Modelling of combustion and soot radiation in a large two stroke marine engine

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IC Engine Group
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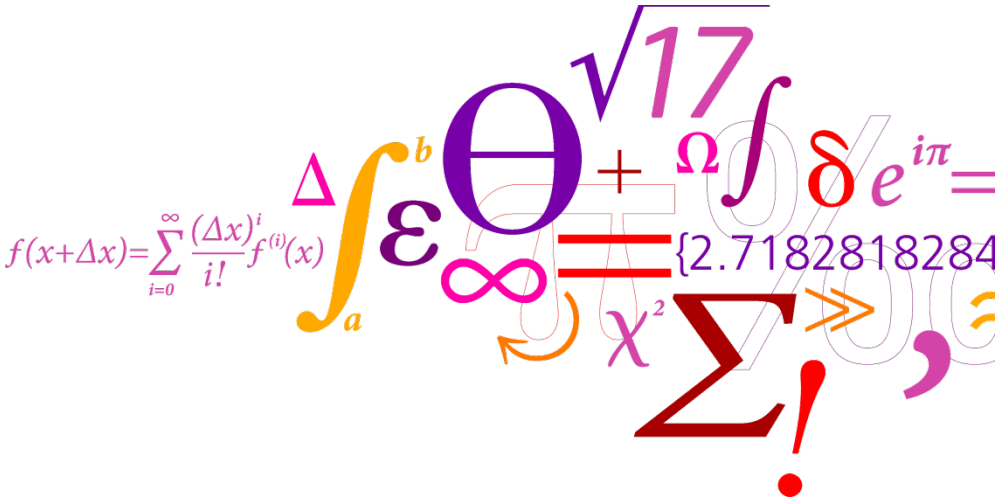
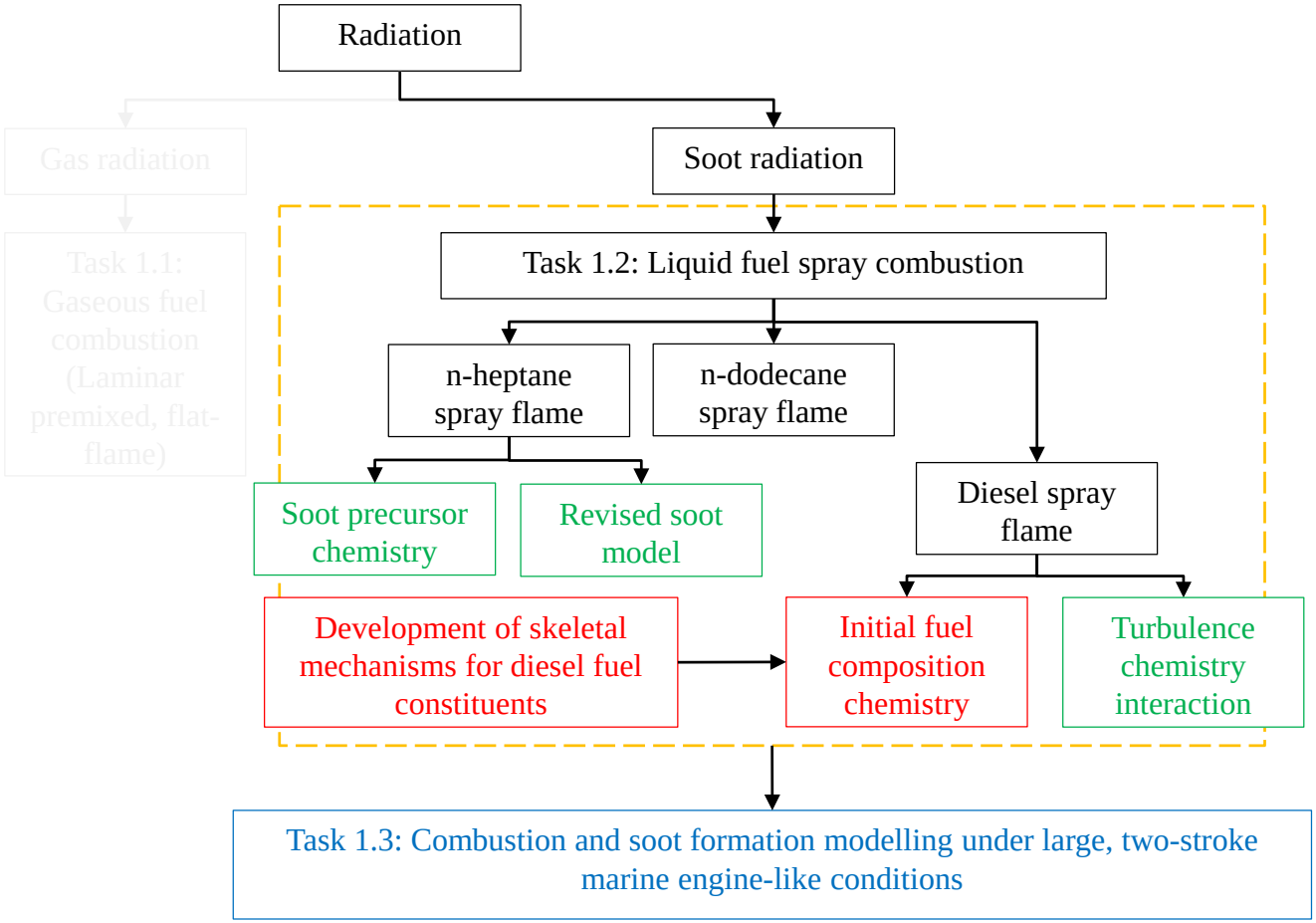


DTU Mechanical Engineering
Department of Mechanical Engineering

Overview of Task 1



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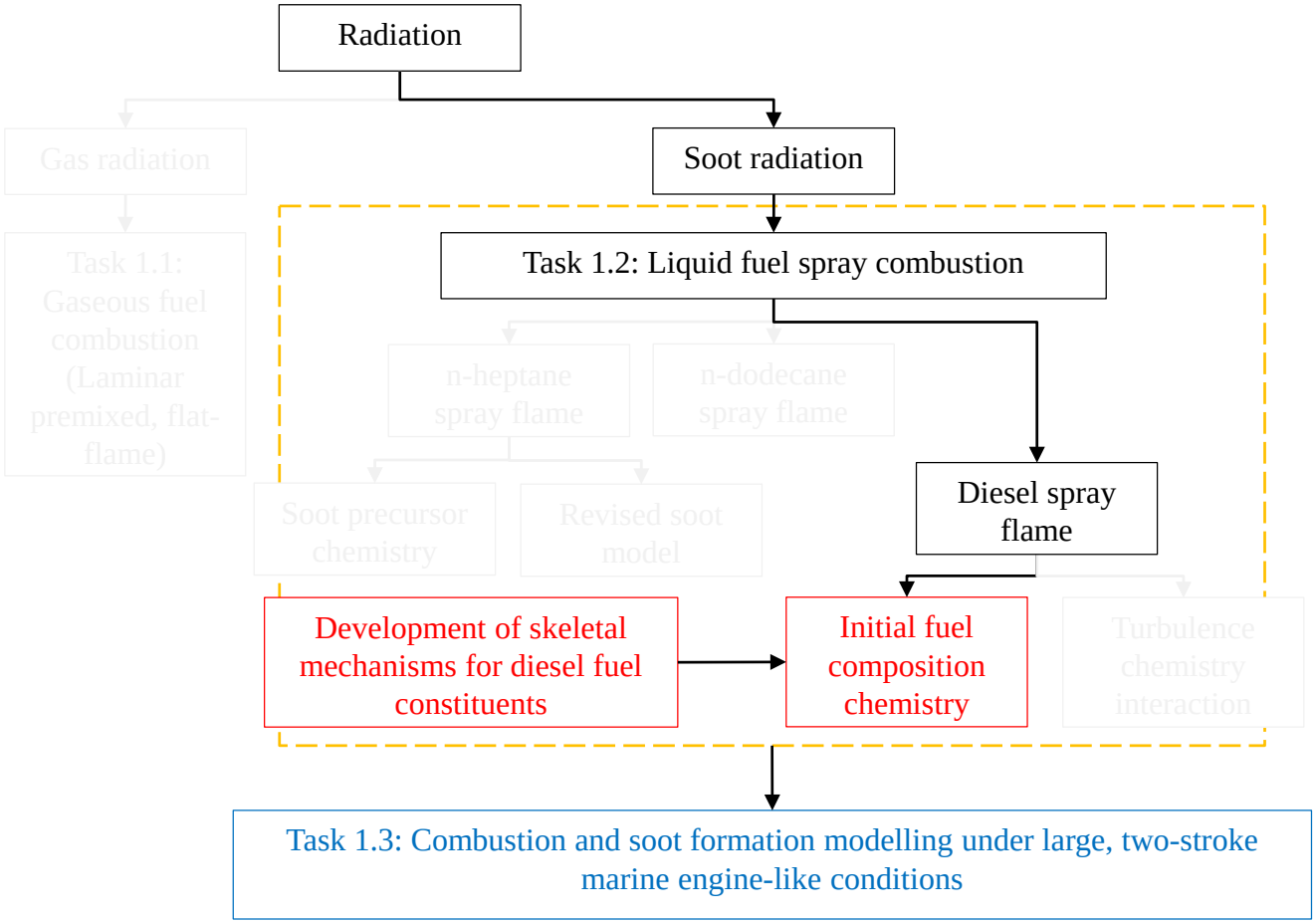


Introduction

Objective(s):

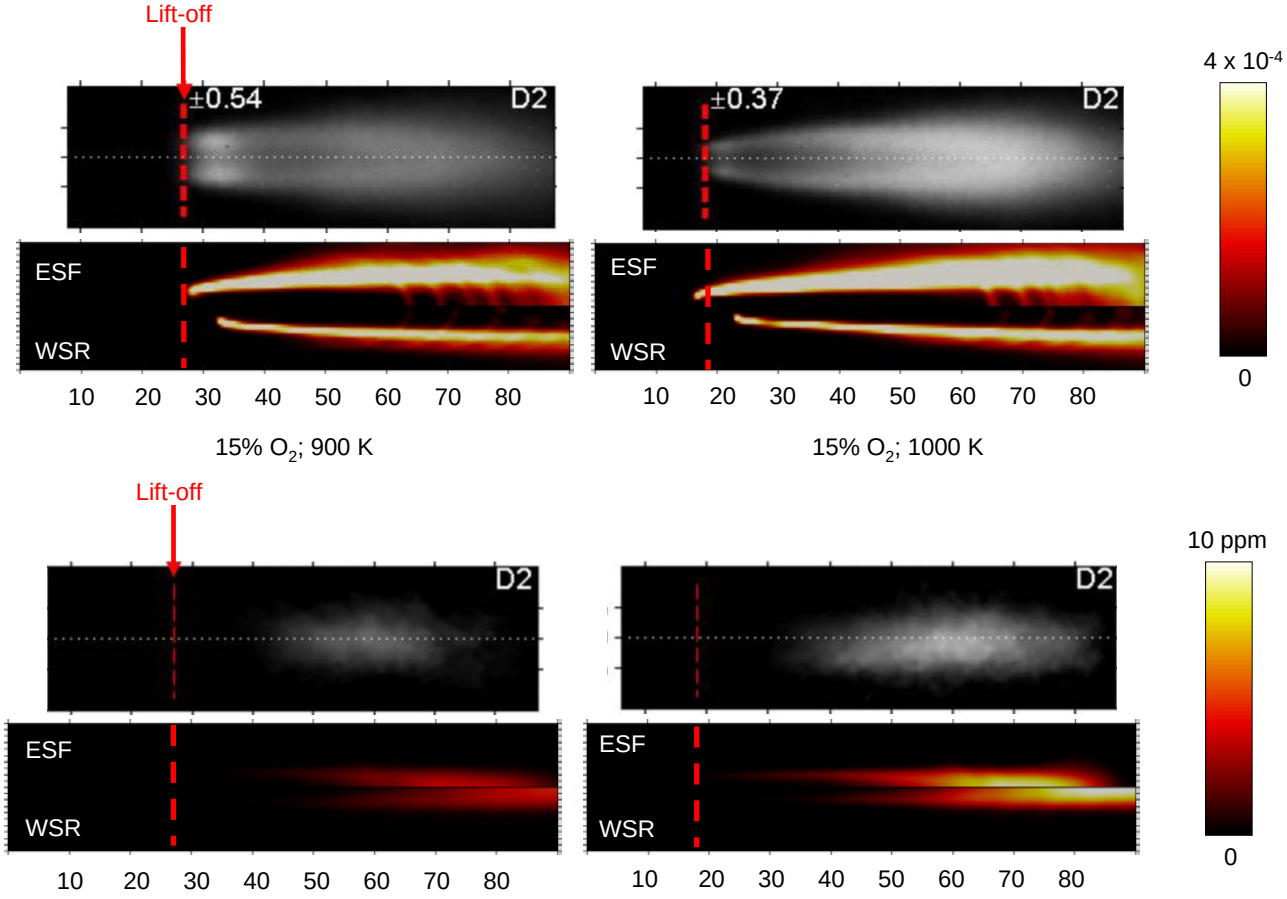
i. To investigate how the soot formation behaves when aromatic compound is considered and is omitted in the surrogate fuel model

ii. To develop and to validate a *skeletal chemical kinetic mechanism* which is computationally efficient for 3-D CFD large bore marine engine simulations yet sufficiently comprehensive to include species essential for pollutant formation predictions

iii. To numerically investigate *in-cylinder phenomena in a large, low-speed uniflow-scavenged marine diesel engine*, operating at full load condition where optical measurements are not available

