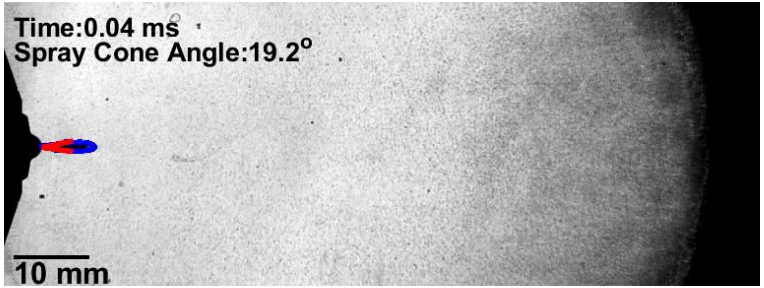
- ✓ Tang, M., Pei, Y., Zhang, Y., Traver, M., Cleary, D.J., Luo, Z., Naber, J., Lee, S.Y., "Numerical Investigation of Fuel Effects on Soot Emissions at Heavy-Duty Diesel Engine Conditions", ASME-ICEF2018-9696, 2018, San Diego, CA.

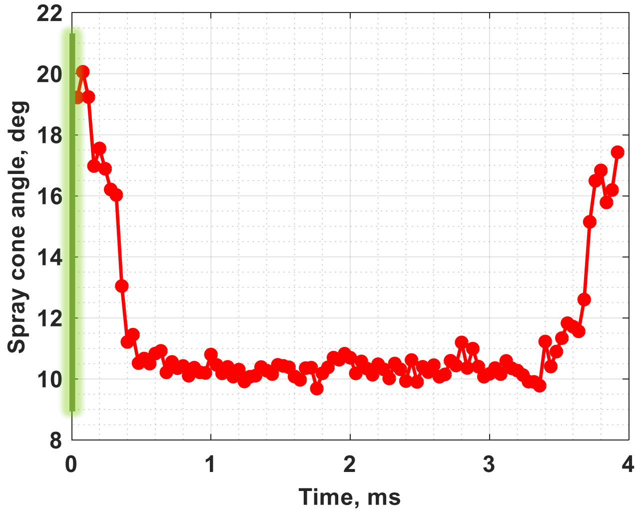
Injector and Fuel Specifications

	Injector at Aramco	ECN Spray D
Outlet Diameter (µm)	176	180
K-factor	1.8	1.5
Cd (Re = 12,000)	0.94	N/A
Description	Central axis, single-hole, solenoid driven, hydraulically lifted needle	

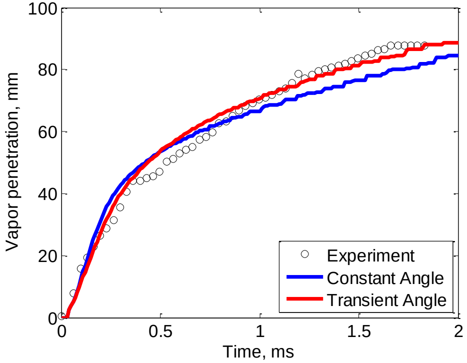
Property	Units	ULSD - Diesel	RON60 Gasoline
IBP	ºC	167	41
T50	ºC	257	67
FBP	ºC	344	134
Density at 15.6 ºC	g/mL	0.845	0.710
Kinematic Viscosity	cSt	2.49	0.58
Aromatics	Vol%	27.7	6.7
Olefins	Vol%	1.8	0.4
Saturates	Vol%	70.5	92.9
Sulfur	ppm	3.9	11.9
H/C Ratio	--	1.79	2.11
Cetane Number (CN)	--	44.2	33.9
AKI	--	n/a	56.8
Lower Heating Value	MJ/kg	42.87	44.15

