Modelling of combustion and soot formation in various spray flame

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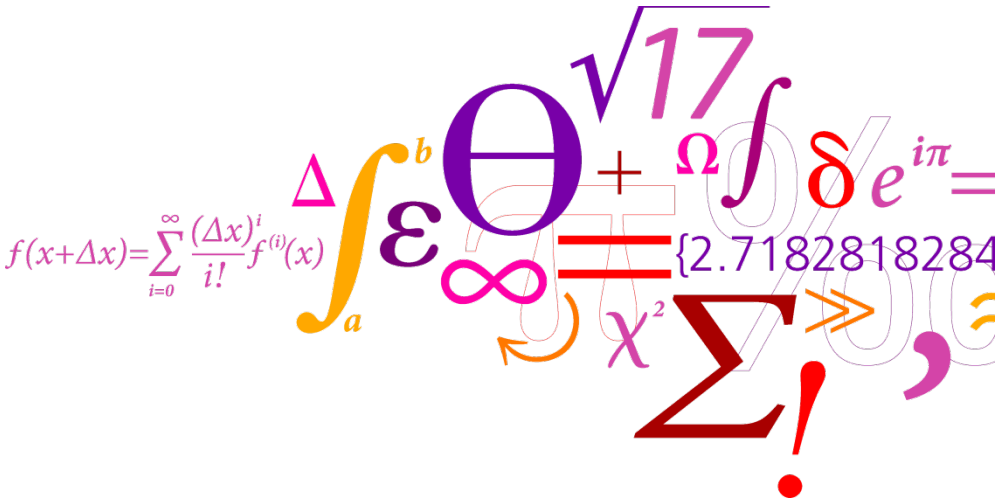
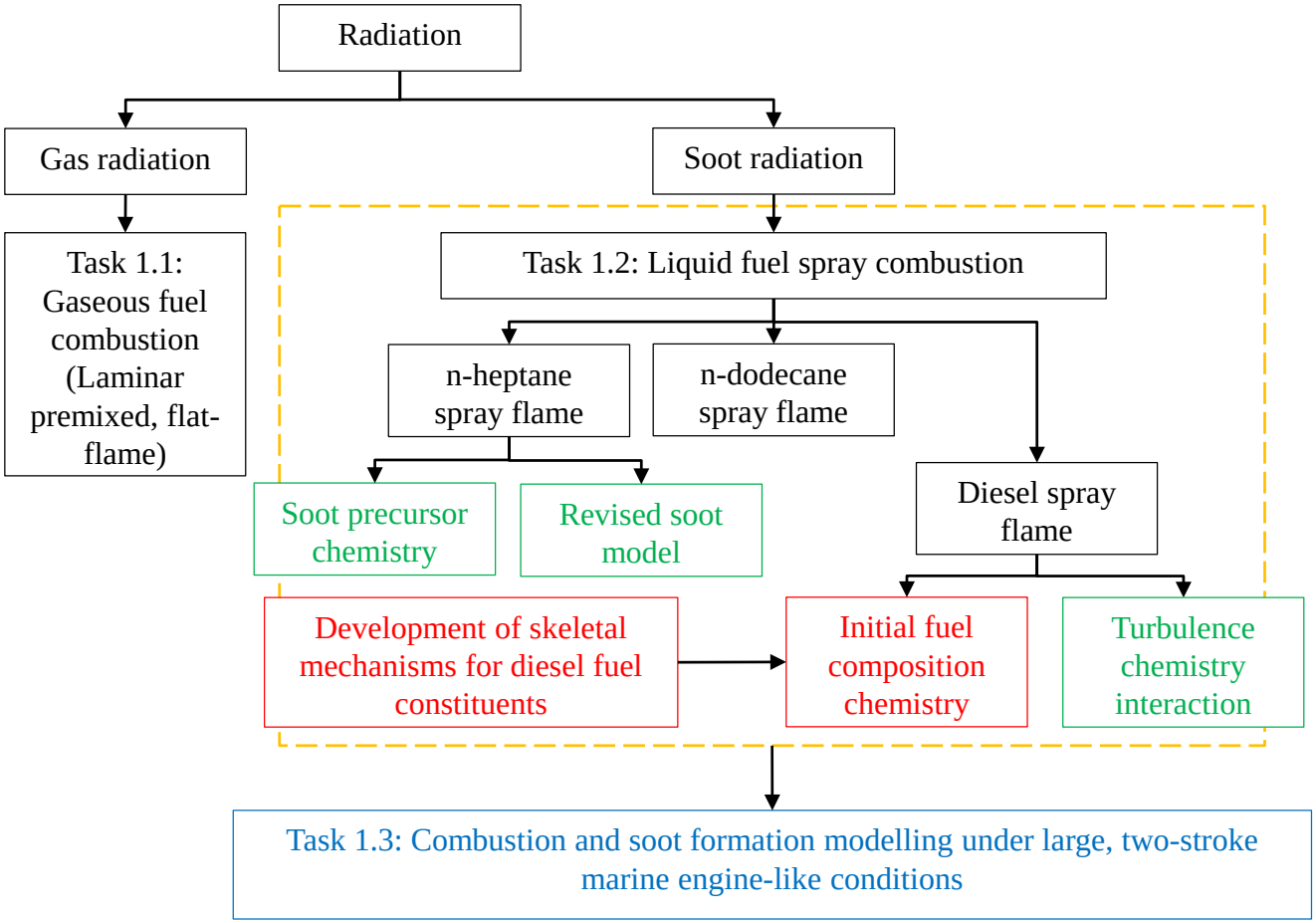


DTU Mechanical Engineering
Department of Mechanical Engineering

Overview of Task 1



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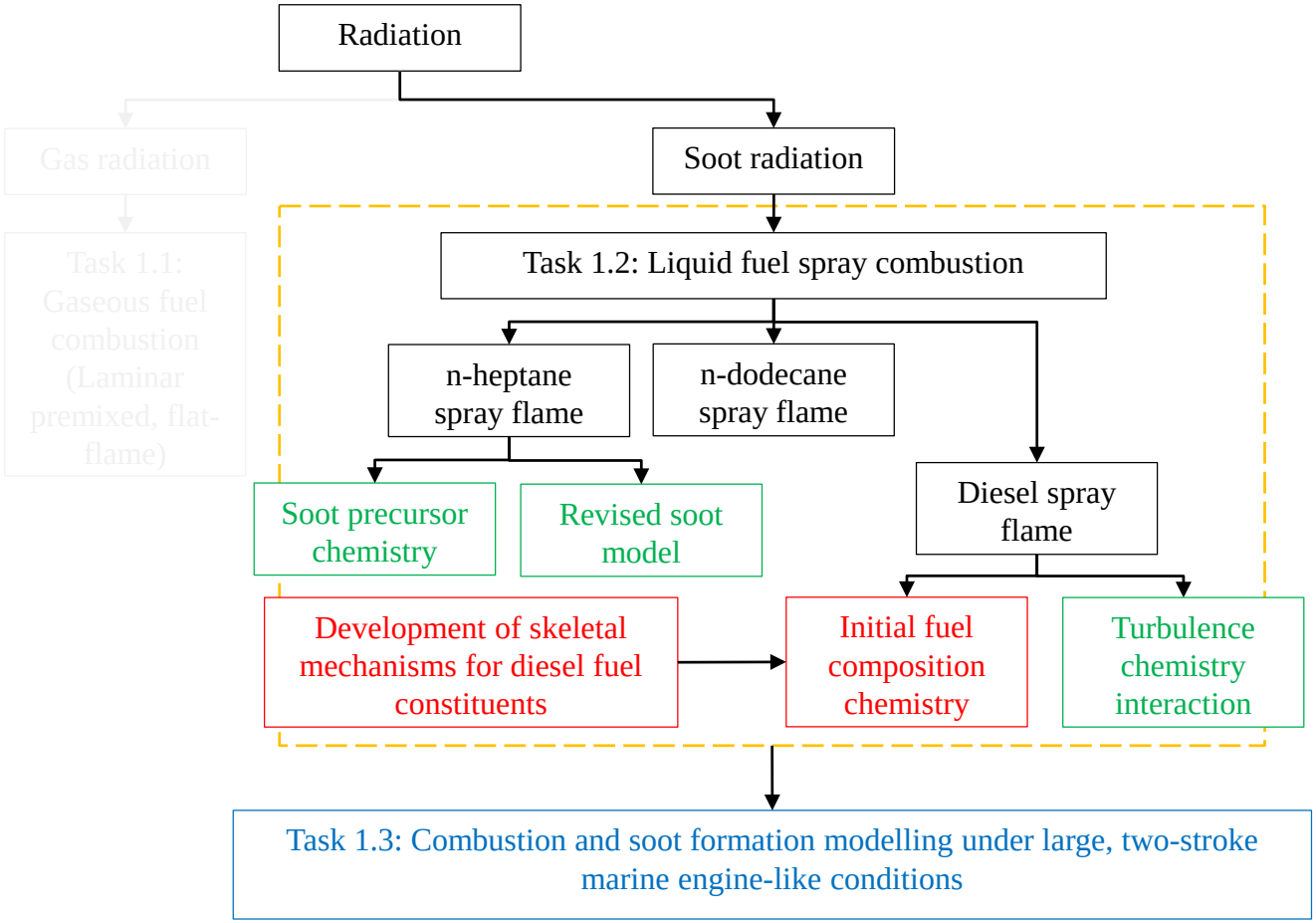