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



Diesel spray combustion

- Single component
  - 68 species by Lu et al. [2009]
  - Pure n-heptane model and no aromatic chemistry is included
  - C_2H_2 is used as soot precursor and surface growth species

- Multi-component
  - 70 species model by Golovitchev et al. [2005]
  - Diesel Oil Surrogate, DOS
  - Integration of n-heptane and toluene mechanisms
  - Widely used in multi-dimensional CFD diesel engine simulations
  - A_2 is used as soot precursor; C_2H_2 is used as surface growth species

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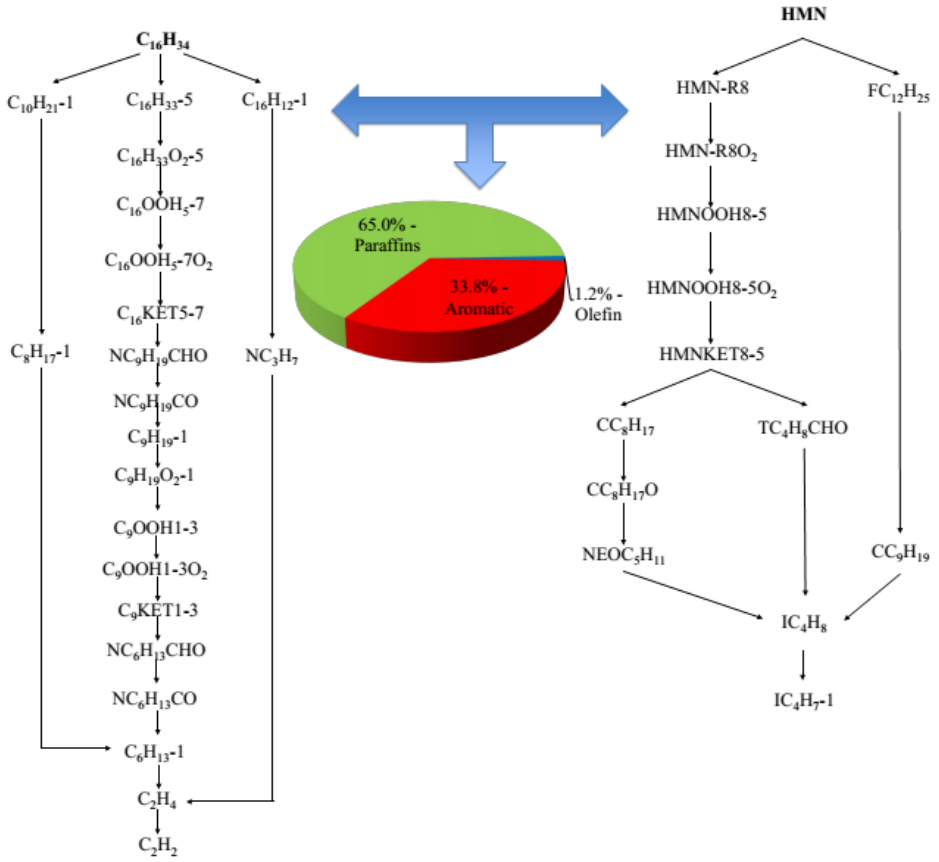
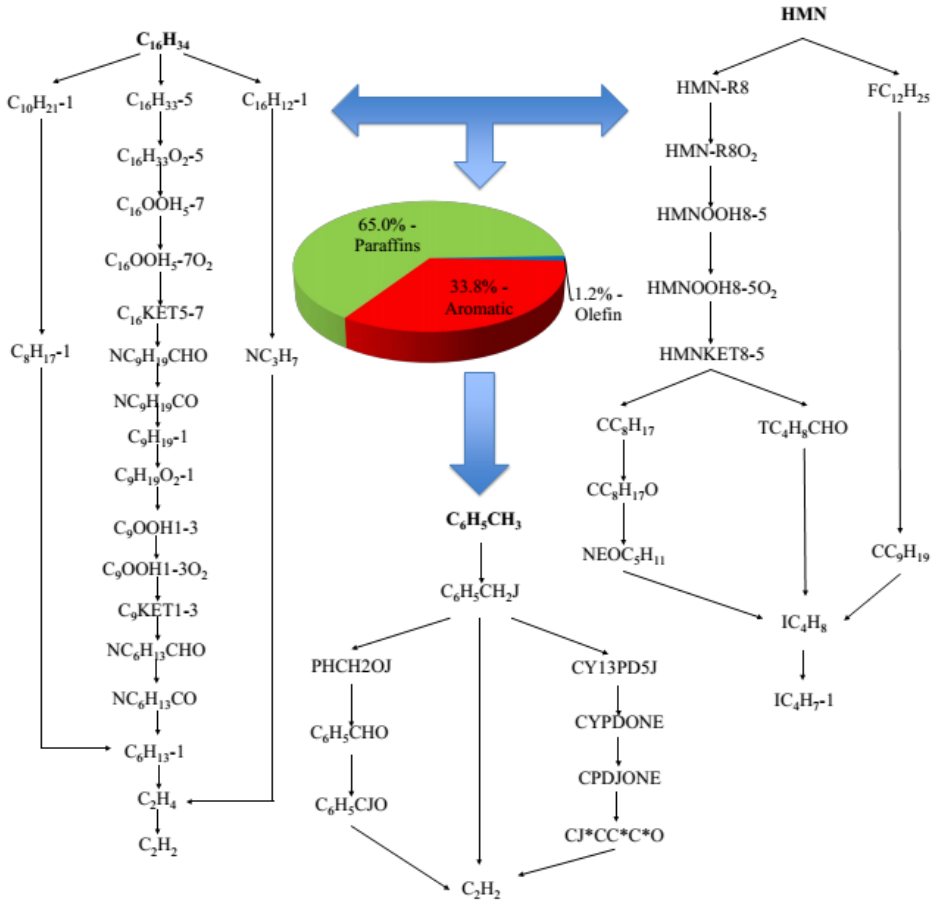
Multi-component, C16 model

- Version I (**C16** model): adding heptamethylnonane, HMN
  - For desired cetane number, $CN = (F_{HXN} + 0.15F_{HMN}) \times 100$
  - F_{HXN} : F_{HMN} = 0.42 : 0.58
  - C_2H_2 is used as soot precursor and surface growth species
  - 88 species



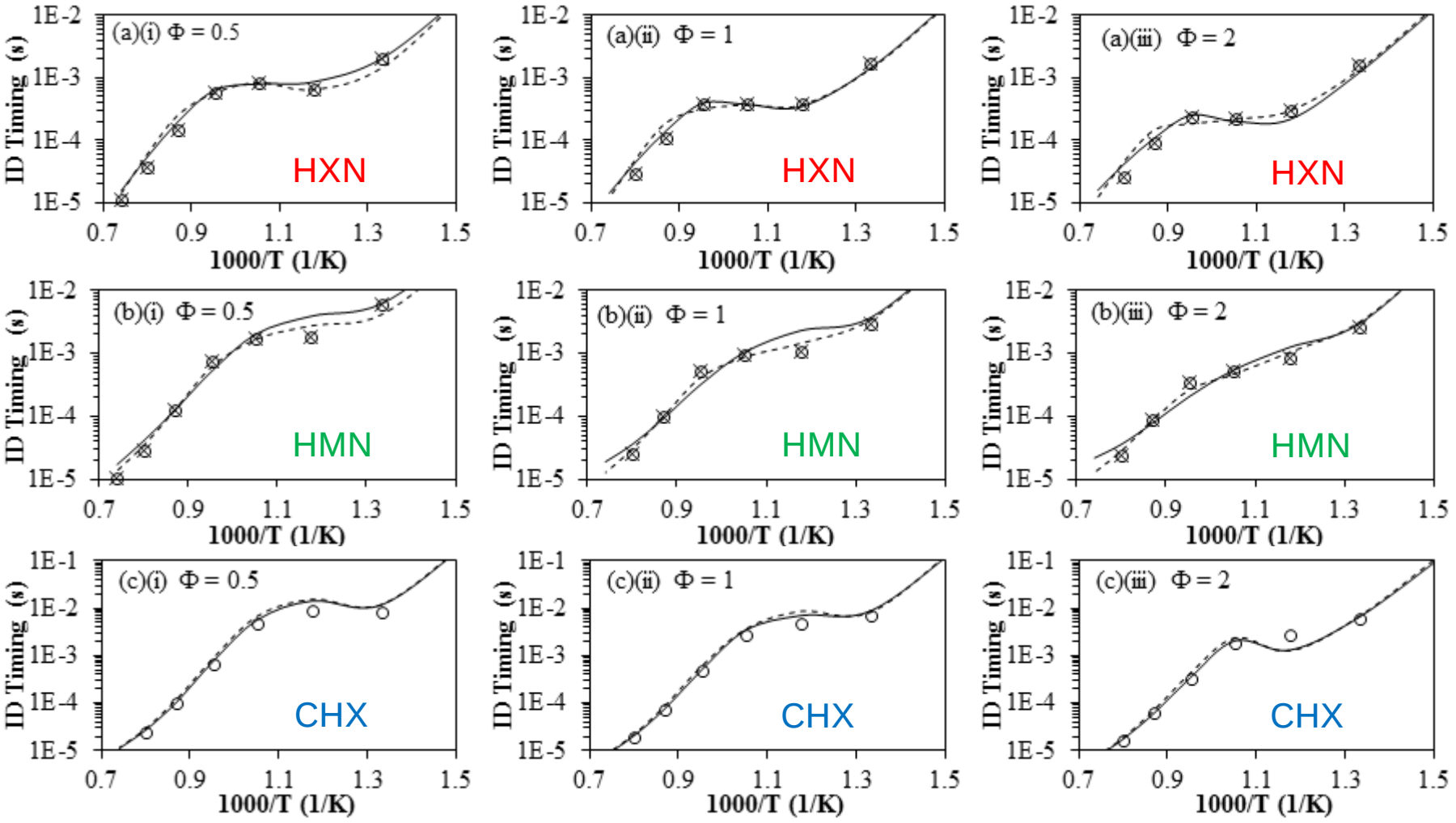
Multi-component, C16 model

- Version II (**Revised C16** model): adding CHX and C_7H_8 into Version I
  - F_{HXN}:F_{HMN}:F_{CHX}:F_{C7H8} = 0.42 : 0.20 : 0.10 : 0.28
  - A_1 is used as soot precursor; C_2H_2 is used as surface growth species
  - 129 species



Multi-component, C16 model

- Validation: shock tube (ST)