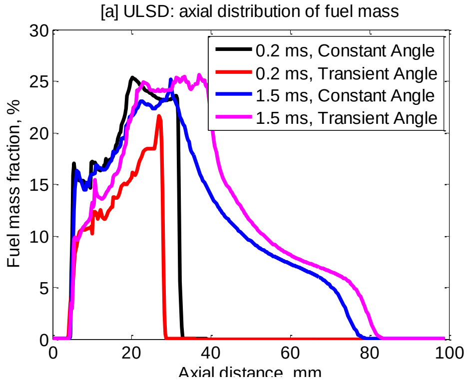
Fuel Effect on Spray Cone Angle



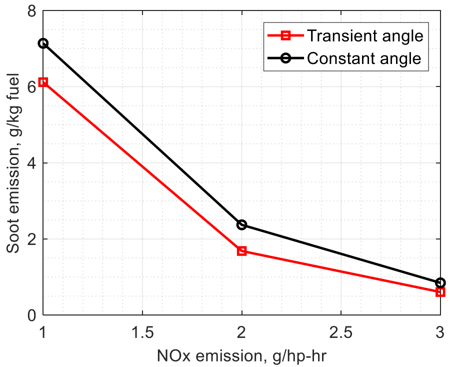


Vapor penetration in spray





Mixing fields in spray



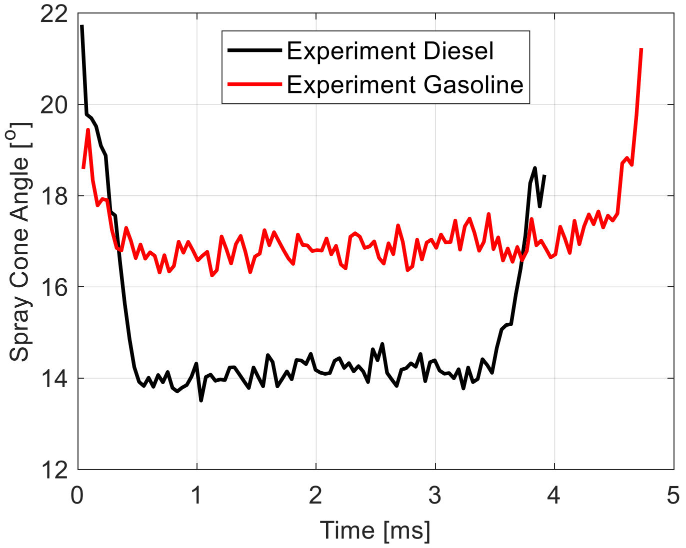
Soot emissions in engines

Have our spray models considered the transient cone angle?

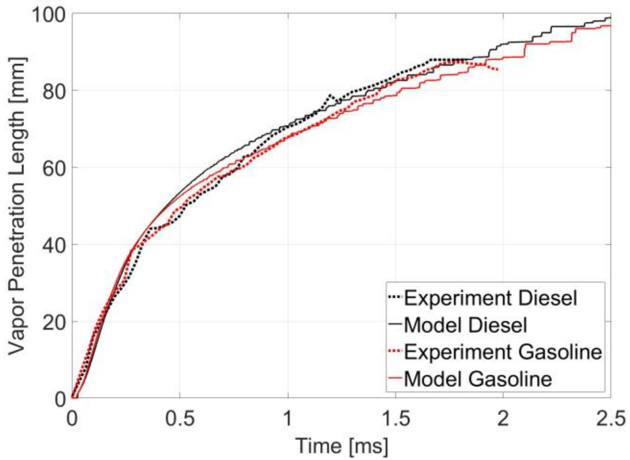
* Tang, M., Pei, Y.*, Zhang, Y., Tzanetakis, T., Traver, M., Cleary, D.J., Quan, S., Naber, J., Lee, S.Y., *SAE Paper*, 2018-01-0304.

Fuel Effect on Spray Cone Angle

0% O_2 – 5 MPa – 150 MPa – 324 K



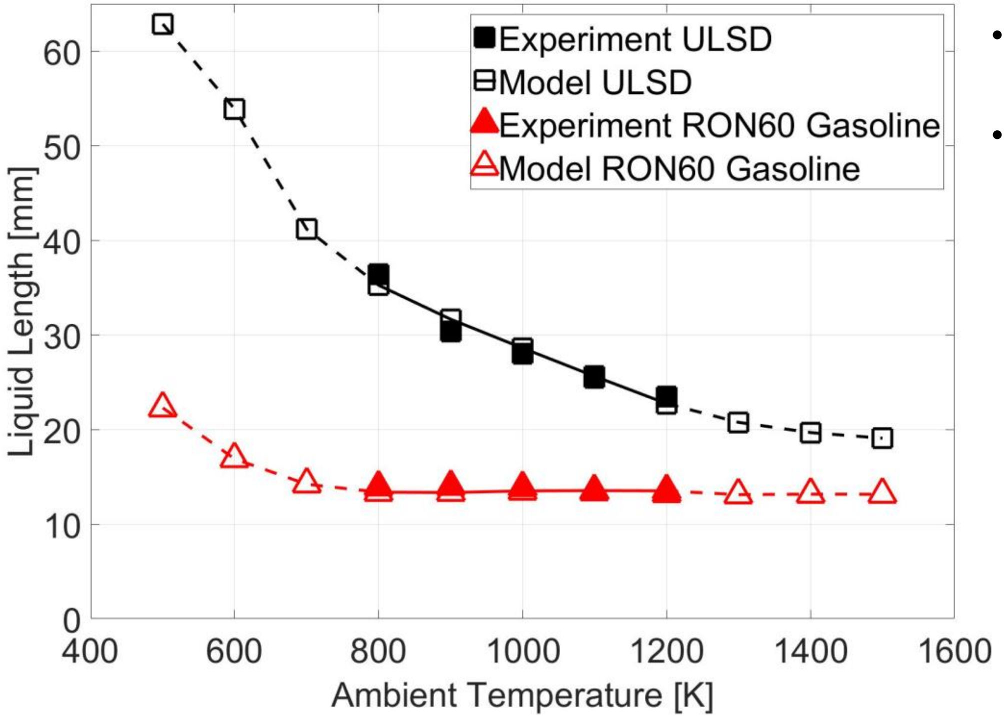
- Lower density gasoline fuel has a wider spray cone angle, leading to shorter vapor penetration
- Spray cone angle accounted for fuel effects is necessary



Have our spray models considered the fuel effect on transient cone angle?