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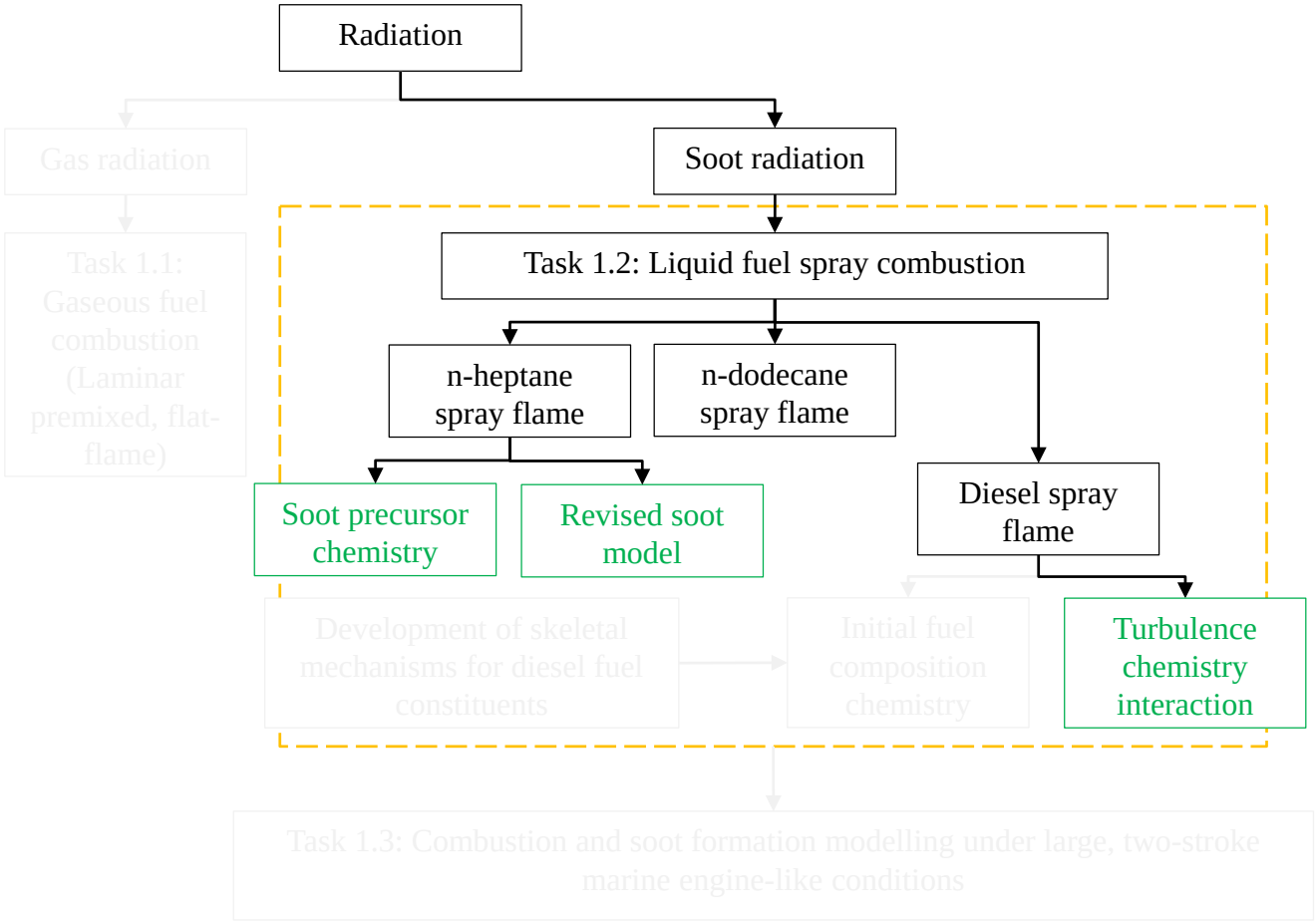

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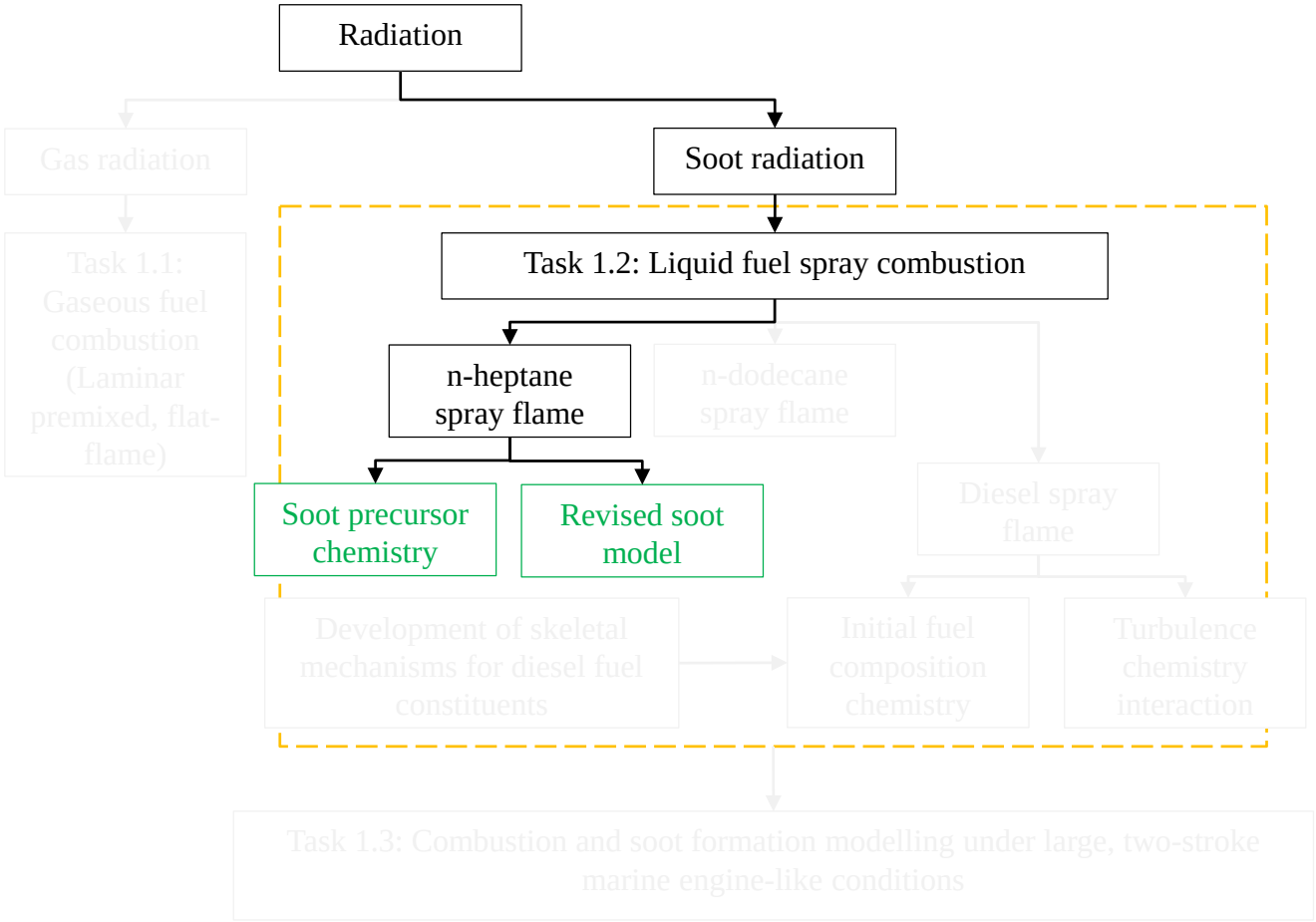

Introduction

Background

- Marine engines operate at various modes, although the operating range is narrower than that of automotive engines.

- At different injection timing, the temperature and pressure are different. Also, EGR may or may not be used. All these initial conditions influence the ignition, combustion and the subsequent emissions formation.

- Diesel soot modelling: Uncertainties at diesel chemistry, soot precursor chemistry and soot model.

- Instead, soot formation of fuel which the chemistry is better understood is first studied.

Introduction

Background

- Prior to the soot formation modelling, it is essential to capture the *formation of soot precursor*
- *Effects of pressure on soot mass production* are not captured

Objectives

- To study the effects of the use of different gas-phase species as soot precursors
- To study the effects of different soot formation/oxidation submodels on estimations of soot particle evolution
- Validate the optimized soot model across wide range of operating conditions using the n-heptane spray measurements
- Further validate the model using the n-dodecane spray measurements (baseline for the D2 spray case)

Experimental data

Descriptions

- n-Heptane measurements provided Engine Combustion Network (ECN)
- Quasi steady state event is reached

Basis of comparison

- ECN experimental measurements of
  - liquid penetration length (LPL)
  - vapour penetration length (VPL)
  - ignition delay time (IDT)
  - liftoff length (LOL)
  - soot volume fraction
- Soot precursor formation derived based on coupling of detailed chemistry and two-stage lagrangian (TSL) approach [Reference: SAE Technical Paper 2006-01-3434]

Test conditions (diesel engine-like)

T (K)	ρ (kg/m3)	$[O_2]$	**Δ** Injection(ms)	Total fuel mass injected (mg)
900	14.8	10.0 %	5.9	15.5
1000	14.8	10.0%	6.9	18.1*,a
1100	14.8	10.0%	6.8	18.0*
750	14.8	21.0 %	6.6	17.4
800	14.8	21.0%	6.6	17.5
850	14.8	21.0%	6.7	17.6
900	14.8	21.0%	6.6	17.5*
950	14.8	21.0%	6.7	17.6
1000	14.8	21.0%	6.8	17.8*,b
1100	14.8	21.0%	6.9	18.1
1000	14.8	8.0 %	6.9	18.1
1000	14.8	10.0 %	6.9	18.1*,a
1000	14.8	12.0 %	6.8	17.8*
1000	14.8	15.0 %	6.8	17.8*
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1000	30.0	8.0 %	6.8	18.0*
1000	30.0	10.0 %	6.8	18.0*
1000	30.0	12.0 %	6.8	17.8*
1000	30.0	15.0 %	6.8	18.0*