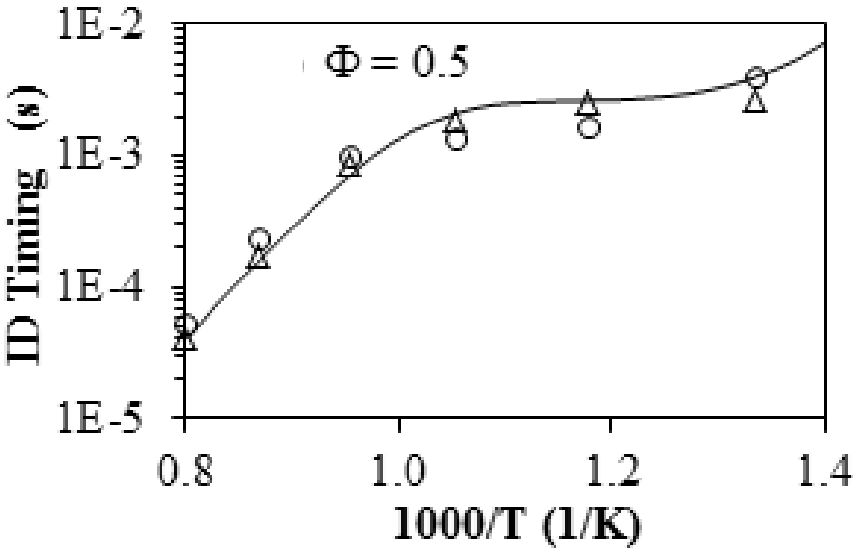
Detailed (solid lines); reduced (dotted lines); C16 (X); Revised C16 (O)

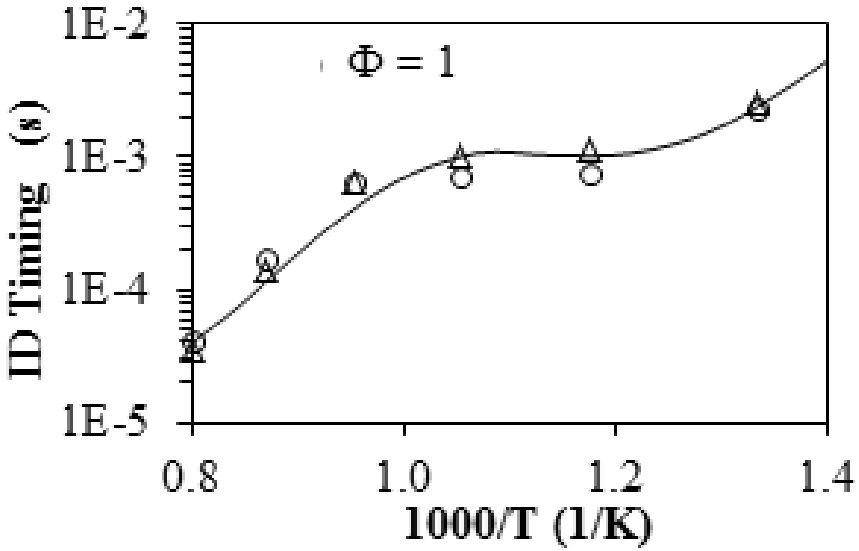
Multi-component, C16 model

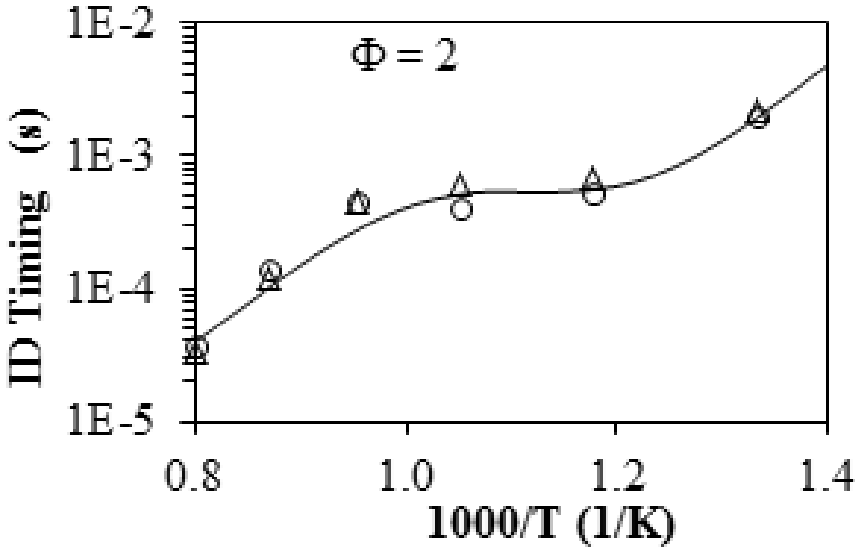
- Validation: shock tube (ST)
  and jet stirred reactor (JSR)

Multi-component, C16 model

- Validation: shock tube (ST) and jet stirred reactor (JSR)



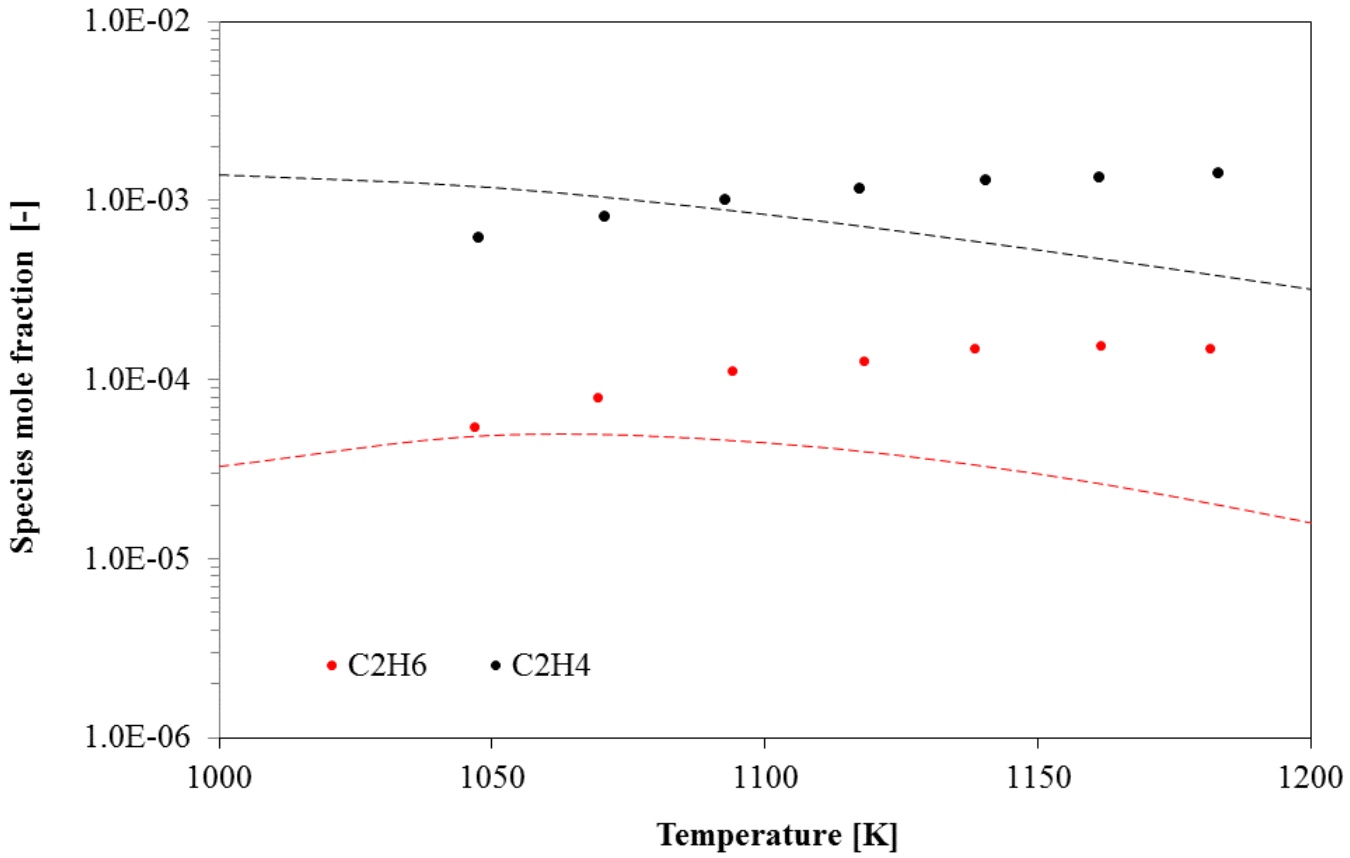




Detailed DPRF58 mechanism (lines)
C16 (Δ)
Revised C16 (○)

Multi-component, C16 model

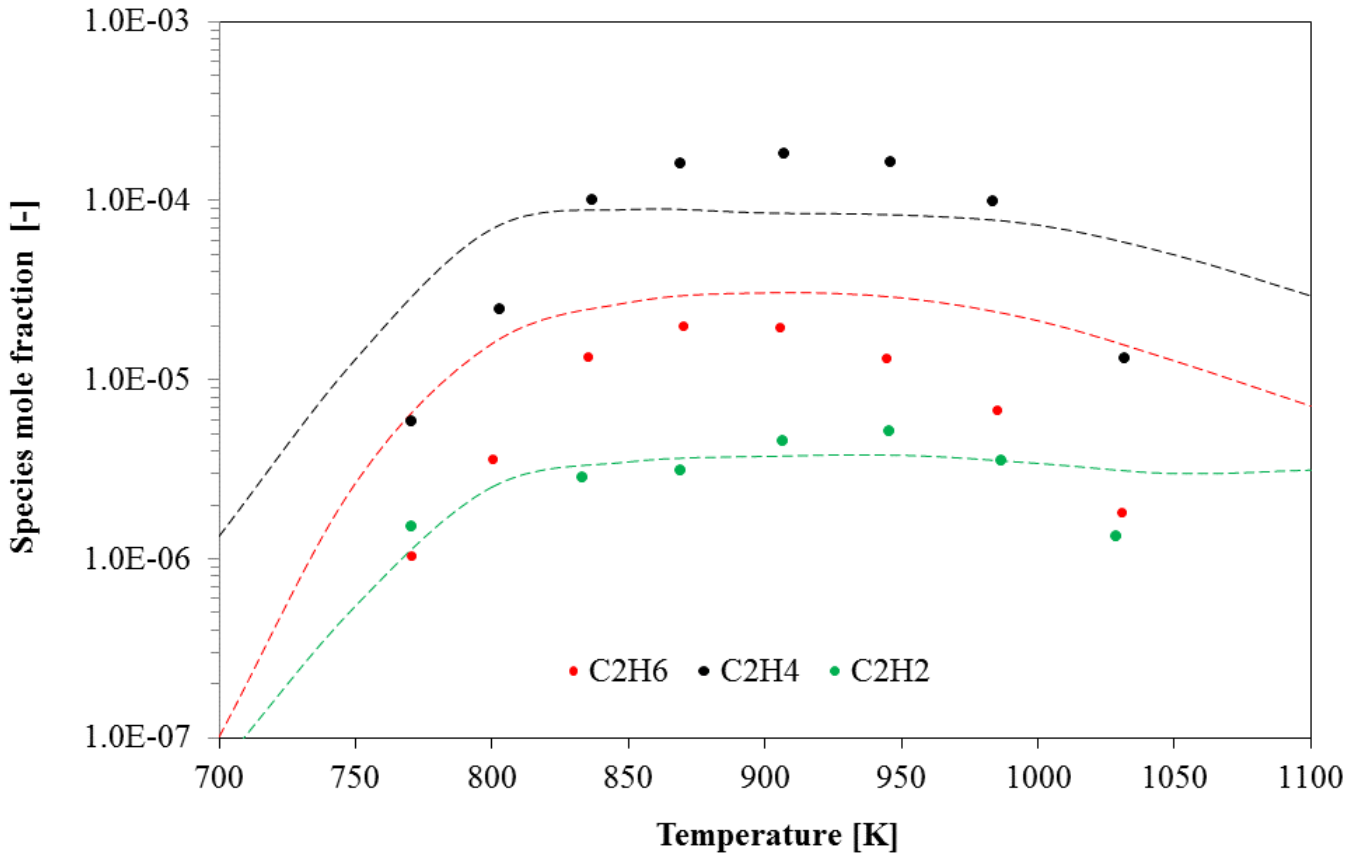
- Validation: shock tube (ST) and jet stirred reactor (JSR)



Experimental (symbols) and computed (lines) mole fractions for the oxidation of HXN at 1 atm in a JSR (0.03% of HXN, 1.47% of O2, 98.5% of N2, Φ = 0.5, τ = 0.07 s).