Fuel Effect on Vaporizing Spray

0% O_2 – 6 MPa - 150 MPa



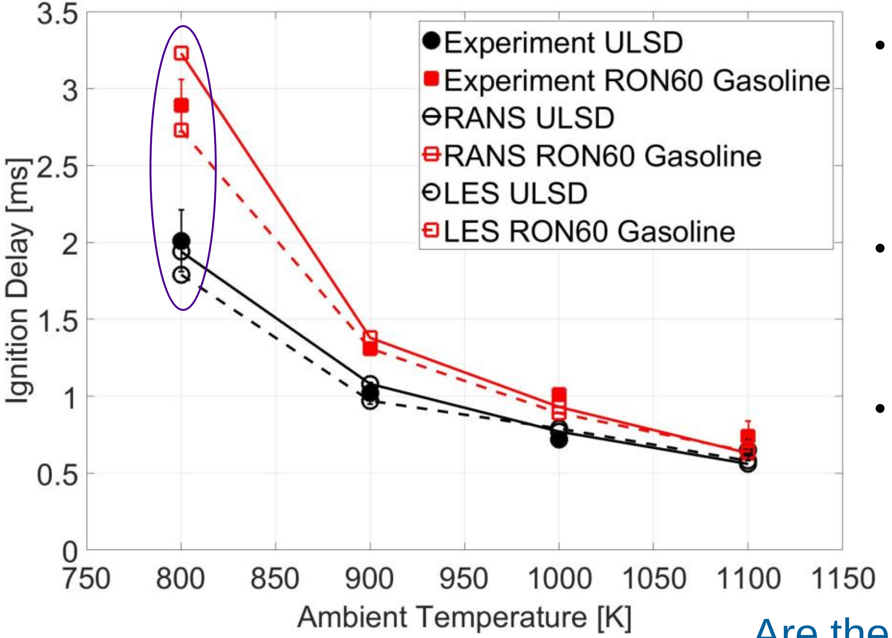
- Different liquid length trend for diesel and gasoline at different ambient temperature
- Lagrangian-type of spray models can capture the interesting behavior – consistent model setup only with different fuel physical properties.

Is it a coincidence?

[1]Pei, Y., Torelli, R., Tzanetakis, T., Zhang, Y., Traver, M., Cleary, D.J., Som, S., *ASME-ICEF2017-3530*, Seattle, WA, 2017.

Fuel Effect on Ignition Delay

15% O_2 – 6 MPa – 150 MPa

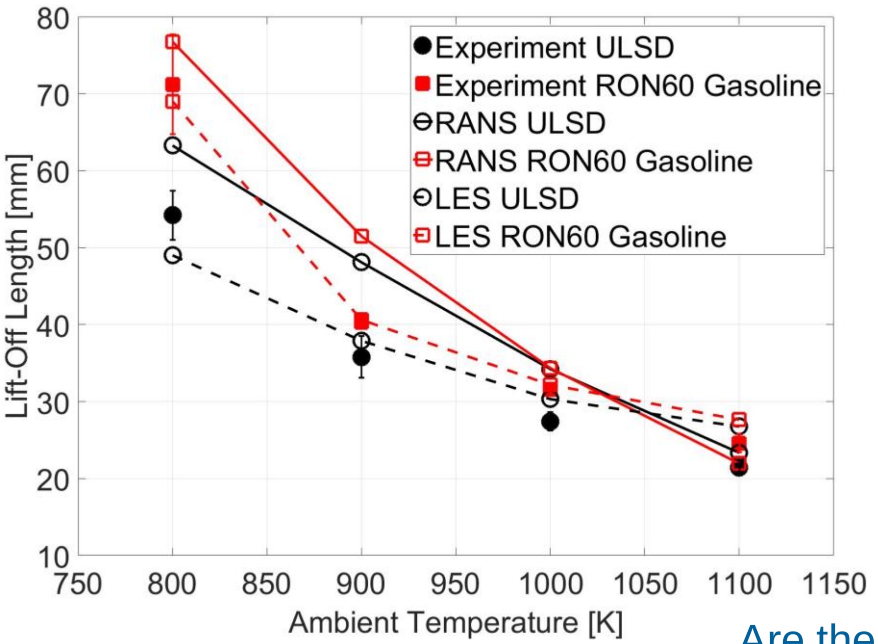


- Difference becomes smaller at higher ambient temperatures
- TRF chemical kinetic model from Wang et al. CnF 2015 is capable of capturing both fuels
  - ✓ ULSD – n-heptane
  - ✓ RON60 Gasoline – n-heptane and iso-octane
- LES compared to RANS:
  - ✓ Shorter ID at lower ambient temperature
  - ✓ Similar ID at higher ambient temperature
- Suggesting TCI is more important for low CN fuels or for low reactive conditions that have a longer ID

Are the chemical kinetic and combustion models good enough to capture the fuel sensitivity?