T ↑

$[O_2]$ ↑

ρ ↑

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1000	30.0	12.0 %	6.8	17.8*
1000	30.0	15.0 %	6.8	18.0*

T ↑

$[O_2]$ ↑

ρ ↑

For soot formation modelling

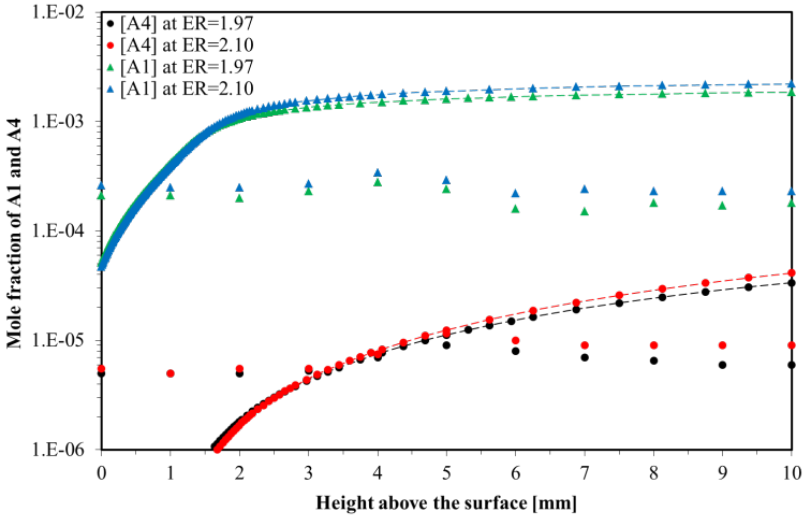
Numerical formulation

- OpenFOAM version 2.0.x

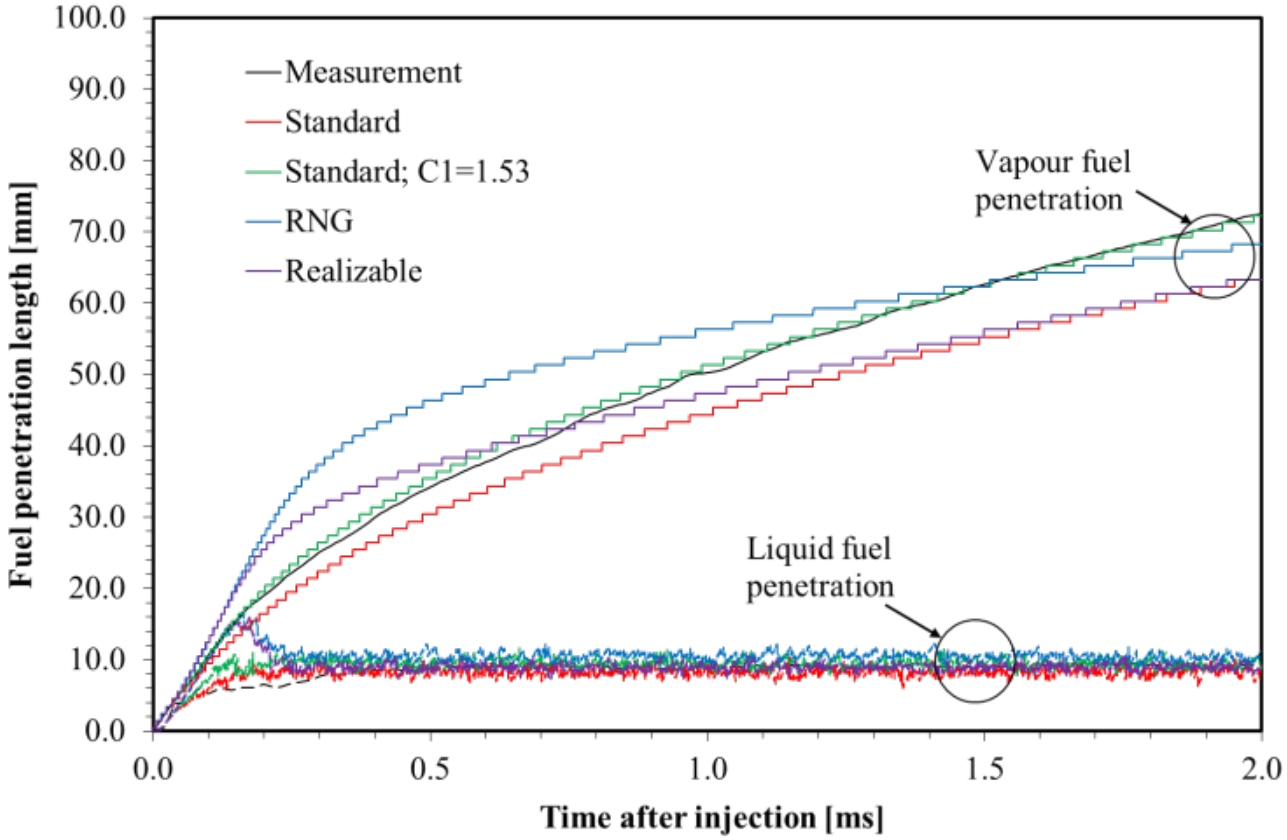
Models	**Descriptions**
Spray breakup model	KH-RT
Turbulence model	Standard k-ε, with C_1 = 1.53
Turbulence-chemistry interaction	Well mixed (Well stirred reactor)
Liquid properties	C_7H_{16}
Combustion chemistry	Lu et al. 2009+skeletal PAH model
Soot model	Phenomenological multi-step model
Radiation model	-
Accelerator	Chemistry coordinate mapping
Resolutions	
Spatial (cell size)	0.5 mm x 1.0 mm
Temporal (timestep size)	2e-7s

Numerical formulation

- *Skeletal n-heptane model developed by Lu et al. 2009* integrated with a skeletal PAH mechanism
- Using 1-D premixed flame code of Cantera 2.0
- Variation of A_1 and A_4 formation trend with respect to the change of equivalence ratio is replicated
- Mole fractions of both A_1 and A_4 are overestimated but retain within one order of magnitude
- Limitation of original mechanism which is not capable to predict the correct laminar premixed flame speed

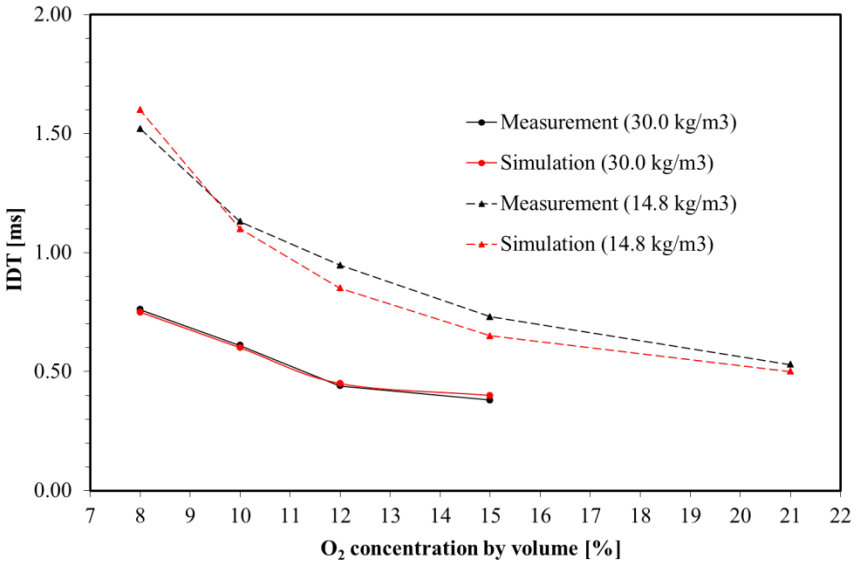


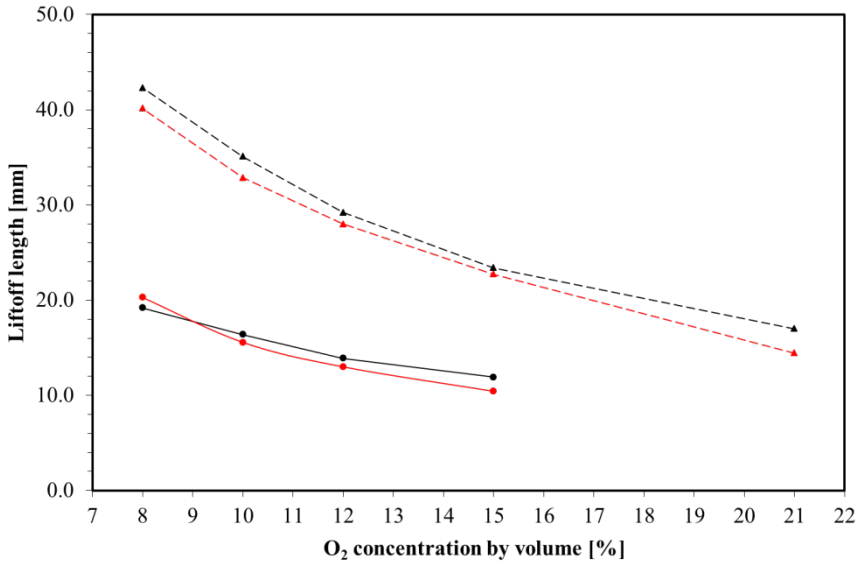
Non-reacting spray results (LPL and VPL)