Multi-component, C16 model

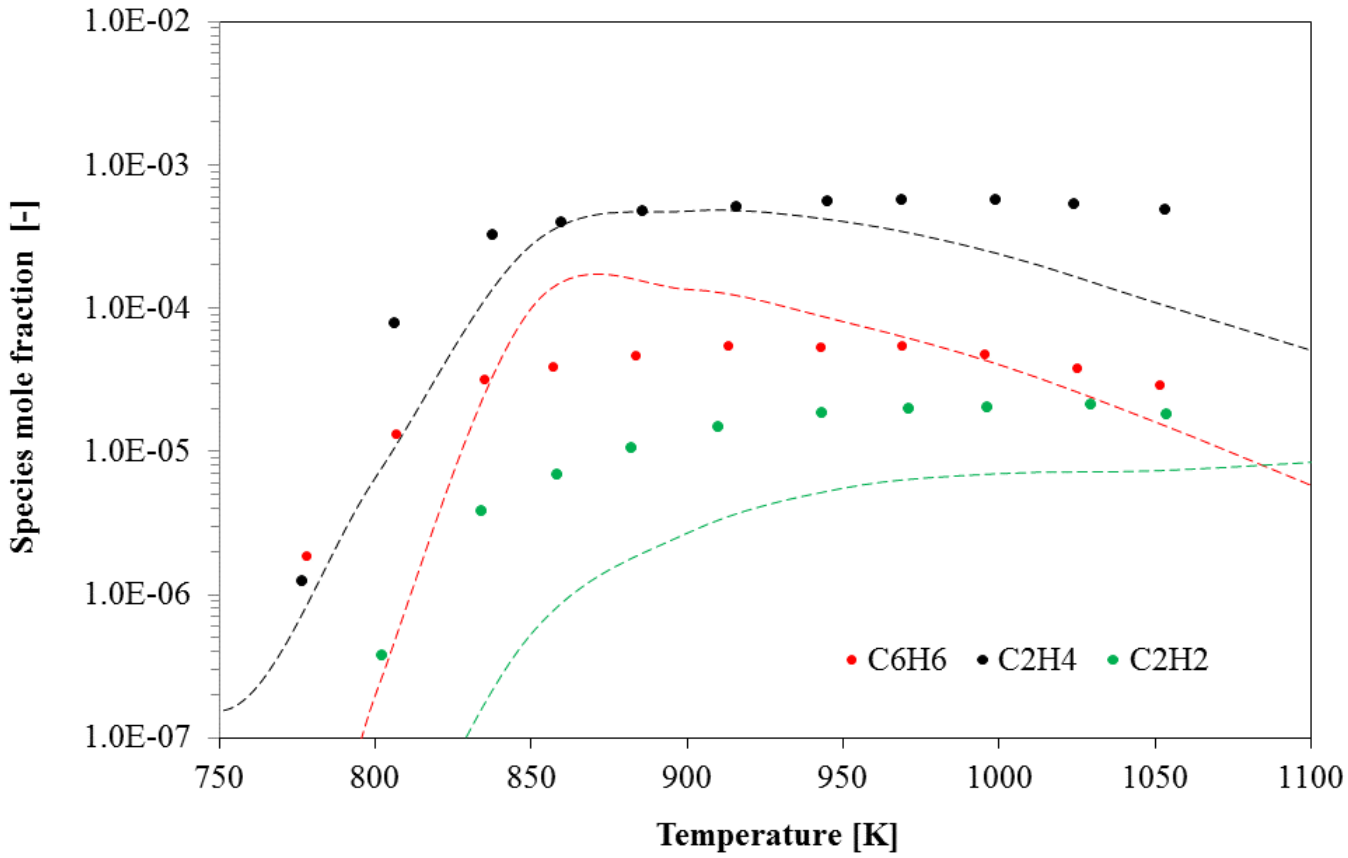
- Validation: shock tube (ST)
  and jet stirred reactor (JSR)



Experimental (symbols) and computed (lines) mole fractions for the oxidation of HMN at 10 atm in a JSR (0.07% of HMN , Φ = 2.0, τ = 1.0 s)

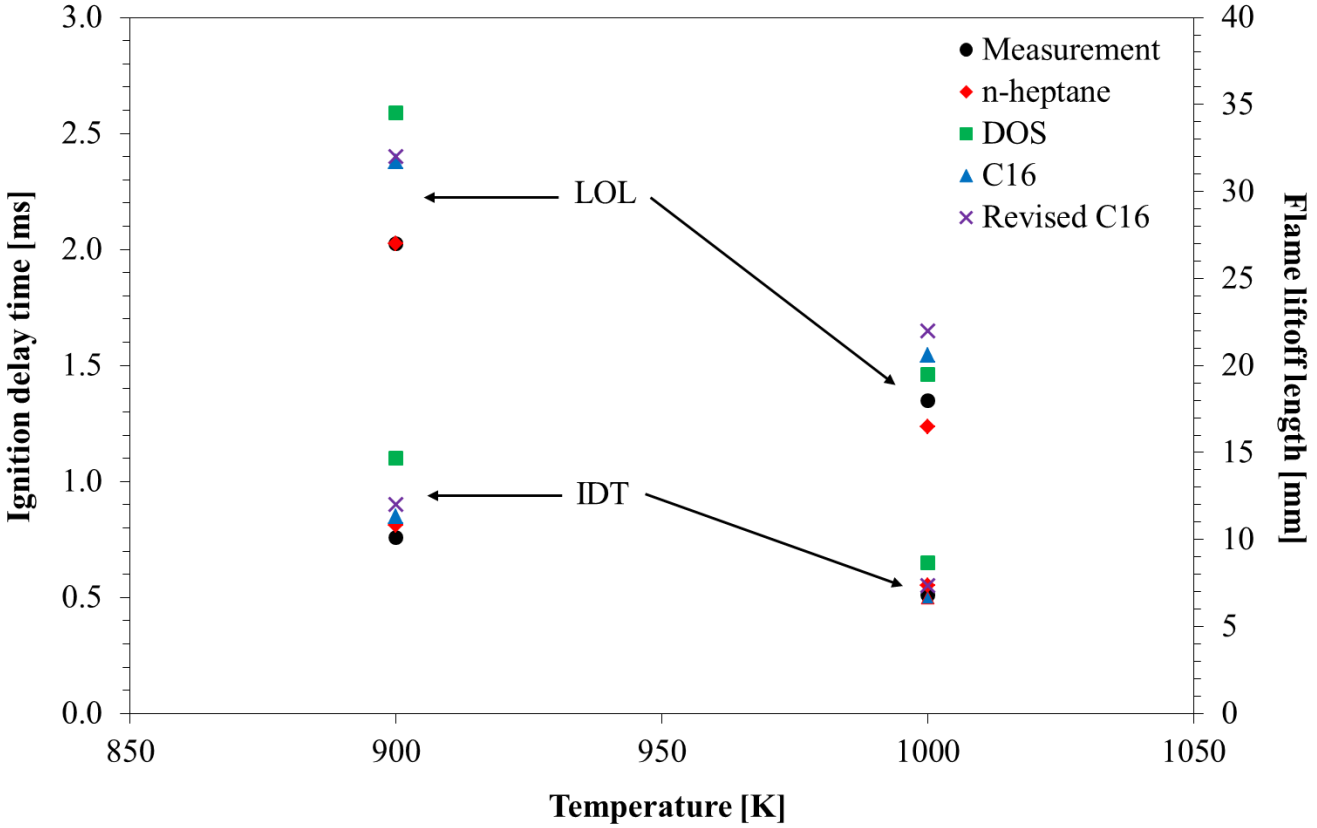
Multi-component, C16 model

- Validation: shock tube (ST) and jet stirred reactor (JSR)



Experimental (symbols) and computed (lines) mole fractions for the oxidation of CHX at 10 atm in a JSR (0.1% of CHX, Φ = 1.5, τ = 0.5 s)

Diesel spray combustion



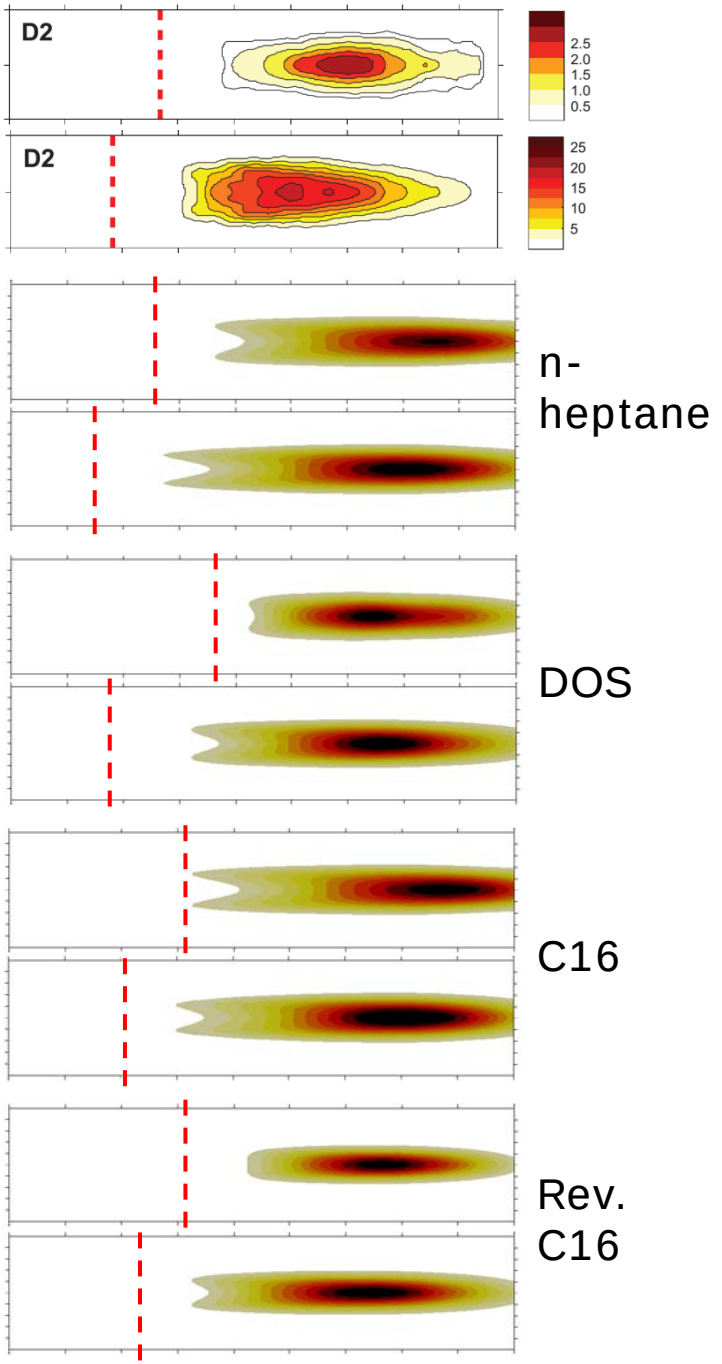
- The n-heptane mechanism performs the best in the current test cases
- C16 and revised C16 models predict the IDTs fairly well but slightly overestimate the LOLs

Diesel spray combustion

- Calculated ratio of maximum SVF is ~2 when fuel mechanisms without toluene is used, agreeing with the measurement in n-dodecane spray combustion data

- The use of DOS is produces a ratio of ~8.5 but IDT and LOL in the 900 K are overestimated

Model	SVF_{max} in 900K case	SVF_{max} in 1000K case	ratio
n-heptane	11.16 ppm	22.0 ppm	1.9
DOS	0.13 ppm	1.10 ppm	8.5
C16	11.3 ppm	21.3 ppm	1.8
Rev. C16	2.60 ppm	9.64 ppm	3.7



Rate of production analysis of DOS

- During the fuel oxidation process and before the ignition, C_2H_2 formed via R1 and R2

$$C_6H_5 + O_2 <=> CH_2CO + HCCO + C_2H_2 \quad (R1)$$
$$C_6H_4O_2 + O => 2CO + C_2H_2 + CH_2CO \quad (R2)$$

  where C_6H_5 and $C_6H_4O_2$ are both compounds formed during the oxidation of toluene

- At higher temperatures after ignition occurs, significant pathways to the formation of C_2H_2 are shown in R3 and R4. Also, C_2H_2 is formed from C_6H_5 via R5.

$$C_2H_4 + M <=> C_2H_2 + H_2 + M \quad (R3)$$
$$C_2H_3 + O_2 <=> C_2H_2 + HO_2 \quad (R4)$$
$$C_4H_3 + C_2H_2 <=> C_6H_5 \quad (R5)$$