Fuel Effect on Lift-Off Length

15% O_2 – 6 MPa – 150 MPa



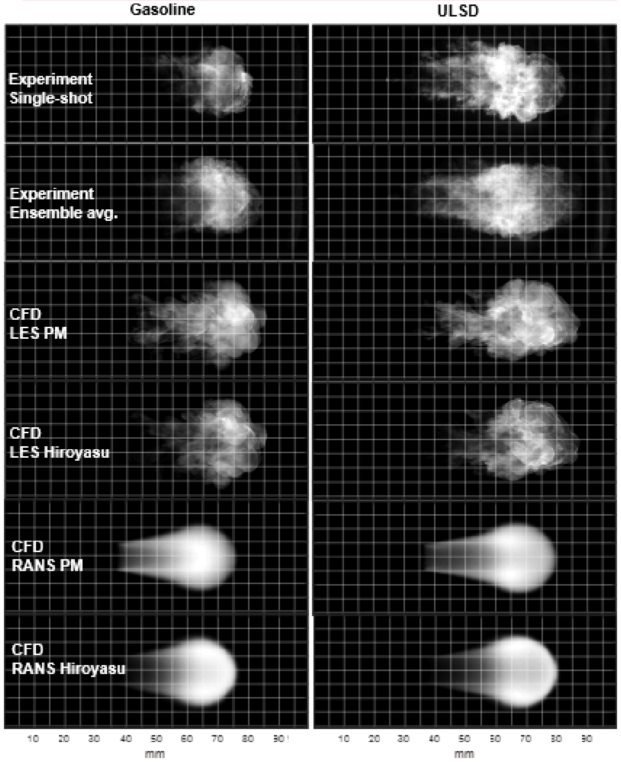
- With a well-mixed combustion model and a TRF mechanism, the sensitivity on LOL is not captured
- Chemical mechanism certainly plays a role
- A LES model improves the predictions suggesting a TCI model might be helpful

Are the chemical kinetic and combustion models good enough to capture the fuel sensitivity?

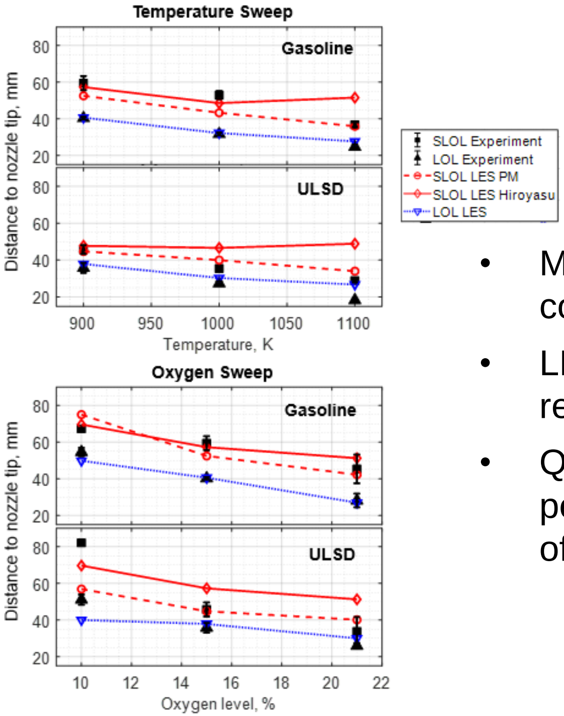
Fuel Effect on Soot

15% O_2 – 6 MPa – 150 MPa – 1000 K

Can soot models capture the fuel sensitivity?



*Experimental natural luminosity and line-of-sight integrated soot field from CFD**



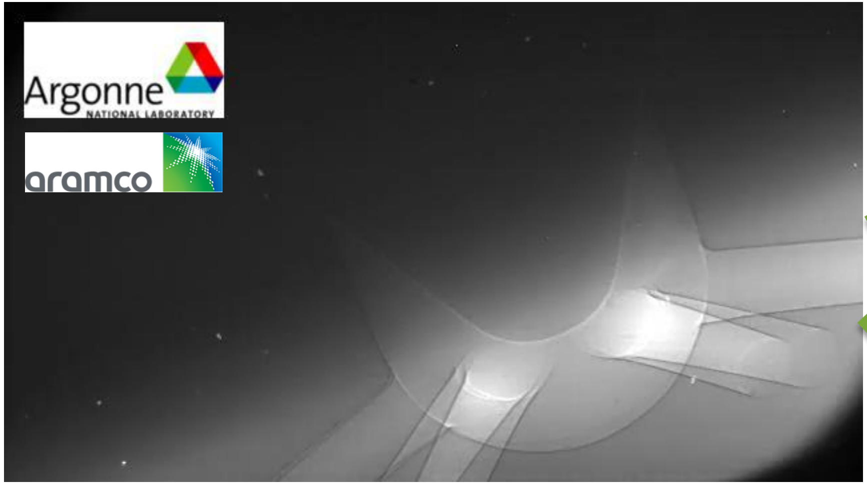
Soot lift-off lengths and lift-off lengths