- LPL and VPL are reproduced by the model

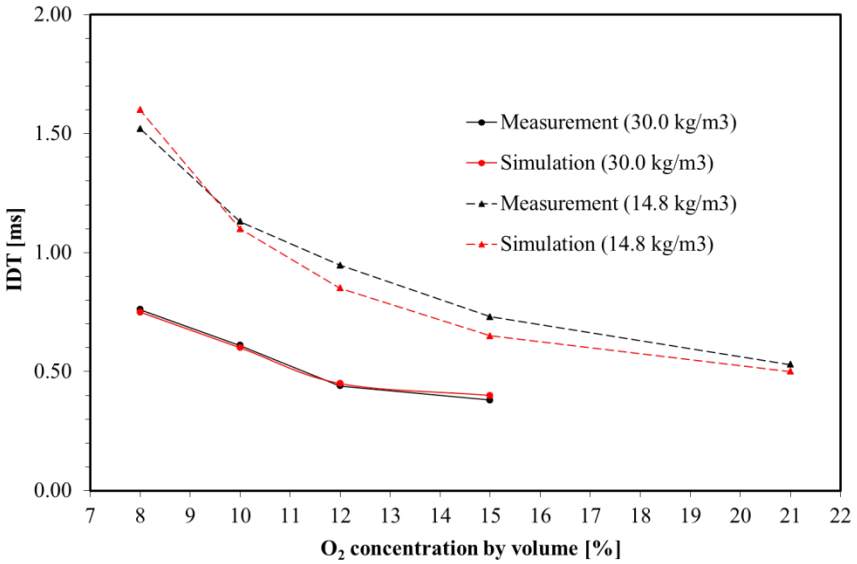
Reacting spray results (IDT and LOL)

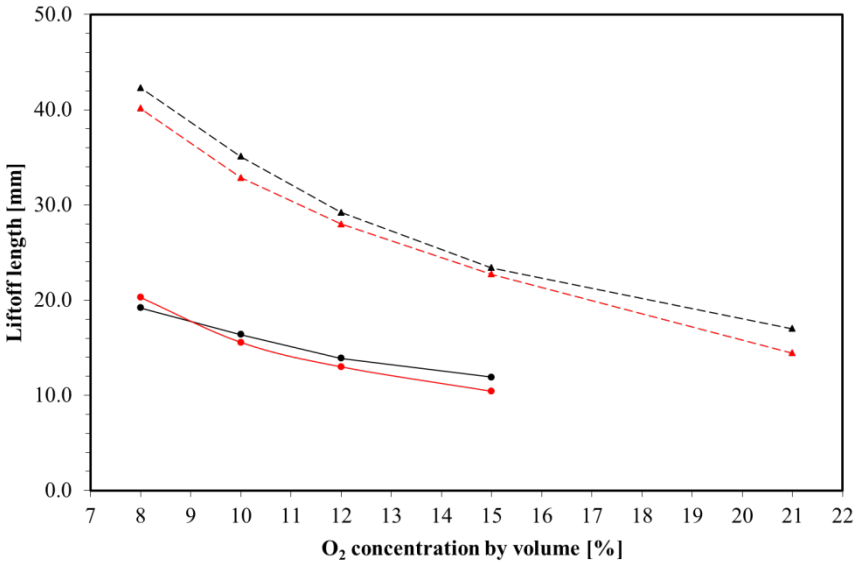




- For high ambient density conditions, the maximum relative error of IDT = 5.3%
- For low ambient density conditions, the maximum relative error of IDT = 11.0%
- All the simulated LOLs match the experimental measurements fairly well (Maximum relative error = 15.1%)
- The model is next used for soot formation study

Combustion results (IDT and LOL)





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- All the simulated LOLs match the experimental measurements fairly well (Maximum relative error = 15.1%)
- The model is next used for soot formation study

Soot model sensitivity analysis

Physical processes	Configuration	Descriptions
Precursor formation	A1	Selecting A_4 as the soot precursor
Inception	B1	Omitting the activation temperature
	B2	Adding a pressure dependence model constant
Mass growth	C1	Increasing the model constant value
	C2	Using a linear dependence of S_{soot}
	C3	Adding a pressure dependence model constant
	C4	Adding PAH condensation term
Coagulation	D1	Varying model constant values when $k_{sgs} = f(S_{soot}^{0.5})$
	D2	Varying model constant values when $k_{sgs} = f(S_{soot})$
Oxidation (OH)	E1	Increasing collision efficiency
	E2	Deactivating the OH oxidation model
Oxidation (O_2)	F1	Replacing the Lee model with NSC model
	F2	Deactivating the O_2 oxidation model

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Soot model sensitivity analysis (A1)

T (K)	ρ (kg/m3)	$[O_2]$	**Δ** Injection(ms)	Total fuel mass injected (mg)
900	14.8	10.0 %	5.9	15.5
1000	14.8	10.0%	6.9	18.1*,a
1100	14.8	10.0%	6.8	18.0*
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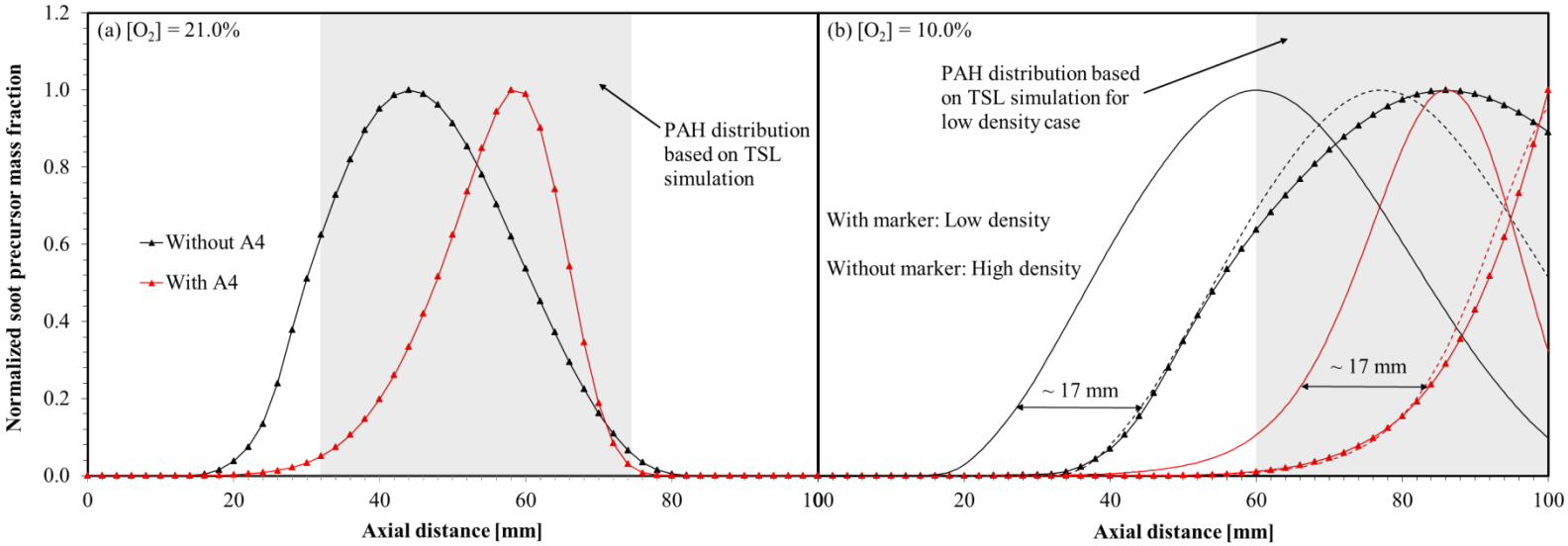
Soot model sensitivity analysis (A1)



- Relative change of spatial soot precursor evolution predicted by both models in response to decrease of ambient $[O_2]$ is captured
- The use of C_2H_2 as soot precursor leads to the associated formation appears to be nearer to the injection tip
- With the implementation of A_4 as soot precursor, the associated distribution is shifted to a location further downstream

Soot model sensitivity analysis (C1 to C4)

T (K)	ρ (kg/m3)	$[O_2]$	**Δ** Injection(ms)	Total fuel mass injected (mg)
900	14.8	10.0 %	5.9	15.5
1000	14.8	10.0%	6.9	18.1*,a
1100	14.8	10.0%	6.8	18.0*
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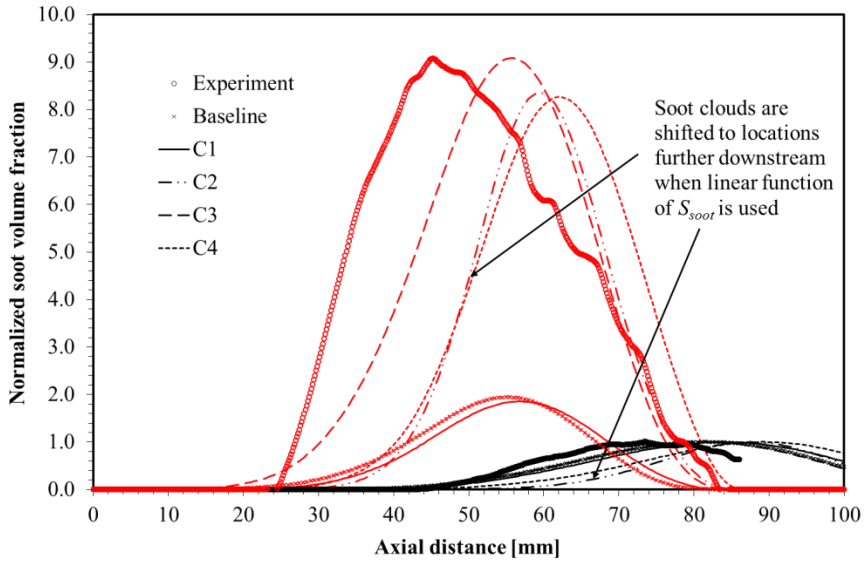
Soot model sensitivity analysis (C1 to C4)