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Reactions in single component mechanism

$$C_2H_4 + M <=> C_2H_2 + H_2 + M \quad (R3)$$
$$C_2H_3 + O_2 <=> C_2H_2 + HO_2 \quad (R4)$$
$$C_4H_3 + C_2H_2 <=> C_6H_5 \quad (R5)$$

- Not in the revised C16 model

To-date observations

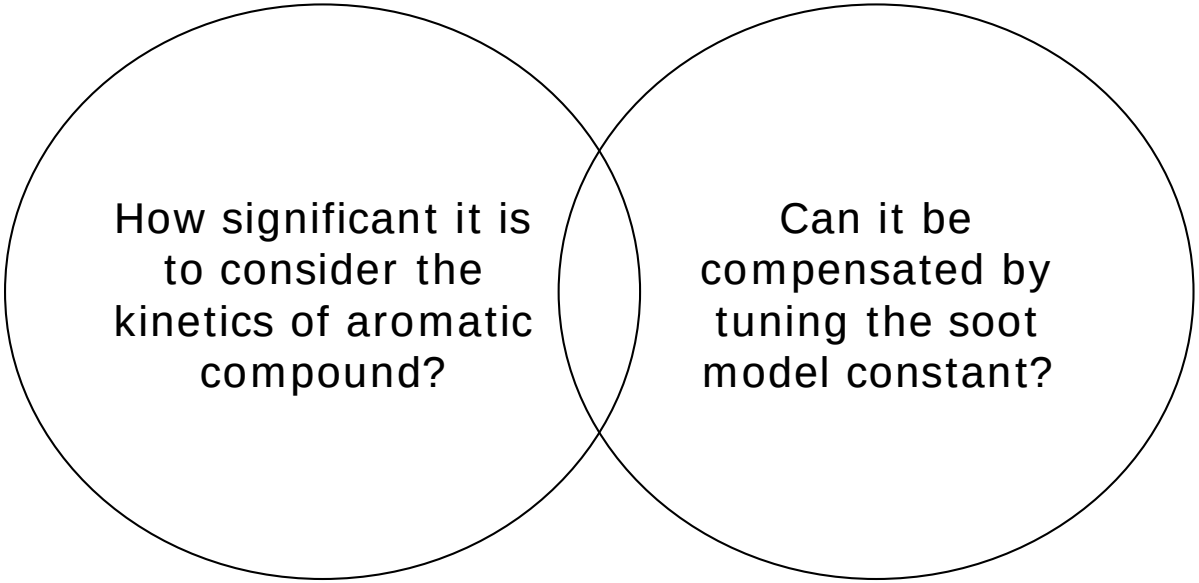
- Calculated ratio of maximum SVF is ~2 when fuel mechanisms without toluene is used, agreeing with the measurement in n-dodecane spray combustion data

- The use of DOS is more promising, producing a ratio of ~8.5 but IDT and LOL in the 900 K are overestimated

- The used of revised C16 model (which is validated using jet stirred reactor oxidation results) produces a ratio of ~ 3.7

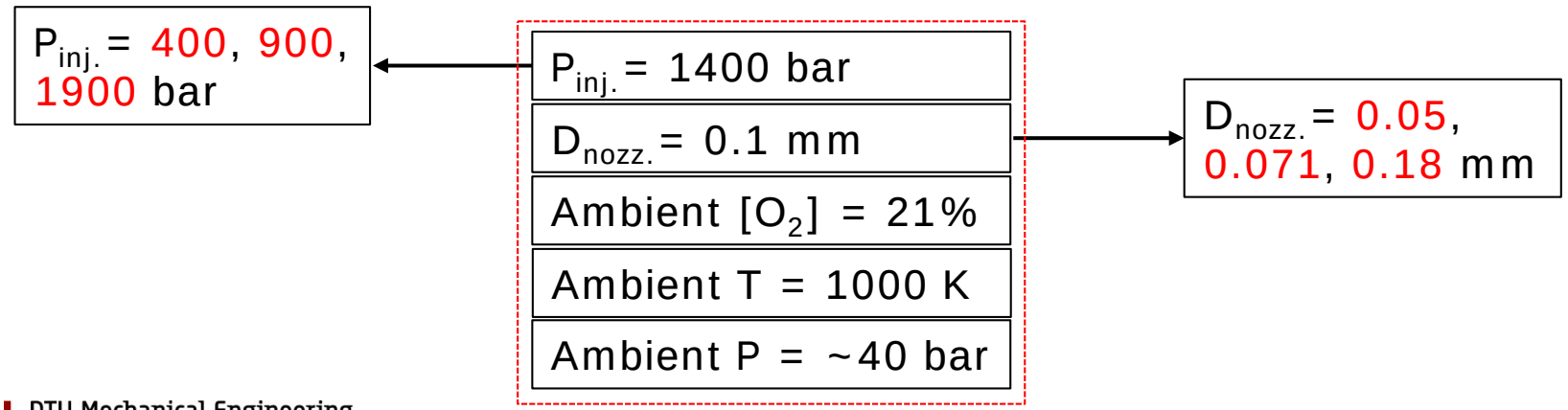
- Co-oxidation reactions are unknown

‘From Sandia spray to engine’



‘From Sandia spray to engine’

- Diesel soot modelling at different ambient temperature is challenging – a single injection case is selected
- Potentially greatest amount of in-cylinder soot (hence greatest soot radiative heat loss) – a high load case is selected
- Main differences in the Sandia constant vessel and MDT marine engine cases are
  - i) Injection pressure
  - ii) Nozzle hole diameter
  - iii) In-cylinder pressure (during start of injection)



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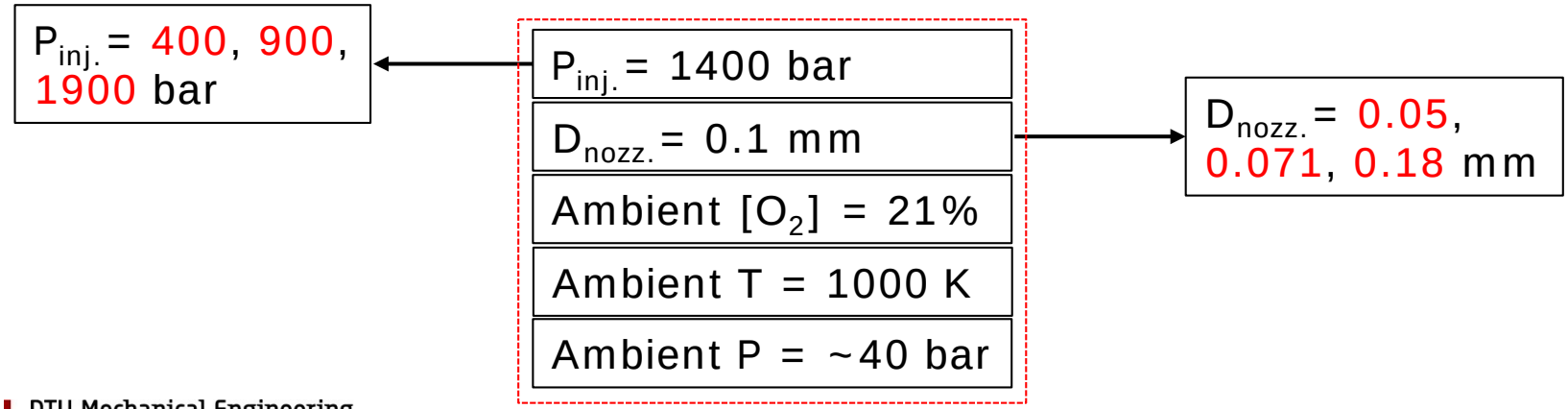

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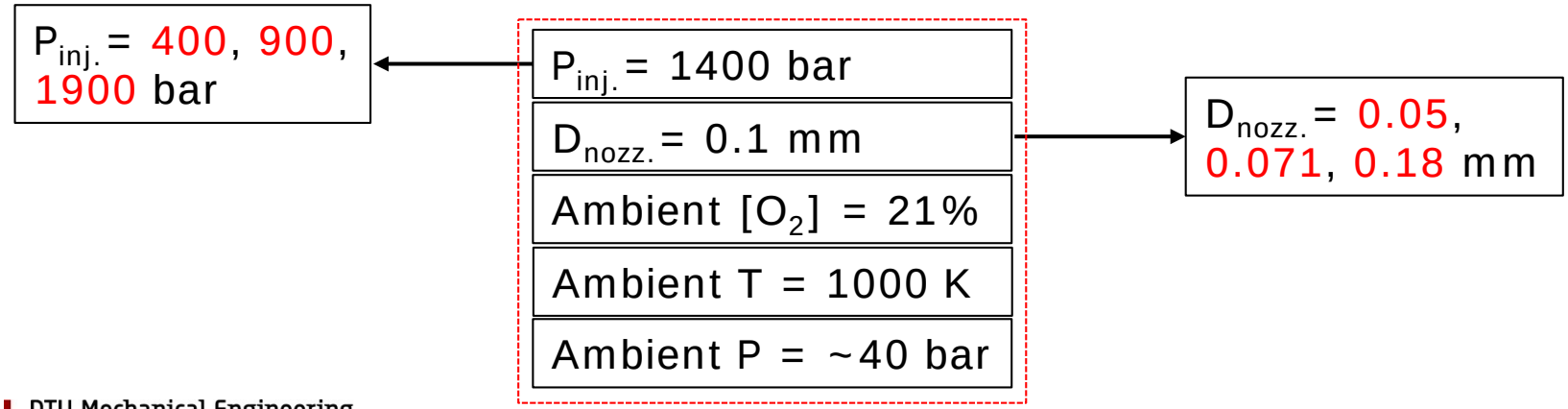
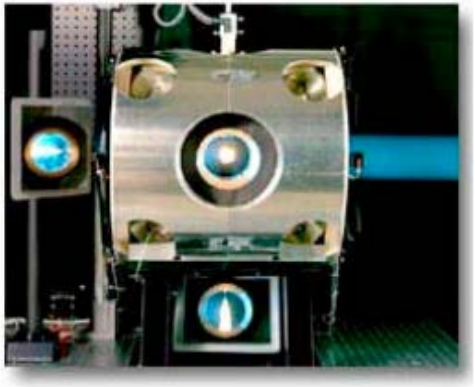


Operating conditions / injection specifications

	Constant volume combustion chamber (t=0)			
$[O_2]$	21 %	21 %	21 %	21 %
T [K]	950	950	950	950
ρ (kg / m^3)	7.3	14.8	30.0	56.3
P [bar]	19.6	38.6	80.0	150.0
orifice diameter (mm)	0.1	0.1	0.1	0.1
Fuel mass delivered [g]	0.0178	0.0135	0.0139	0.0139
Injection duration [ms]	6.5	4.9	4.87	4.87



Operating conditions / injection specifications

	Constant volume combustion chamber (t=0)				Marine engine (at TDC)
$[O_2]$	21 %	21 %	21 %	21 %	21 %
T [K]	950	950	950	950	924
ρ (kg / m^3)	7.3	14.8	30.0	56.3	57.3
P [bar]	19.6	38.6	80.0	150.0	152.9
orifice diameter (mm)	0.1	0.1	0.1	0.1	1.0
Fuel mass delivered [g]	0.0178	0.0135	0.0139	0.0139	44.6
Injection duration [ms]	6.5	4.9	4.87	4.87	31.2

Numerical formulation (STAR-CCM+)

Models / Resolution	Descriptions
Spray breakup model	KH-RT, B1 = 25
Turbulence model	Standard k-ε, with C_1 = 1.55 / k-omega SST
Turbulence-chemistry interaction	None i.e. Well-stirred reactor
Liquid properties	$C_{14}H_{30}$
n-Heptane combustion chemistry	In-house; 30 species
Soot model	Pang et al. [2015] model
Radiation model	None / DOM; $K_a = 1862 \cdot f_v \cdot T$
Smallest cell size	0.25 mm / 2.5mm
Timestep size	4×10^{-7} s / 4×10^{-6} s