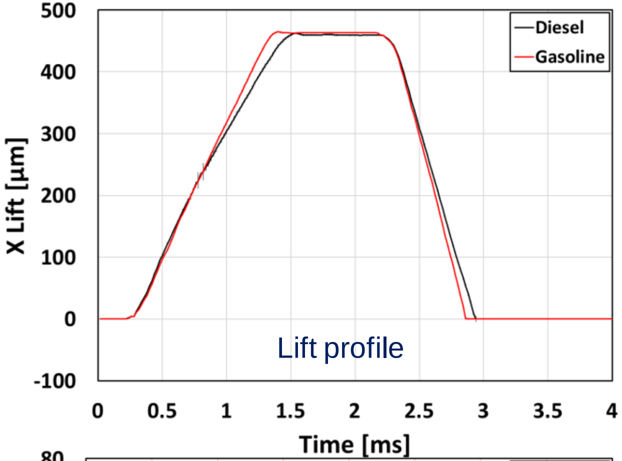
- Much lower soot for gasoline compared to diesel
- LES+Hiroyasu might be able to reproduce soot cloud
- Quantitatively, a detailed soot model performs better in terms of soot lift-off length prediction

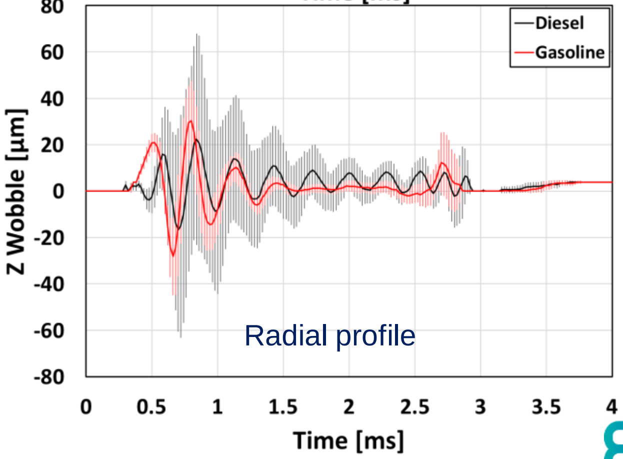
* Tang, M., Pei, Y., Zhang, Y., Traver, M., Cleary, D.J., Luo, Z., Naber, J., Lee, S.Y., ASME-ICEF2018-9696, 2018, San Diego, CA.