Black - Low ambient density
Red - High ambient density

C1 - Increasing the model constant value
C2 - Using a linear dependence of S_{soot}
C3 - Adding a pressure dependence model constant
C4 - Adding PAH condensation term

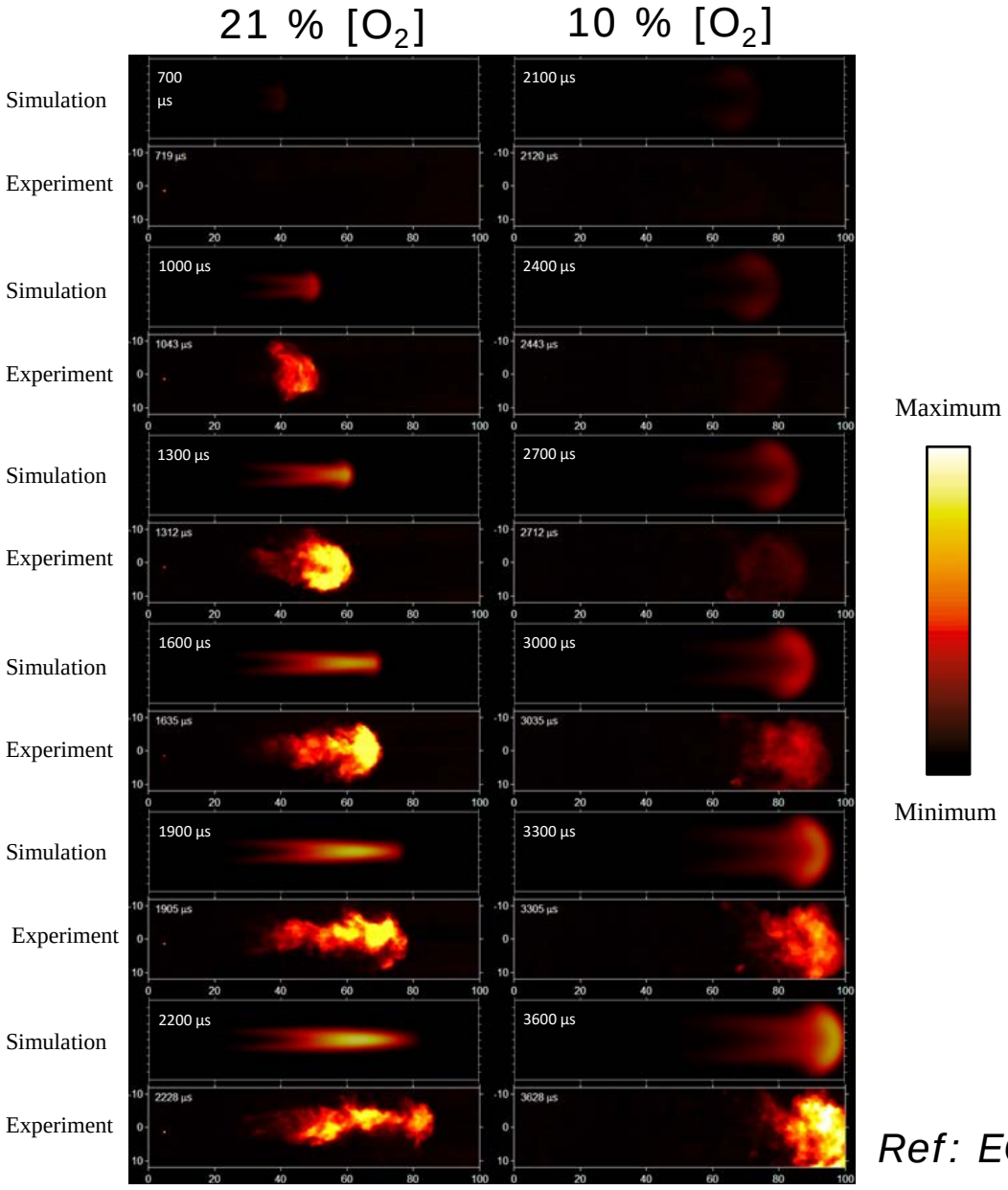
- Experimental $ratio_{pa}$ is approximately nine-fold
- Simulated $ratio_{pa}$ is only approximately two-fold
- R$atio_{pa}$ is sensitive to S_{soot}.
- As $k_{sgs} = f(S_{soot})$, $ratio_{pa} = 8.35$ is obtained, *but* soot cloud is shifted to a location further downstream
- An alternative is by taking a pressure dependence model constant into consideration (power exponent of 1.4)

Soot model sensitivity analysis (Optimized)

Physical processes	Descriptions	Mathematical expressions
Precursor formation	A_4 is selected as soot precursor	
Inception	Baseline inception submodel is implemented	$\omega_{inc} = 10000 \cdot \exp(\frac{21000}{T}) \cdot [A_4]$
Surface growth	Square root function of S_{soot} is chosen and a pressure dependence model constant is introduced	$\omega_{sg} = 14(\frac{P}{P_{ref}})^{1.4} \cdot \exp(\frac{12100}{T}) \cdot S_{soot}{}^{0.5} \cdot [C_2H_2]$
Coagulation	Baseline coagulation submodel is implemented	$\omega_{coag} = 3.0\left(\frac{24RT}{\rho_{soot} N_A}\right)^{0.5}\left(\frac{6M}{\pi\rho_{soot}}\right)^{1/6} N_{soot}{}^{11/6}$
OH oxidation	Increasing the collision efficiency to 0.13	$\omega_{OH} = 1.146 \cdot T^{0.5} \cdot S_{soot} \cdot [OH]$
O_2 oxidation	Baseline O_2 oxidation submodel is implemented	$\omega_{O2} = 10000 \cdot T^{0.5} \cdot \exp(\frac{19778}{T}) \cdot S_{soot} \cdot [O_2]$

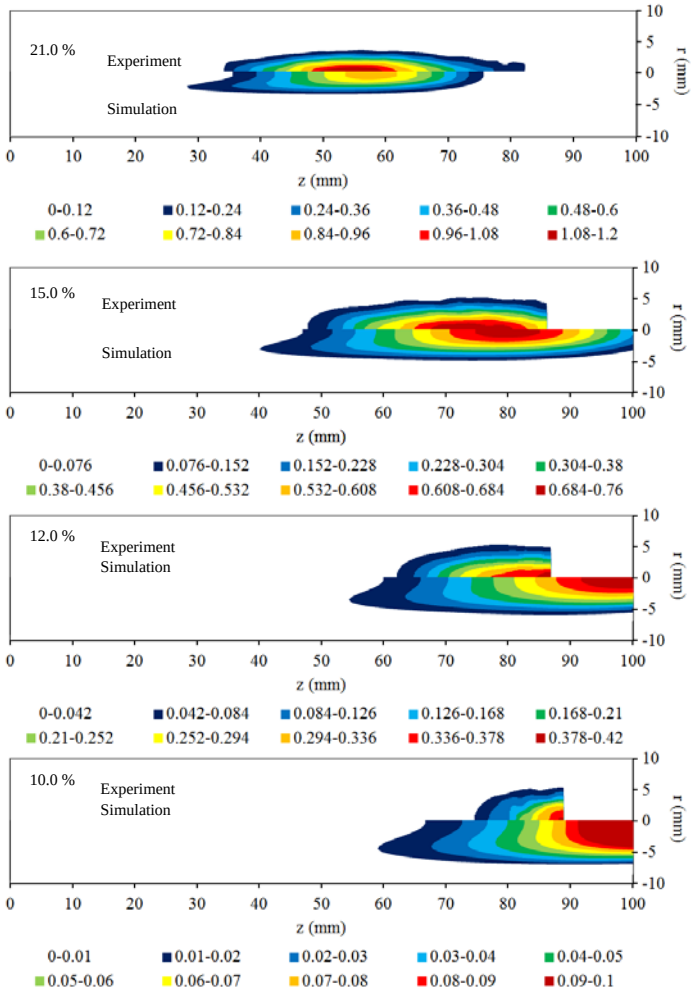
Validation of optimized soot model (Spray H)

- Temporal and spatial soot evolution at different ambient oxygen levels is reproduced by the model.