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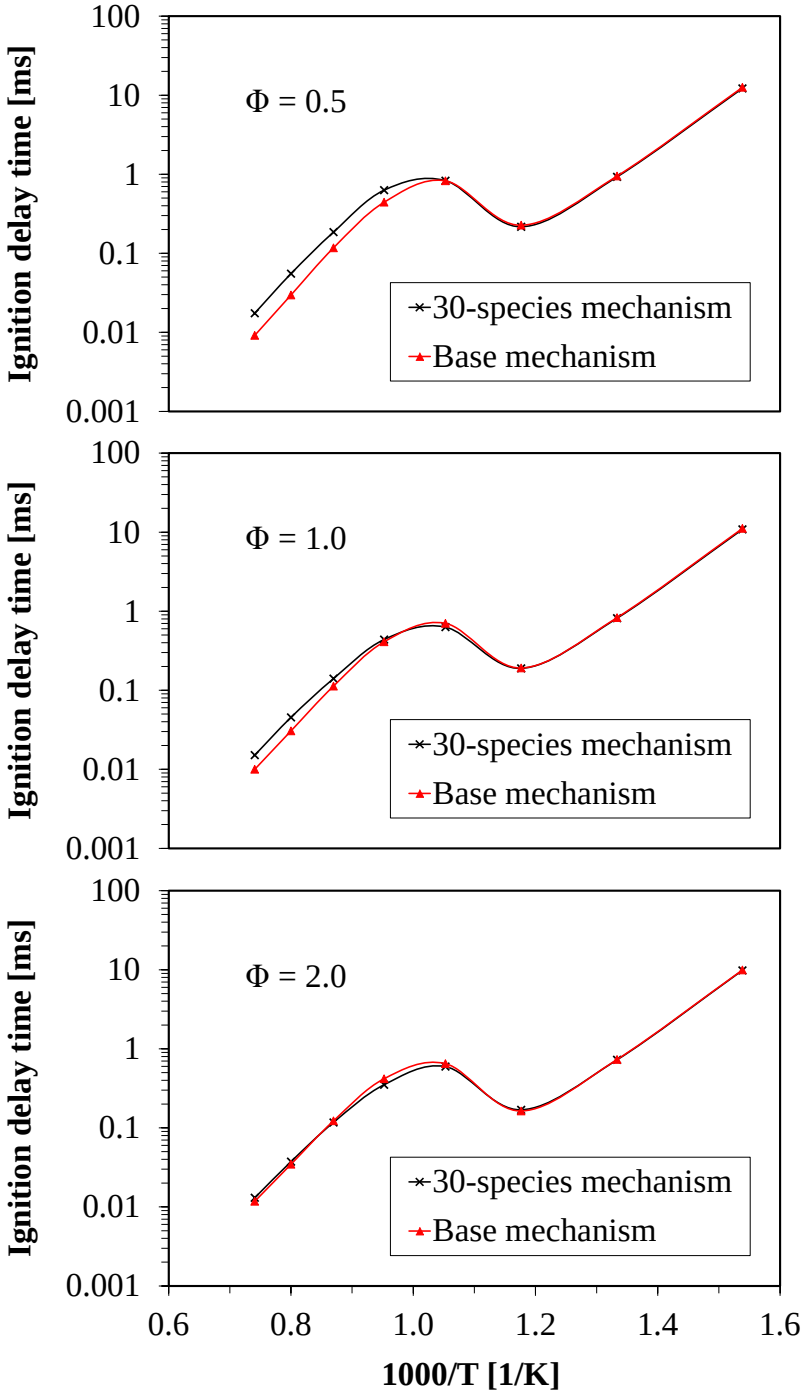
Reference: Haider S, Ivarsson A, Pang KM, Schramm J, Mansouri SH, Proceeding of 12th International Conference on Heat Transfer, Fluid Mechanics and Thermodynamics, 11 to 13 July 2016, Malaga, Spain.

Skeletal n-heptane model

- Previous study:

1. Temporal/spatial evolution of PAH and C_2H_2 are similar at 21% O_2 cases
2. O_2 and OH oxidation are both significant
3. Aromatic chemistry in the initial fuel composition is less influential at varying pressures

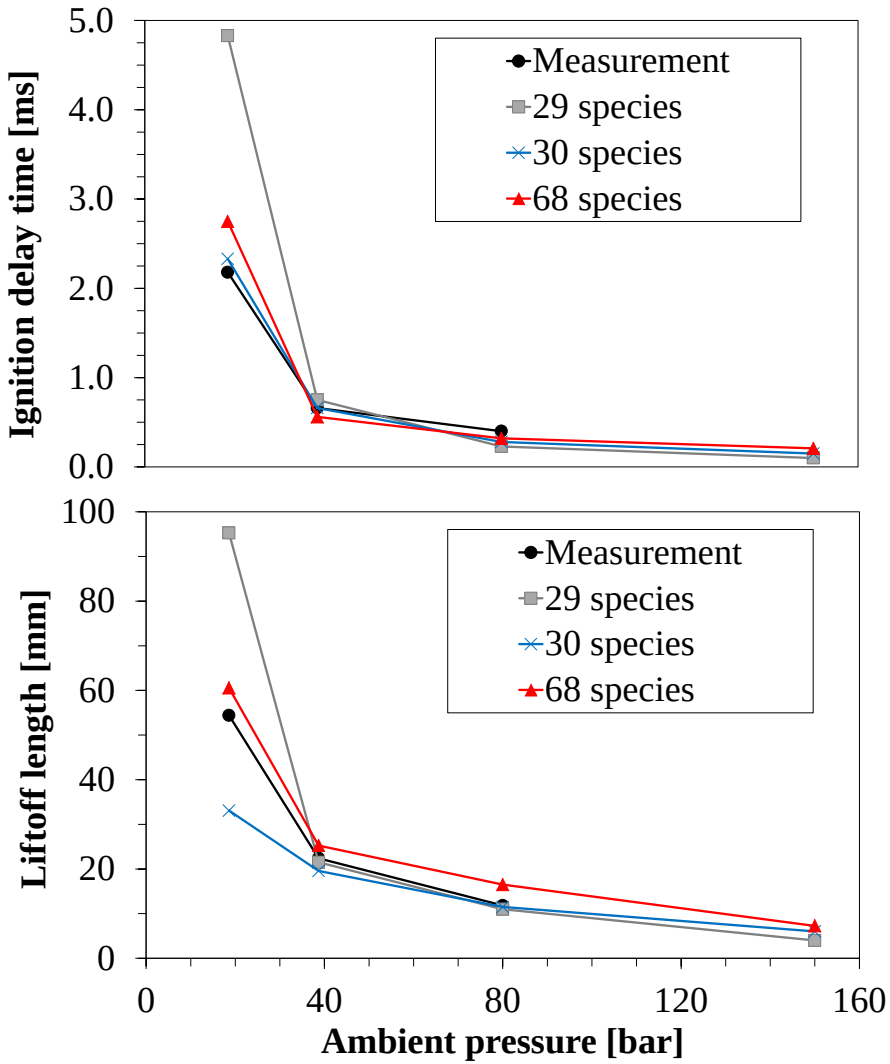
- Reduced from 44 species to 30 species



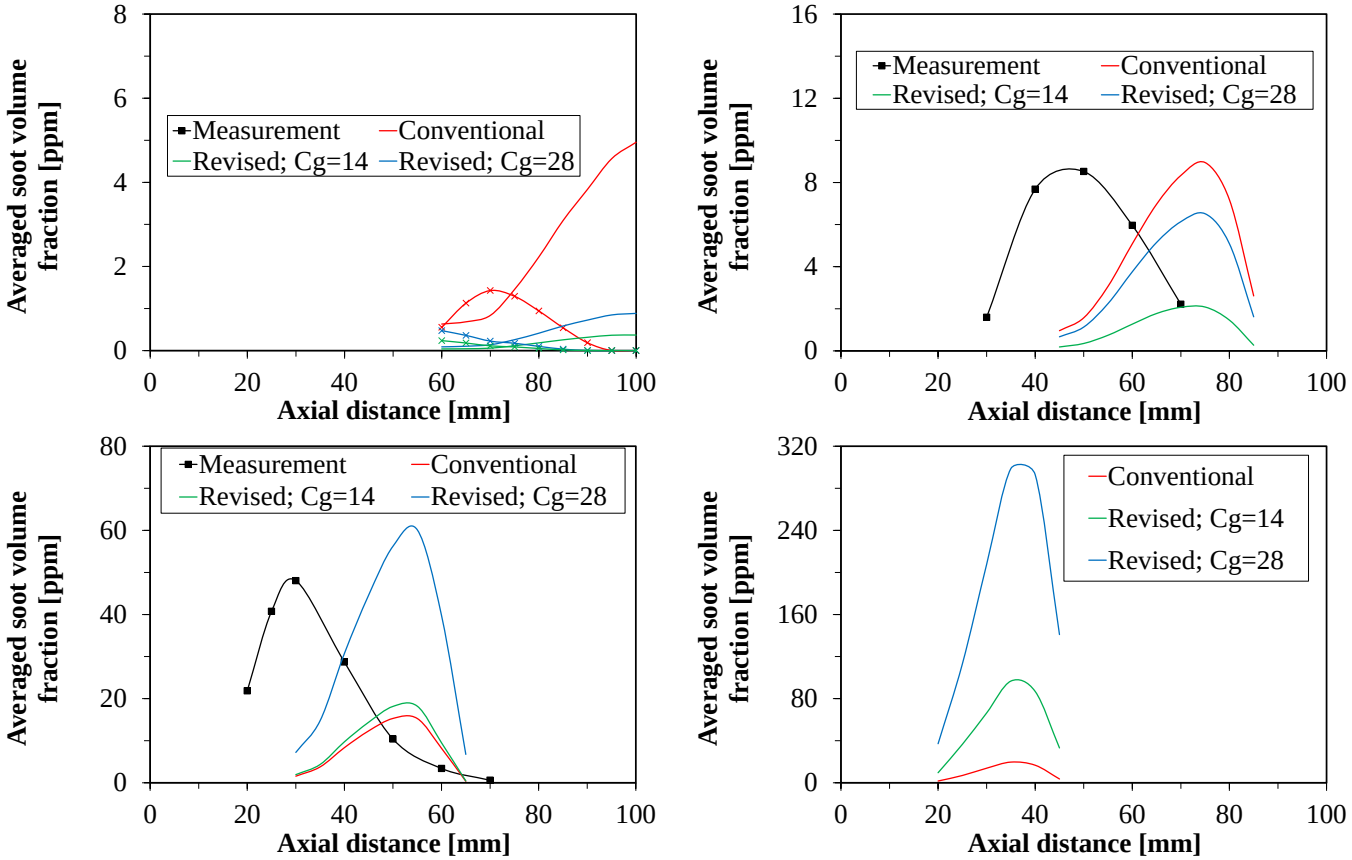
Model validation I

- Ignition delays and lift-off lengths calculated by different mechanisms are compared

- The use of 30 species strikes a balance between accuracy and efficiency



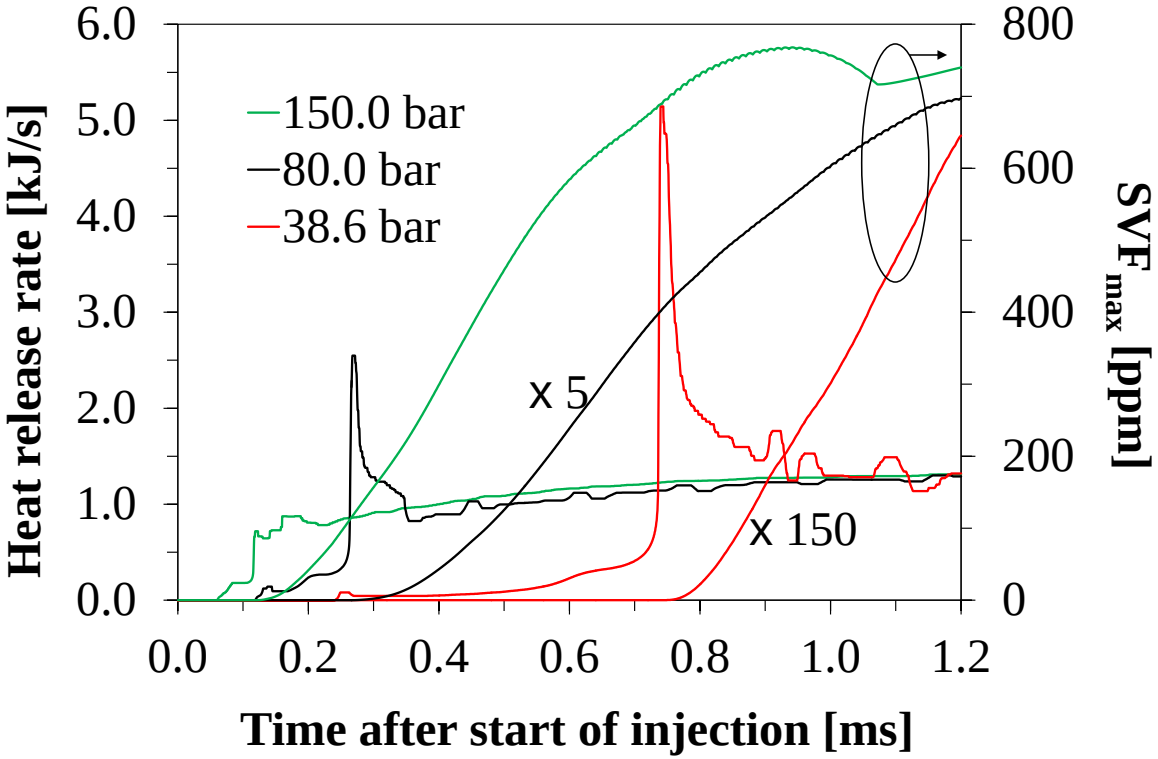
Model validation II



- Revised soot model predicts soot volume fraction (SVF) at different ambient pressures