Fuel Effect on Injector Needle Motion

A HD 8-hole injector measured at Argonne APS by Chris Powell

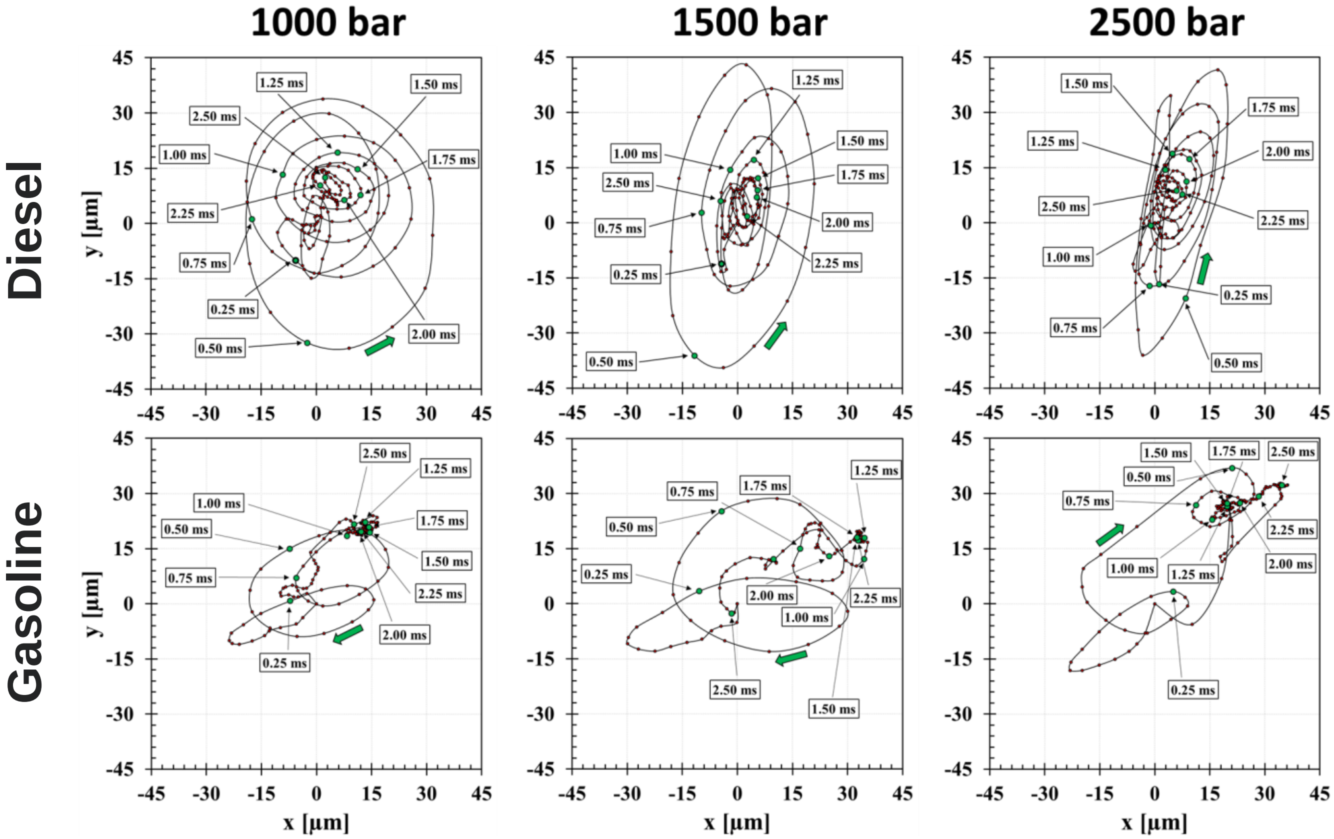






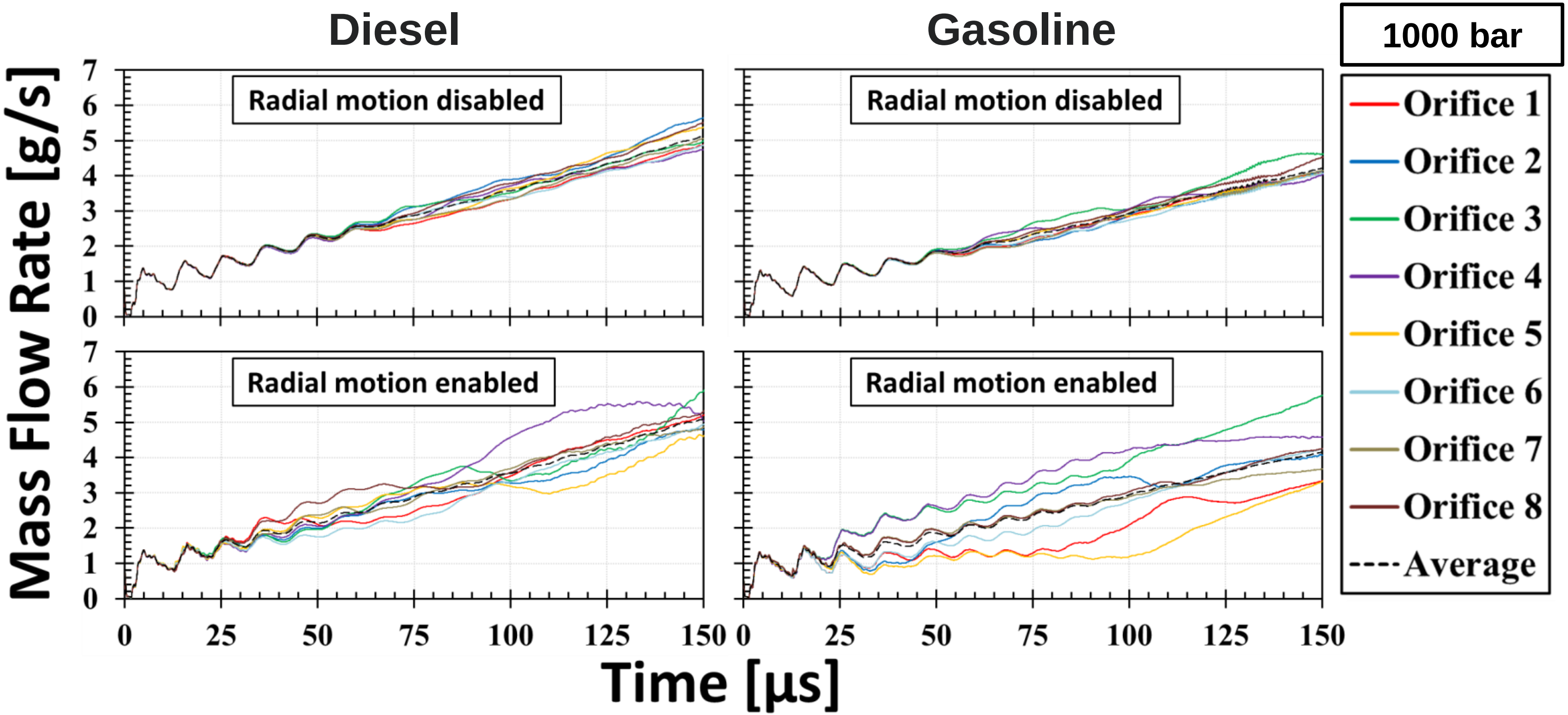
- Diesel lift slope slightly shallower
- Diesel wobbles throughout injection