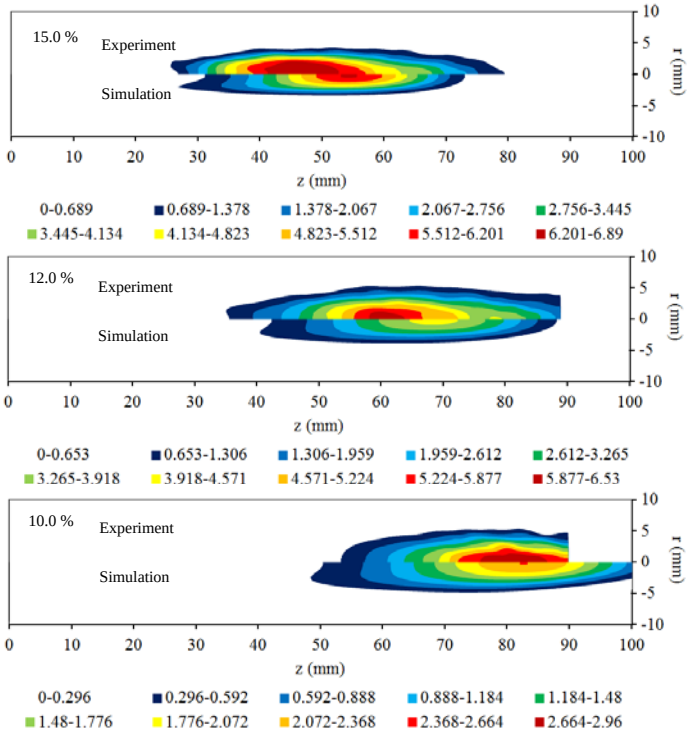


Ref: ECN

Validation of optimized soot model (Spray H)

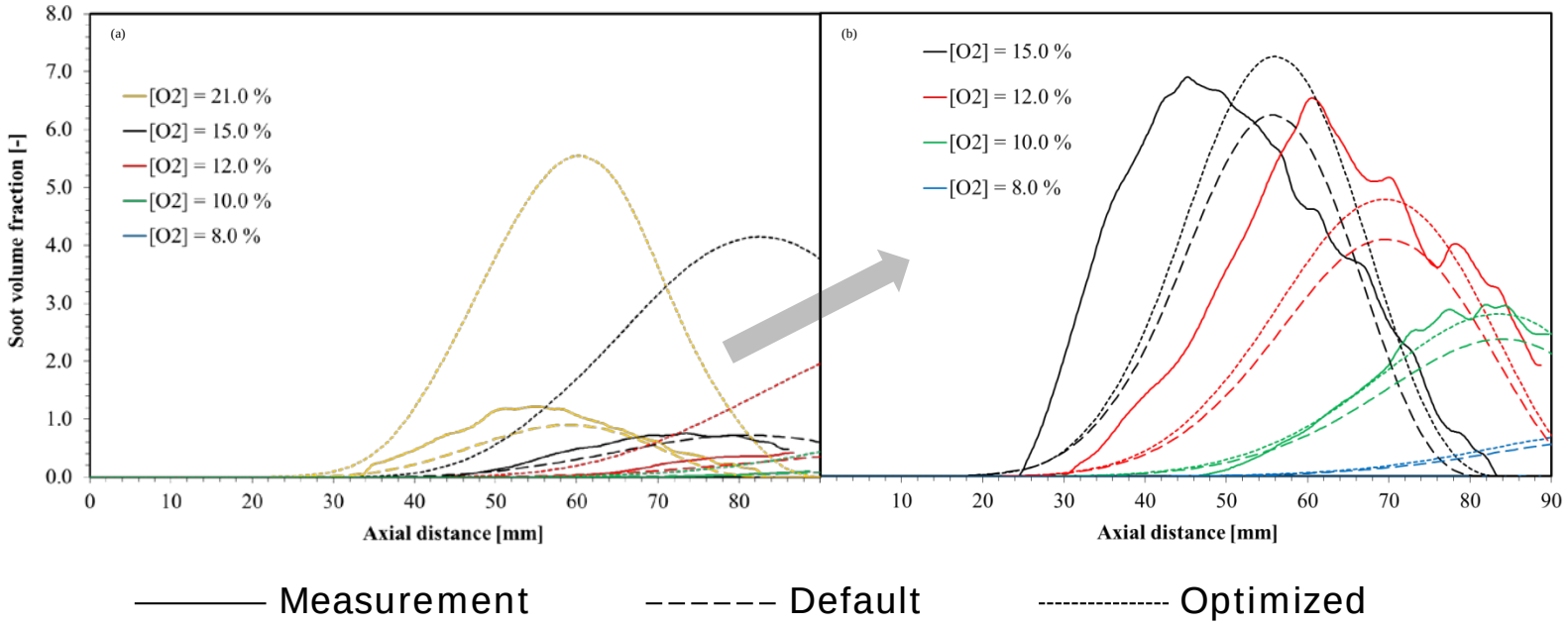


(a) Low ambient density



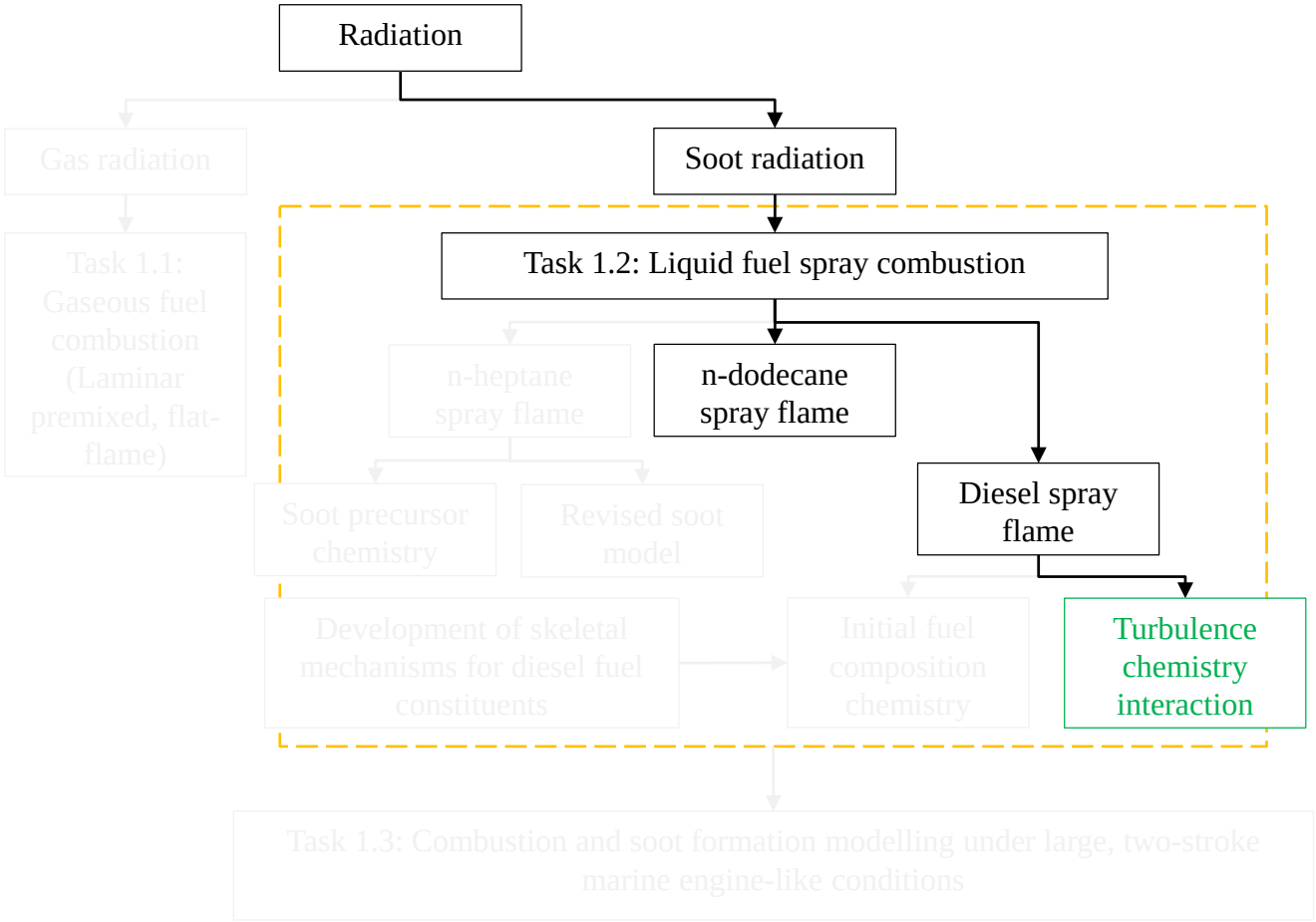
(b) High ambient density

Validation of optimized soot model (Spray H)



- Drop of peak value with respect to ambient $[O_2]$ drop is reproduced by both default and optimized models
- Default soot model overestimates soot volume fraction in low density cases (and hence fails to calculate ratio$_{\rho a}$ values)
- With optimized model, predictions of ratio$_{\rho a}$ are improved

Overview of Task 1

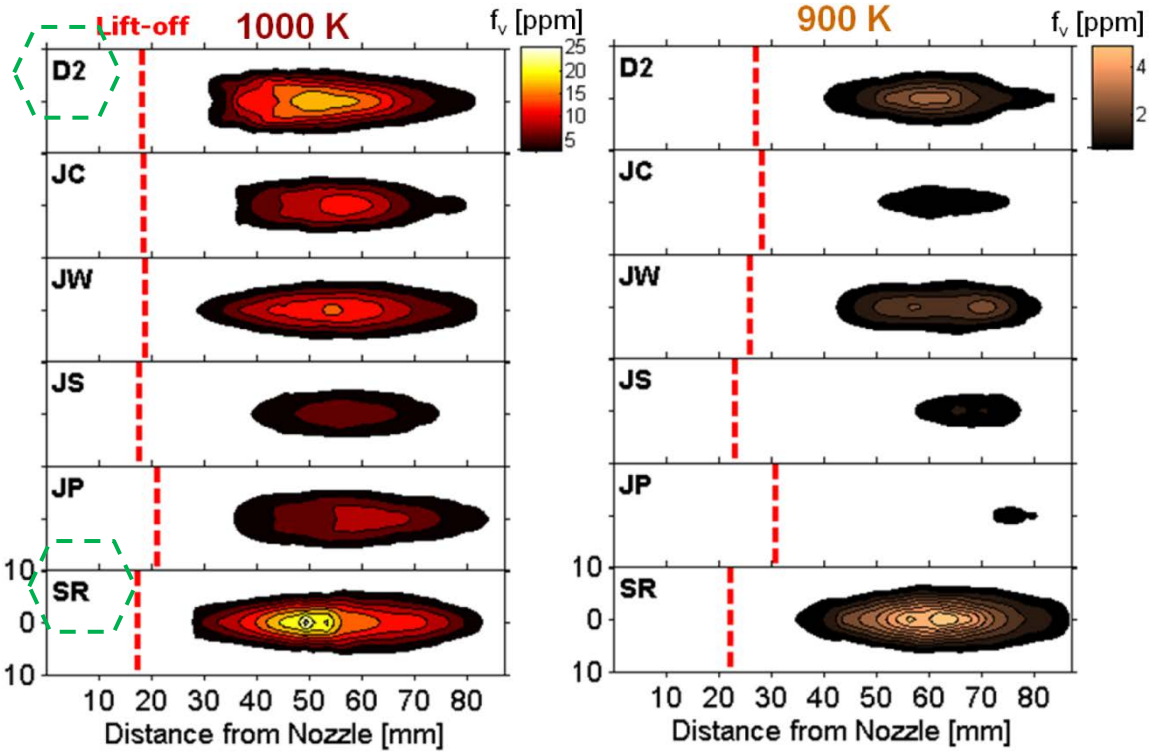


Further validation under the Spray A condition

- Experimental measurement shows that SVF of fuels with 20-30% aromatic compound rises by factors of ~5-7 when ambient temperature increases from 900 K to 1000 K