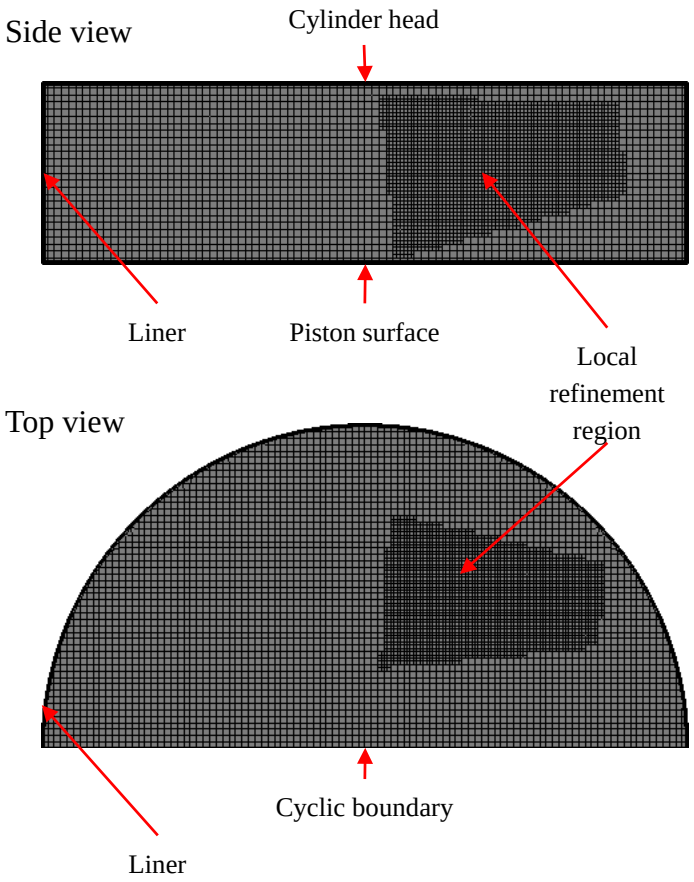
- Maximum SVF predicted by revised model is 15-fold higher at 150 bar

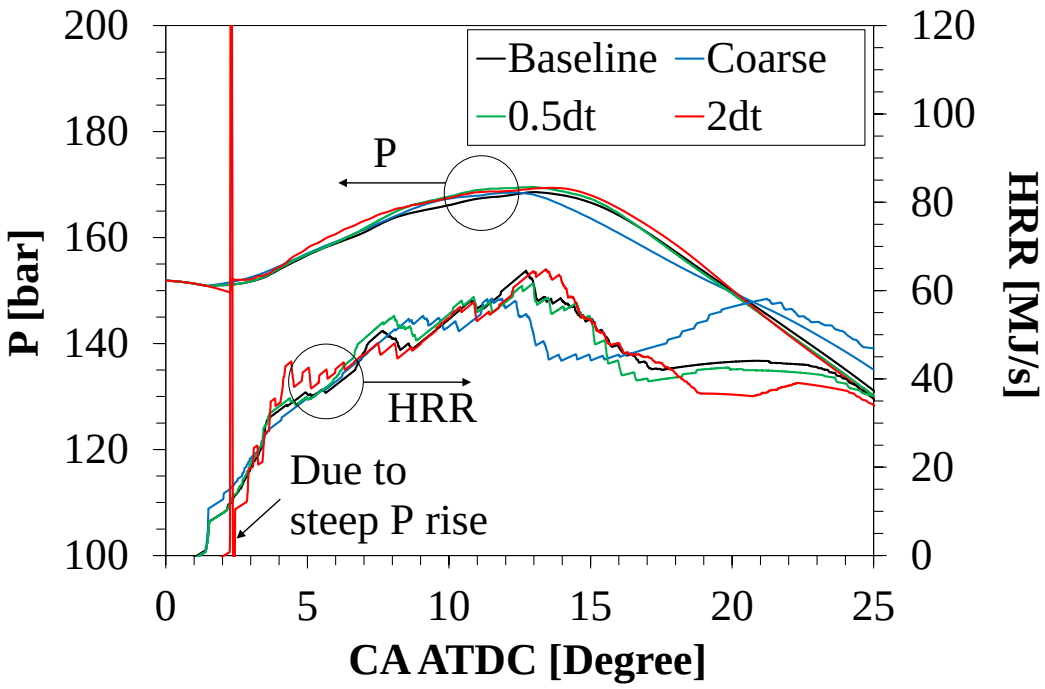
Model validation II



- Soot inception is observed at peak of PMC HRR

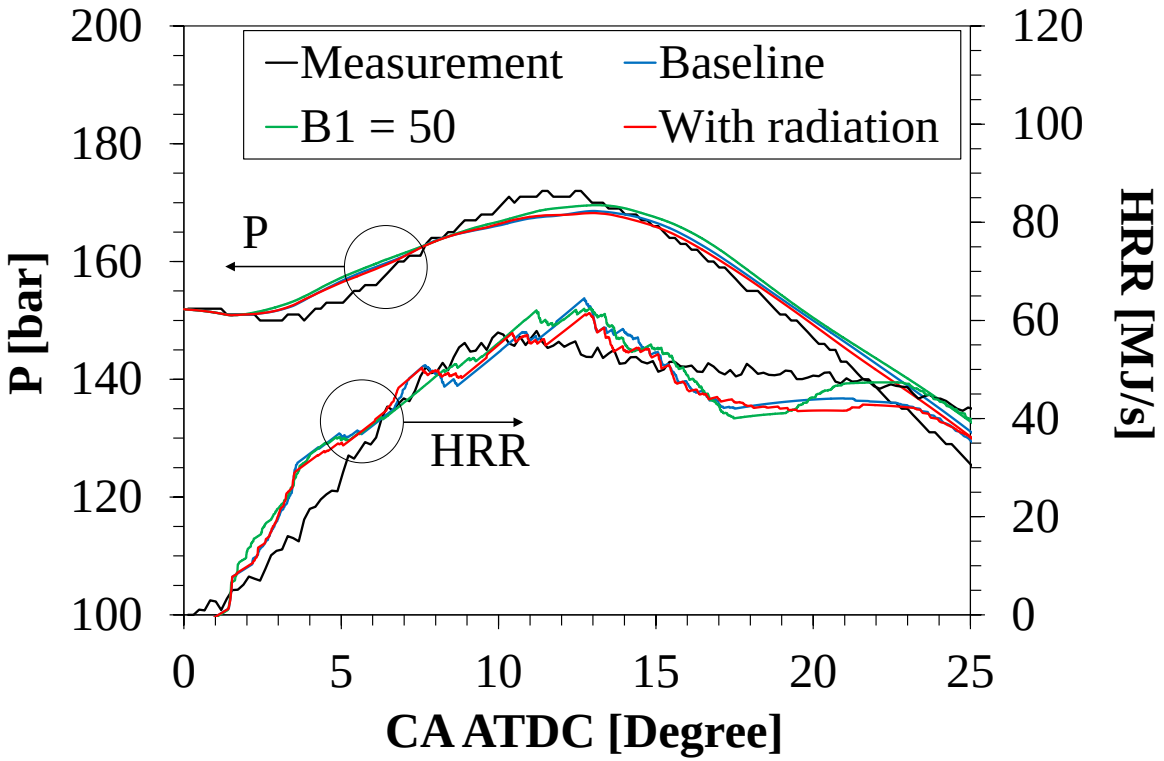
Mesh configuration and convergence studies





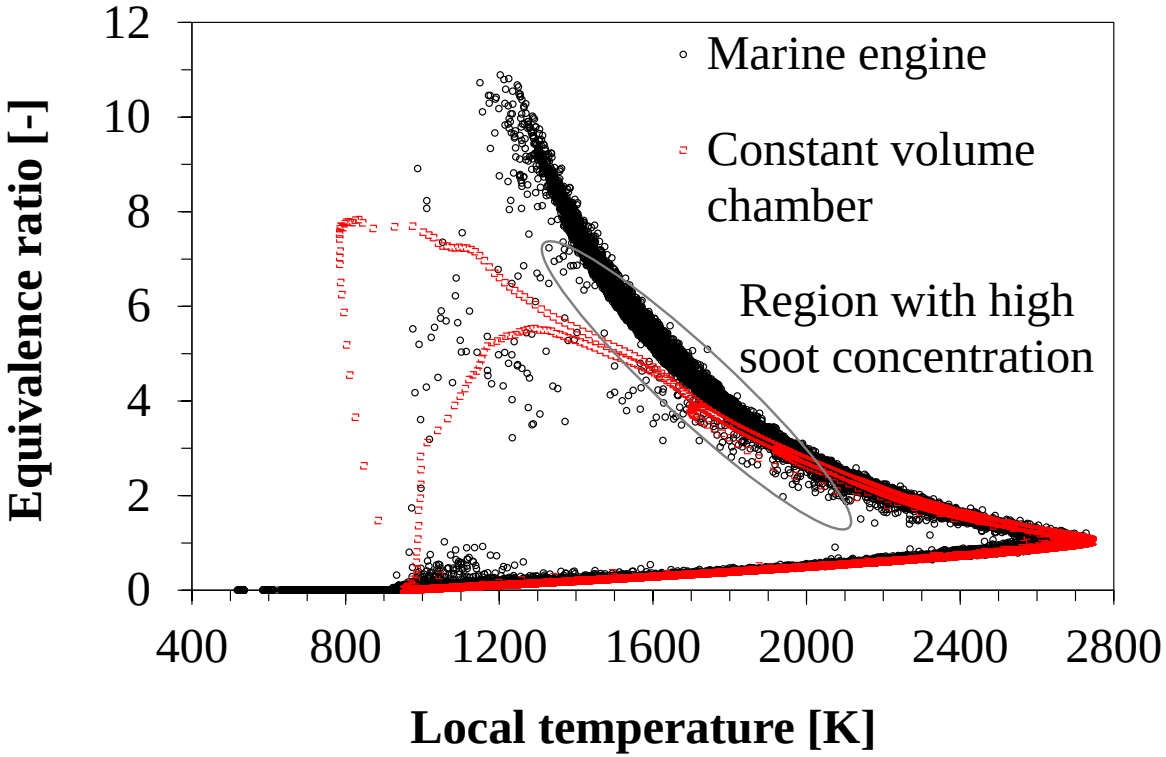
- Local refinement is found to be essential
- The large timestep causes a steep pressure gradient near ignition