Fuel Effect on Needle Radial Motion



- Fuel physical properties has a significant effect on needle radial motion

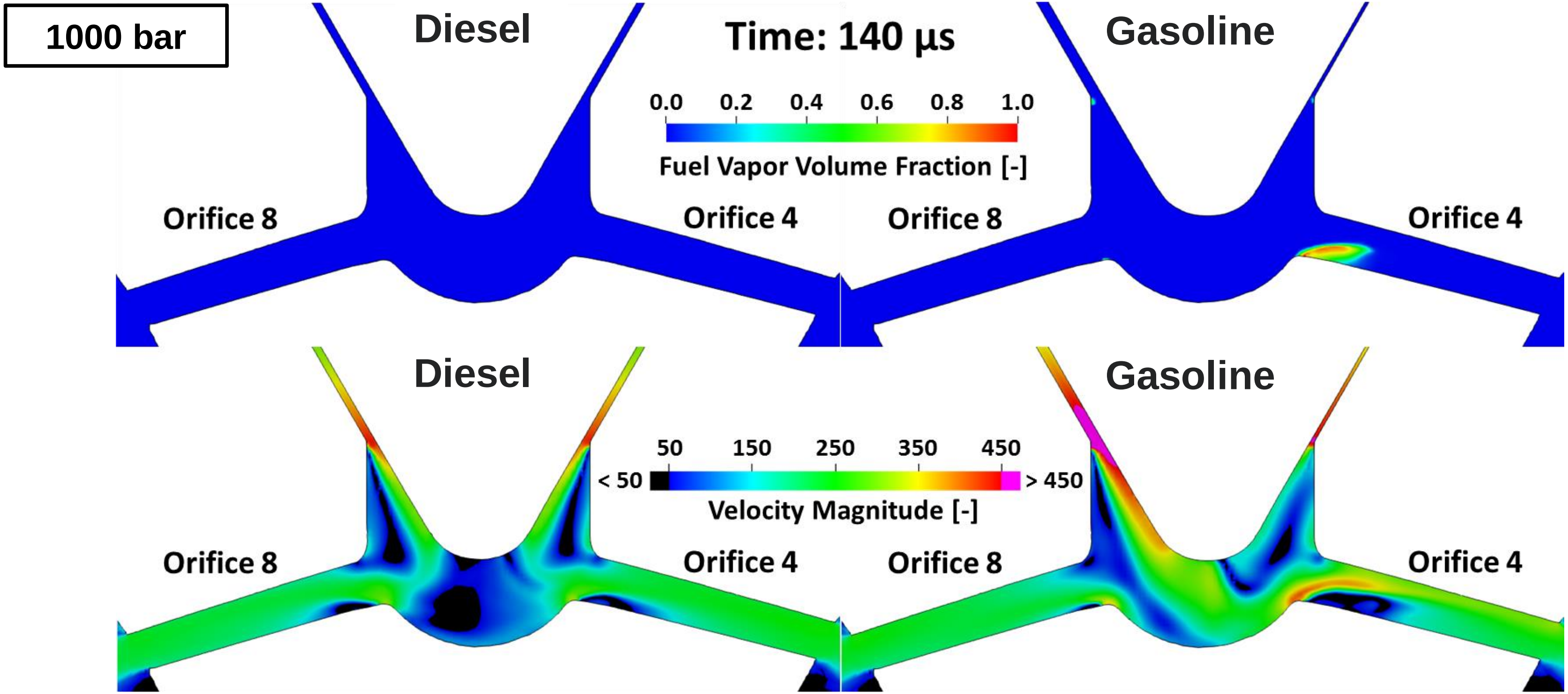
Fuel Effect on Mass Flow Rate



- Radial motion is necessary to realistically examine the flow behavior
- Much higher orifice-to-orifice variation for gasoline