~27%

~23%



Ref: Kook et al. [2012]

Operating conditions

- Two different fuels are used but operating conditions are similar

ρ (kg/m^3)	T (K)	[O_2]	Fuel	m_f [mg]	Δ_{inj} [ms]
22.8	900	0%	n-dodecane	13.77	6.1
22.8	900	15%	n-dodecane	13.77	6.1
22.8	1000	15%	n-dodecane	13.77	6.1
22.8	900	0%	diesel	19.70	7.1
22.8	900	15%	diesel	19.70	7.1
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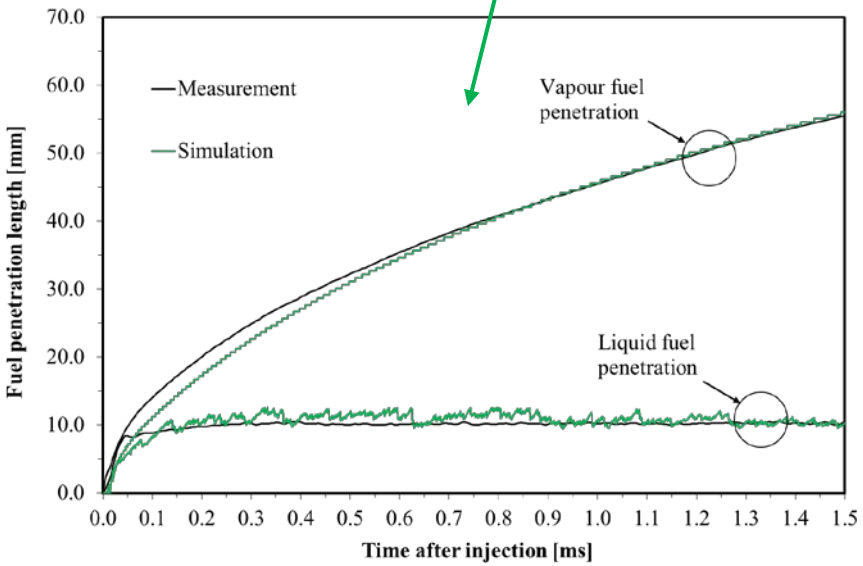

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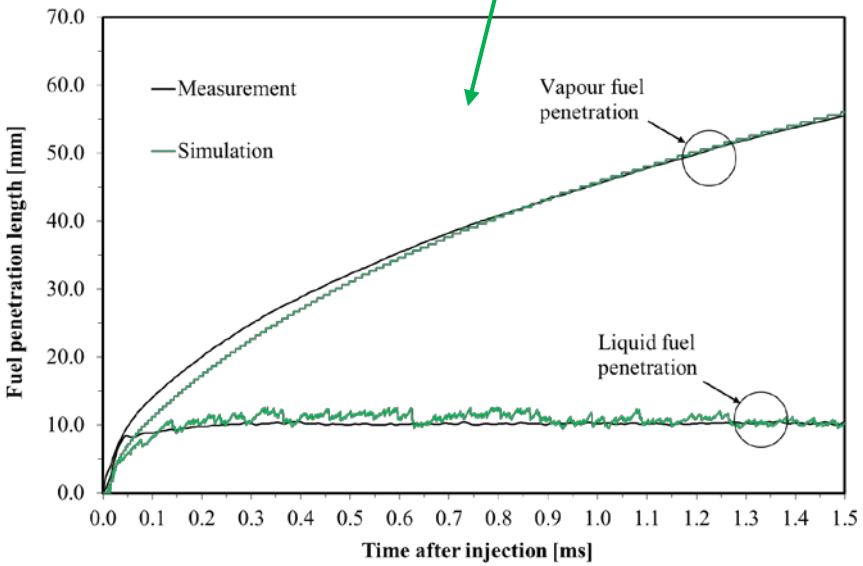
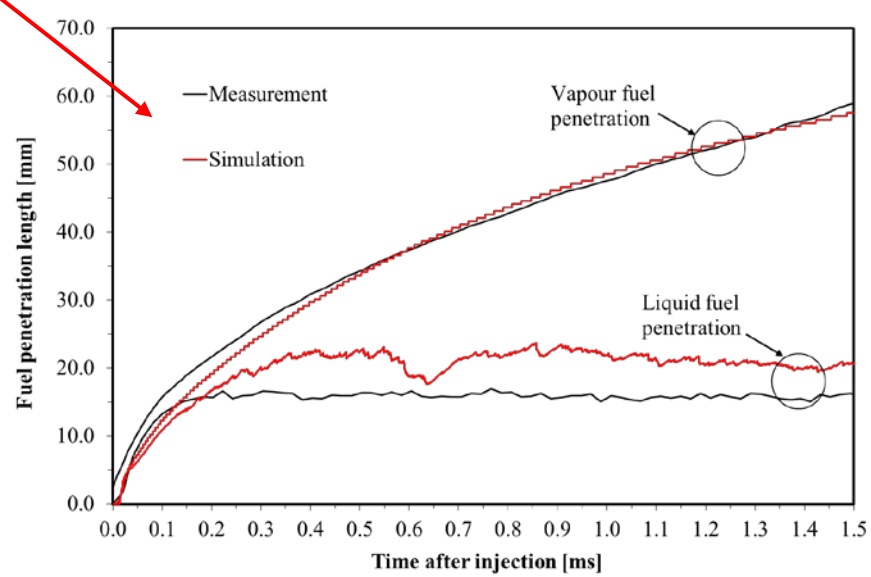