Comparisons of different physical models



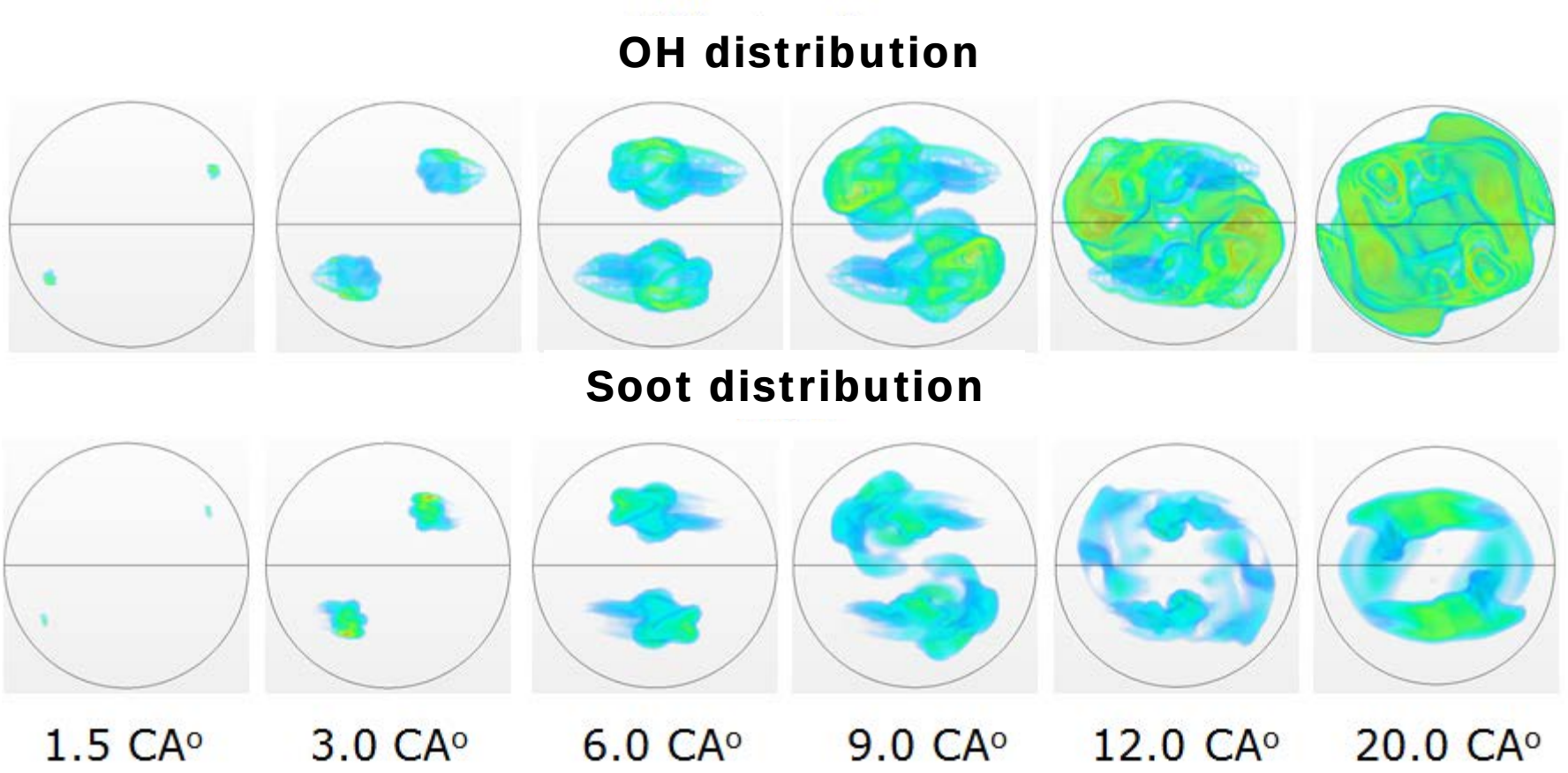
- Ignition delay is slightly underpredicted
- Maximum relative difference in term of peak pressure is < 1.7 %
- Using a larger breakup rate constant value changes the HRR shape

Temperature-equivalence ratio map



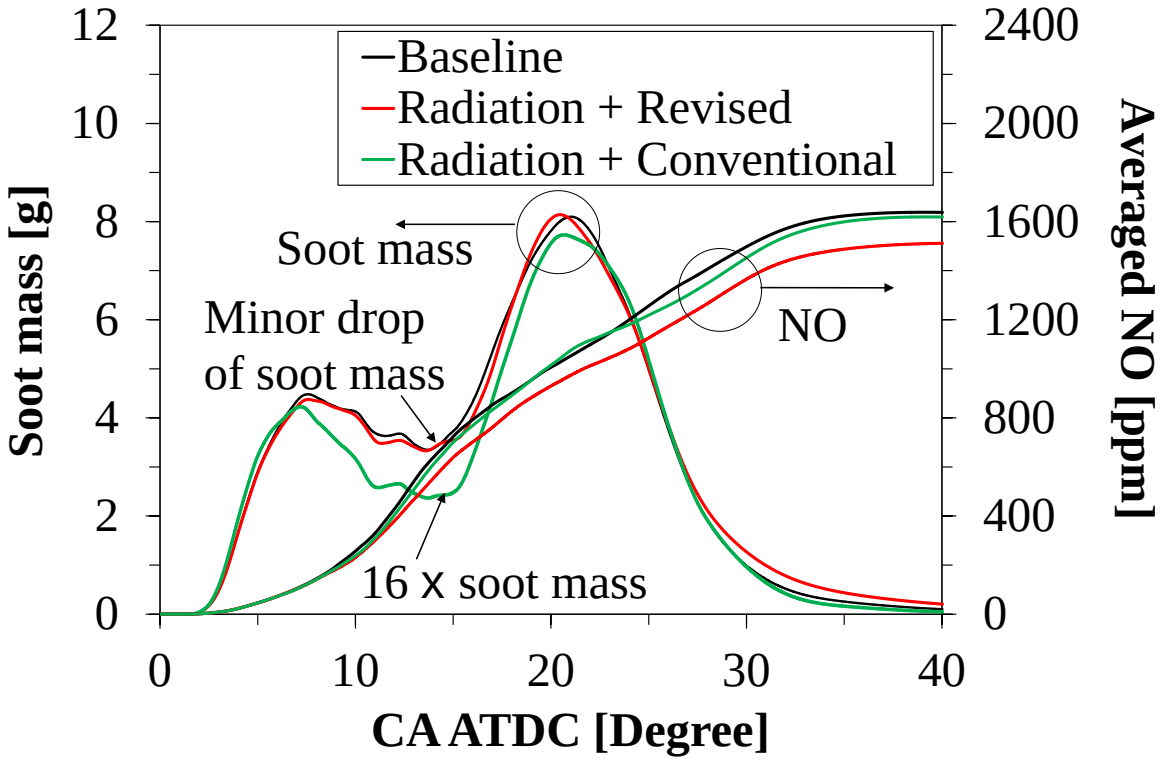
- Liff-off length in marine diesel engine case is much lower
- The local equivalence ratio and soot volume fraction are much higher

OH and soot distributions



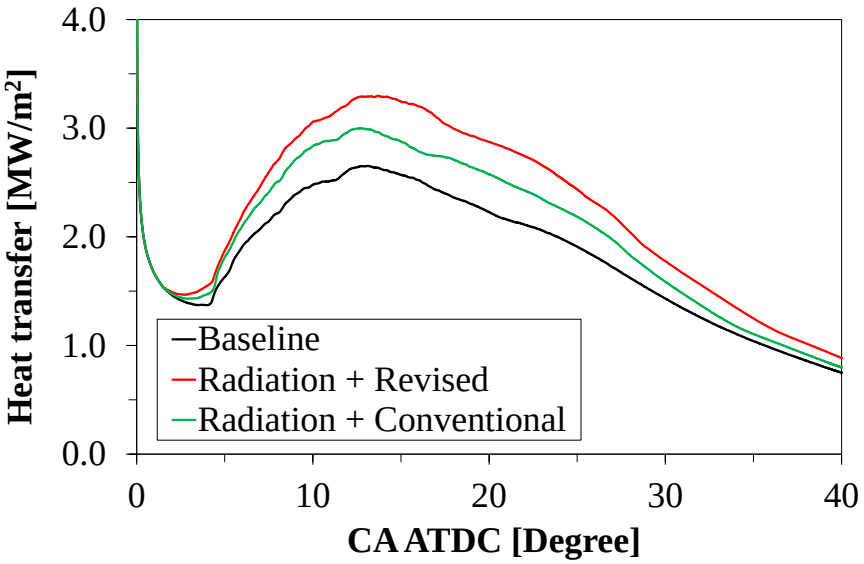
- Flame impingement starts at approximately 12 CAD ATDC

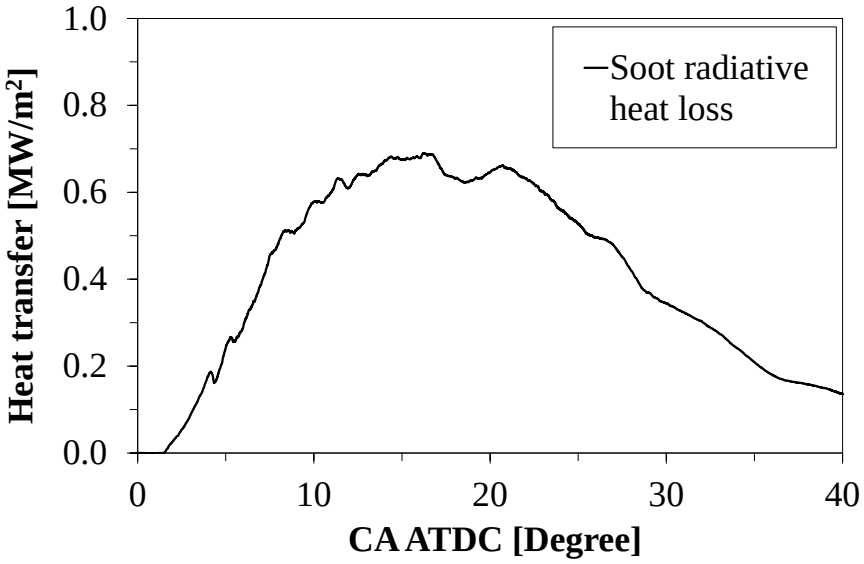
Pollutant formation



- Soot radiation does not influence the total soot mass significantly
- The NO_x level is 7.7% lower when soot radiation is considered

Heat transfer





- 30% higher when soot radiative heat loss is taken into consideration
- Sensitivity studies on Planck mean absorption expression, C_0

Conclusions

- A new skeletal diesel surrogate model is developed for combustion and soot modelling
- In-cylinder phenomena in a two-stroke, uniflow-scavenged marine engine are studied
- The averaged NO concentration is 7.7% lower as soot radiation is considered
- Special attention has to be given in the simulation of in-cylinder, peak soot concentration for different SOI or load
- The model can be integrated with SO_x chemistry to investigate the SO_x and H_2SO_4 formation in marine engine

Numerical tools (for MAN Diesel & Turbo SE)

- Soot library
  - OpenFOAM 2.0.x
  - OpenFOAM 2.3.x

- Chemical kinetic mechanism
  - Skeletal n-heptane mechanism
  - Multicomponent diesel surrogate model

- STARCCM combustion engine model

Thank you

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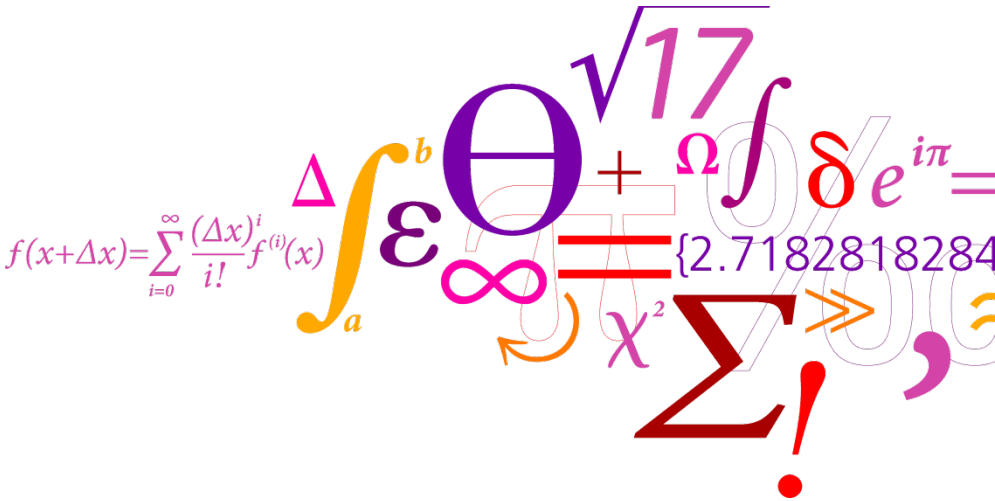

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