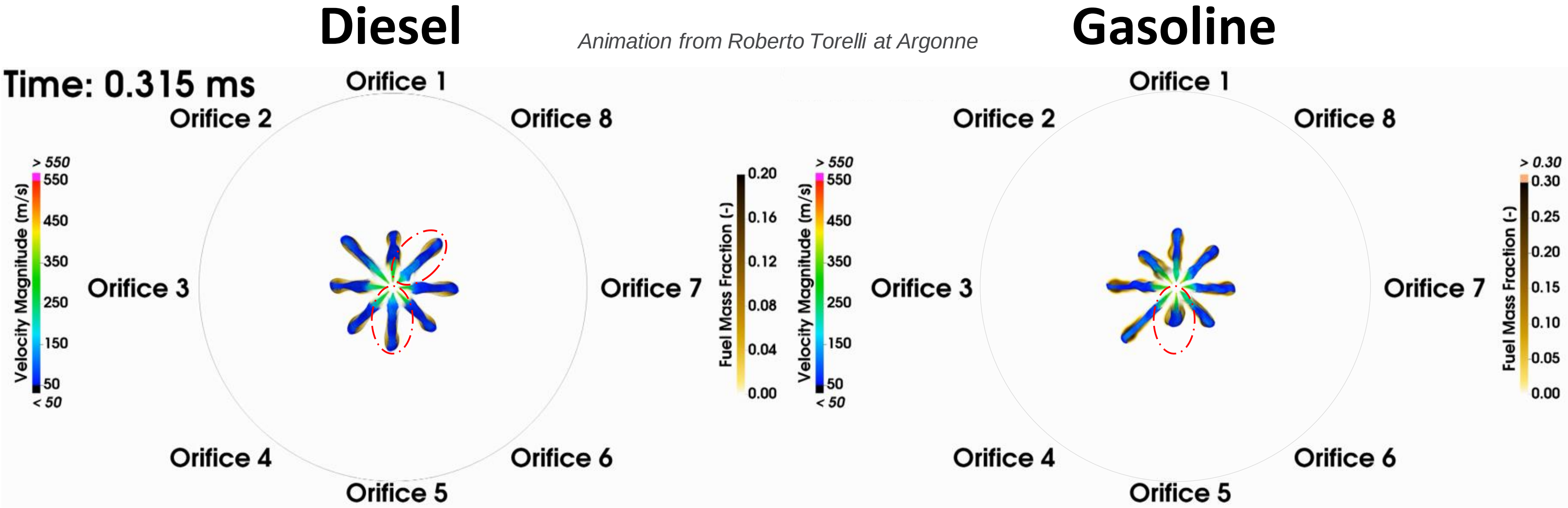
Fuel Effect on Flow Structure

Image from Roberto Torelli at Argonne



- More cavitation for gasoline
- A jet-like structure for gasoline due to needle wobble motion

Fuel Effect on Plume-to-Plume Variability



- Plume-to-plume differences in liquid and vapor penetration
- Wider spreading angles at the beginning and end of the injection

Summary

- Spray
  - ✓ Lighter fuel has a wider spray cone angle and shorter vapor penetration – spray cone angle needs to be properly accounted for
  - ✓ Gasoline has a much shorter liquid length compared to diesel – Lagrangian-type of spray models seem doing well
  - ✓ Ignition delay could be properly captured – TCI more important for longer ID
  - ✓ Lift-off length prediction is more challenging
  - ✓ Detailed soot model performs better

- In-nozzle flow:
  - ✓ Fuel physical properties have effect on needle lift and radial motion
  - ✓ Needle radial motion is necessary for realistic flow structure prediction
  - ✓ Higher plume-to-plume variation and cavitation for gasoline

Acknowledgement

- Jose M. Garcia-Oliver and Leonardo Pachano at CMT for providing the PRF spray data and useful discussion
- Lyle Pickett at SNL for sharing data through the ECN website
- IFPEN spray data from the published paper
- Roberto Torelli, Brandon Sforzo, Muhsin Ameen, Sibendu Som, and Chris Powell at Argonne National Laboratory for providing some data and useful discussion
- Yu Zhang, Meng Tang, Michael Traver, David Cleary at Aramco Research Center – Detroit for their support and useful discussion
- Tom Tzanetakis at Aramco Research Center - Detroit coordinated the HD spray experiments at MTU in collaboration with KAUST
- Might miss some experimental studies, please get in touch!

What would be a realistic “Fuel” variation for ECN7?

- A PRF blend seems a good option:
  - ✓ Simple, but vastly different to n-dodecane
    - ❖ Physical properties on light-end
    - ❖ Chemical properties can be tailored
  - ✓ Chemical mechanism is readily available
  - ✓ …

- ECN7 fuel effect planning – PRF blends on Spray A, B, C, D
  - ✓ Experiments:
    - ❖ CMT, Spray A – 2012
    - ❖ SNL, Spray A – 2018
    - ❖ UNSW, Spray A – 2019
    - ❖ …
  - ✓ Simulations:
    - ❖ UNSW - soon
    - ❖ Aramco – Detroit – in progress
    - ❖ …

Thank you!

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Feedback and Future Directions

- Feedback:
  - ✓ Different fuel blends – challenge chemistry, TRF, TRF-E
  - ✓ Measurement techniques revisit to be consistent
  - ✓ Empirical correlations revisit based on the wide range of fuels examined
  - ✓ Work towards experiments and understanding real world fuels
  - ✓ Broad topic of understanding fuel effects, methods, and related towards predictive soot modeling

- Future direction:
  - ✓ PRF – as a starting point
  - ✓ Combination of PRF, TRF, TRF-E
  - ✓ Real world fuels
  - ✓ Oxygenated fuels