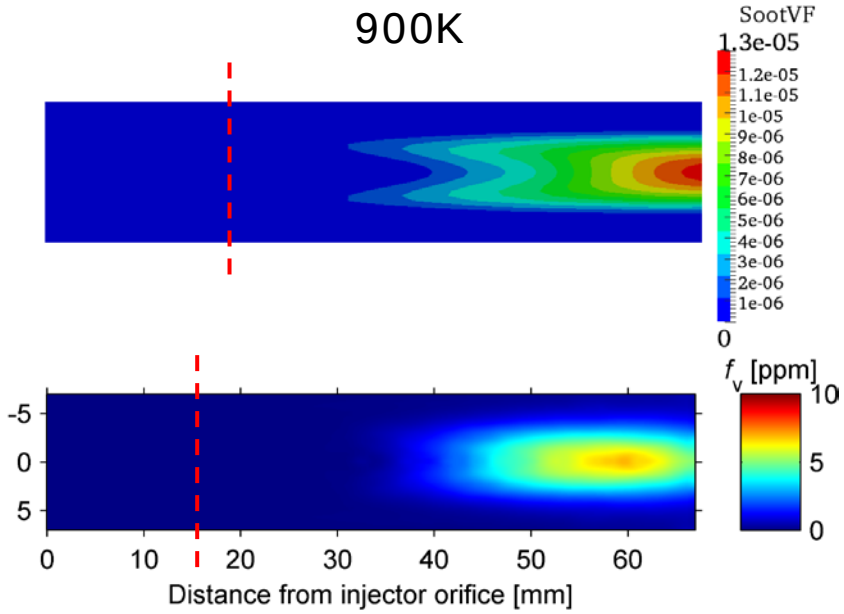


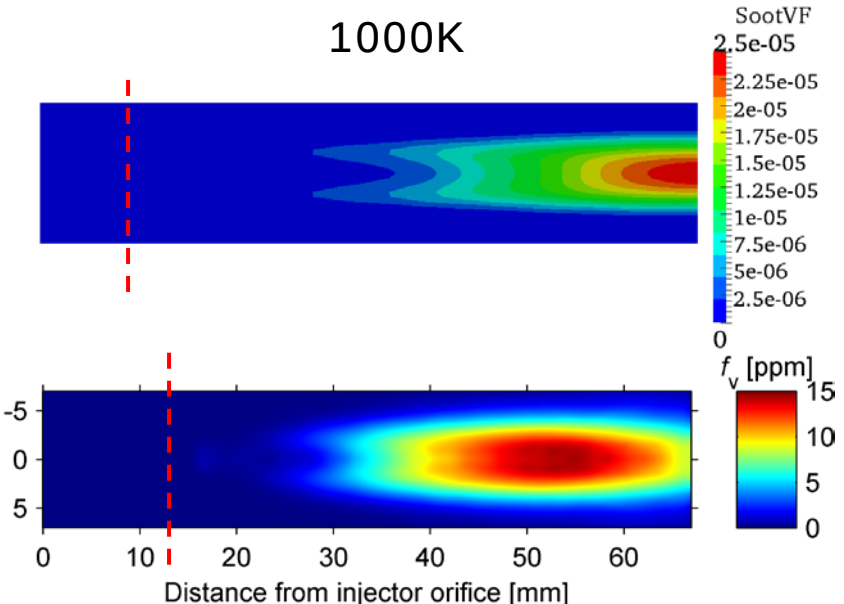
Numerical model formulation

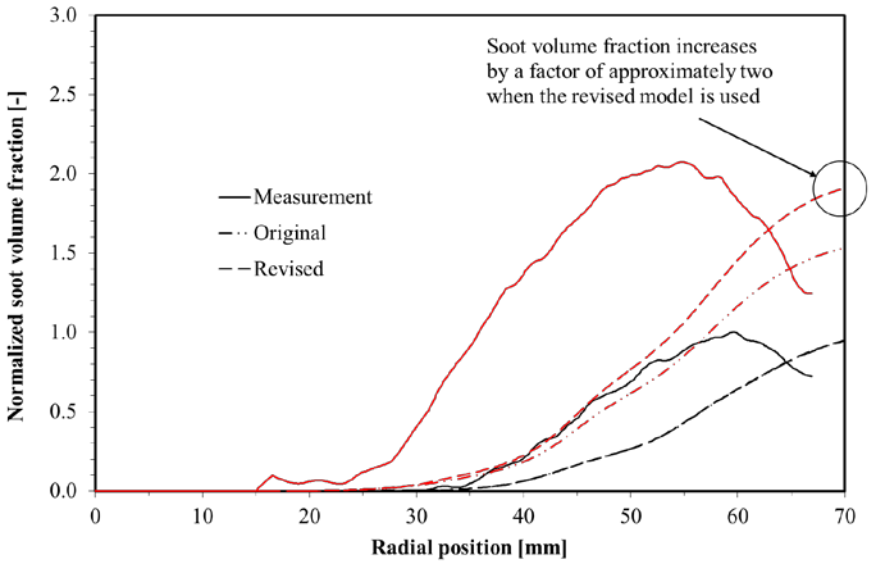
- OpenFOAM version 2.0.x

Models	Descriptions
Spray breakup model	Reitz-Diwakar
Turbulence model	Standard k-ε, with C_1 = 1.58
Turbulence-chemistry interaction	Well Stirred Reactor Eulerian Stochastic Fields (D2)
Liquid properties	$C_{12}H_{26}$;$C_{14}H_{30}$
Combustion chemistry	n-dodecane: Luo et al. 2014 D2: Liu et al. 2002
Soot model	Revised phenomenological multi-step model (Pang et al. 2015)
Radiation model	-
Resolutions	
Spatial (cell size)	0.5 mm x 0.5 mm
Temporal (timestep size)	2e-7s

n-Dodecane spray combustion







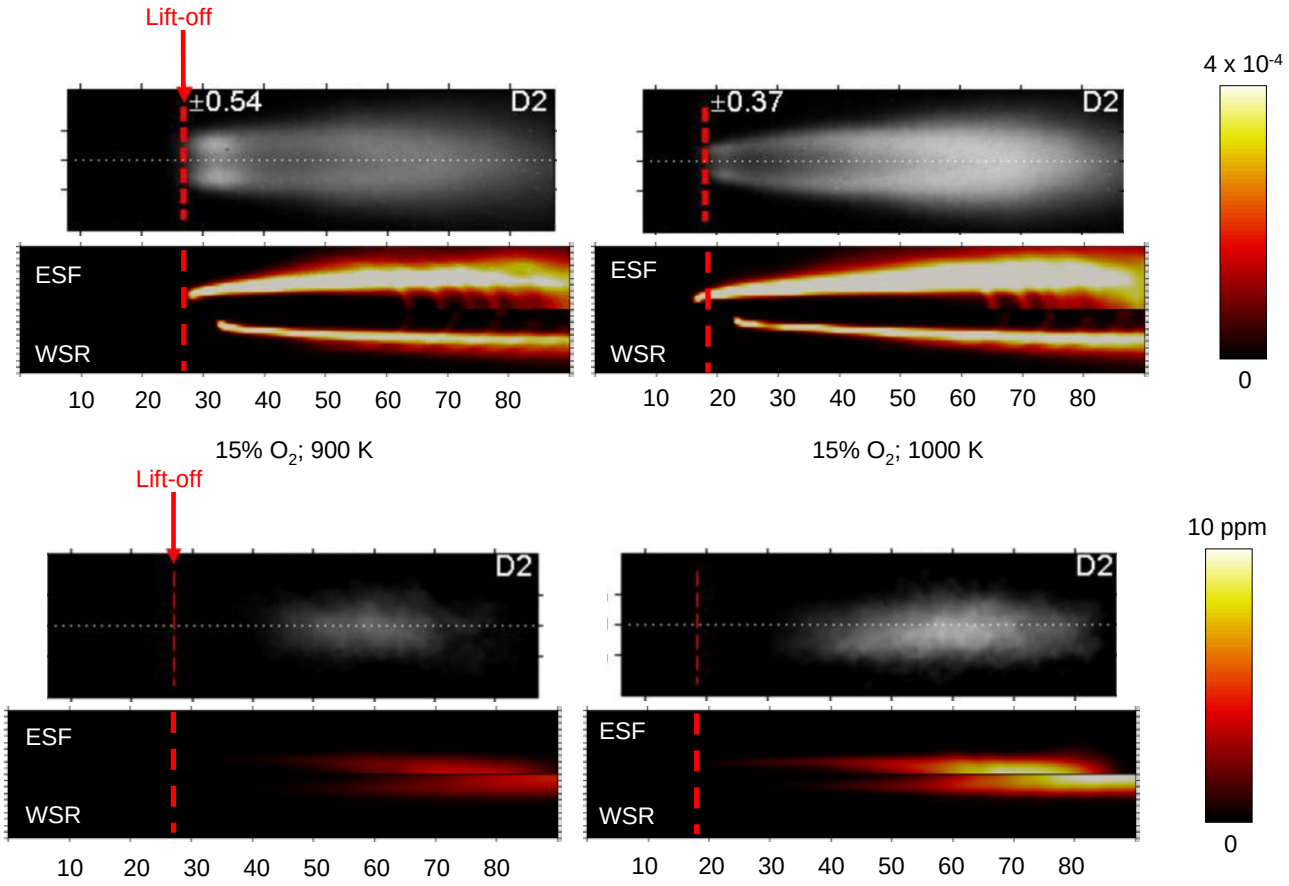
$$\omega_{sg,ori} = 6000 \cdot \exp\left(\frac{12100}{T}\right) \cdot S_{soot}^{\ 0.5} \cdot [C_2H_2]$$

$$\omega_{sg,rev} = 14 \cdot \left(\frac{P}{P_{ref}}\right)^{1.4} \cdot \exp\left(\frac{12100}{T}\right) \cdot S_{soot}^{\ 0.5} \cdot [C_2H_2]$$

- Variation of maximum SVF with respect to the change of ambient temperature (ratio of ~2) in n-Dodecane spray is captured

Diesel spray combustion

- TCI improves the IDT and LOL results
- But, calculated ratio of maximum SVF is ~2 is close to with the measurement in n-dodecane spray combustion data



Concluding remarks

- Overall soot precursor distribution prediction is improved when A_4 is used as soot precursor but C_2H_2 works well in short LOL cases

- Sensitivity analysis indicates that S_{soot} gives a pronounced effect on predictions of *spatial soot distribution* and *soot concentration*

- For n-heptane spray under diesel engine-like operating conditions, the optimized model is applicable to simulate *spatial evolution of soot particle* and *soot volume fraction* at varying levels of EGR for both low and high density conditions

- Increment of maximum SVF with respect to the rise of ambient temperature in the n-dodecane spray cases are replicated

- This is not replicated in the D2 case and the soot formation at the jet core is unaffected by the turbulence chemistry interaction

What's next?

- Modelling of diesel soot formation

- From the Sandia combustion vessel to the MAN Diesel & Turbo A/S marine engine

Thank you

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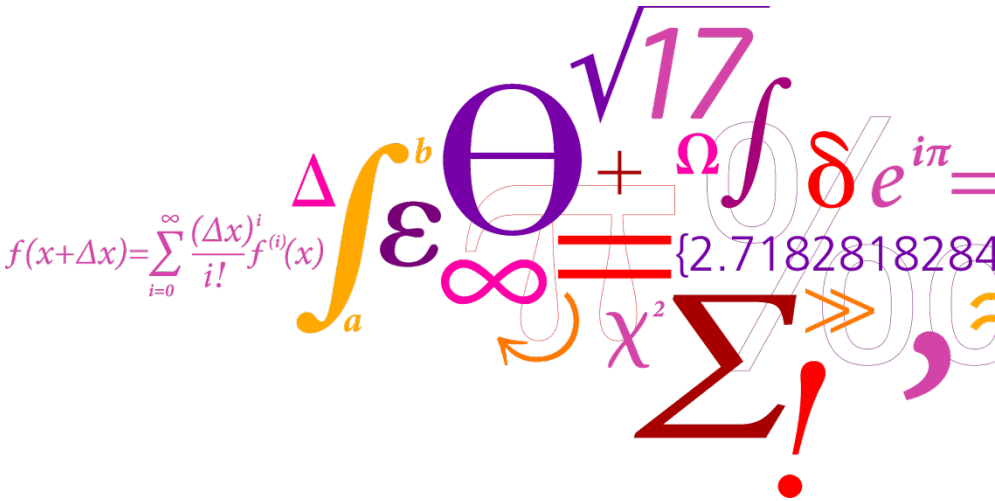

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