Numerical Study on the Combustion and Emission Characteristics of Different Biodiesel Fuel Feedstocks and Blends Using OpenFOAM

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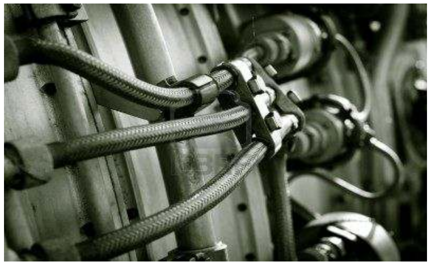
Harun **M. Ismail**[1], Xinwei **Cheng**[1], Hoon Kiat **Ng**[1], Suyin **Gan**[1] and Tommaso **Lucchini**[2]

[1] *Department of Mechanical, Materials and Manufacturing Engineering*
University of Nottingham (Malaysia Campus)

[2] *Dipartimento of Energia, Politecnico di Milano, Italy*



Meeting on Internal Combustion Engine Simulations Using OpenFOAM, Milan, Italy , 2011

Motivation

- Both conventional petroleum industry and bio-fuel industry (Palm Oil) is a multi-million dollar business in Malaysia (biggest Palm Oil exporter in the world)
- Limited petroleum resources and increasing emission standards
- Bio-fuels still at its infancy stage, the development of theories to understand its combustion and emission nature is not widely available

Objectives of this work

- Development and applications fuel thermo-physical and transport properties of Coconut (CME), Palm (PME) and Soy methyl-esters (SME) for in-cylinder (IC) spray combustion CFD modelling
- Development and applications of generic reduced combustions kinetics suitable for CME, PME and SME for CFD , IC engine applications
- Analyse the influence and relation between fuel properties and fuel spray structures for different biodiesel/diesel blend levels (B0 – B100) and fuel type
- Investigate combustion and emission characteristics for different blend levels and fuel type (CME, PME and SME)

Biodiesel Thermo-physical & Transport Properties

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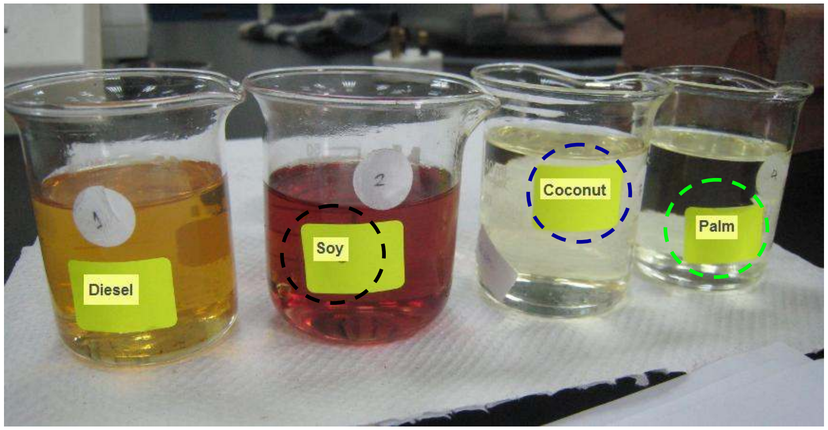
- Properties calculated using "Group contribution method"
- Evaluation of fuel thermo-physical properties & transport properties up to the critical temperature of a respected fuel

Type of Fatty-acids	Chemical Formula	Soy %	Palm %	Coconut %
Saturated	$C_{12}H_{26}O_2$	-	-	48
Saturated	$C_{15}H_{30}O_2$	-	-	17
Saturated	$C_{11}H_{22}O_2$	-	-	9
Saturated	$C_{17}H_{34}O_2$	18	42	8
Saturated	$C_{19}H_{38}O_2$	7	5	-
Unsaturated	$C_{19}H_{36}O_2$	10	41	18
Unsaturated	$C_{19}H_{34}O_2$	60	10	-
Unsaturated	$C_{19}H_{32}O_2$	10	2	-

Bio-fuel components

- Based on information compiled from open literature and lab fuel test
- Five largest contributing components of ME are identified for properties computation

Property	CME	PME	SME
Critical Temperature (K)	773.5	789.2	721.2
Critical Pressure (bar)	14.0	13.0	15.3
Critical Volume (ml/mole)	1064.0	1084.0	885.0



Biodiesel Thermo-physical & Transport Properties

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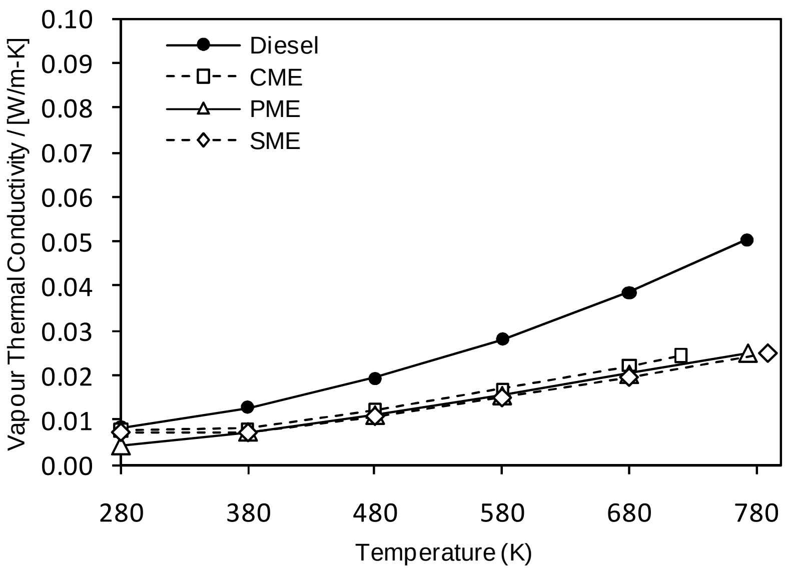
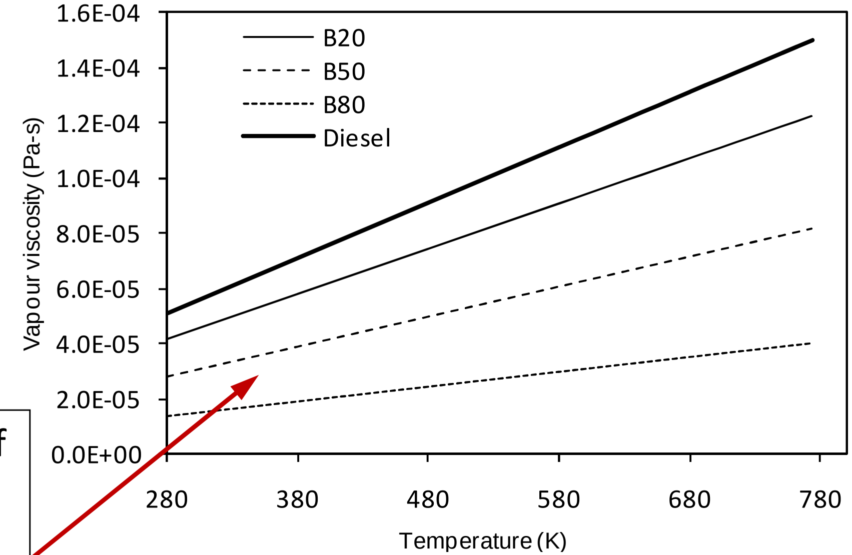
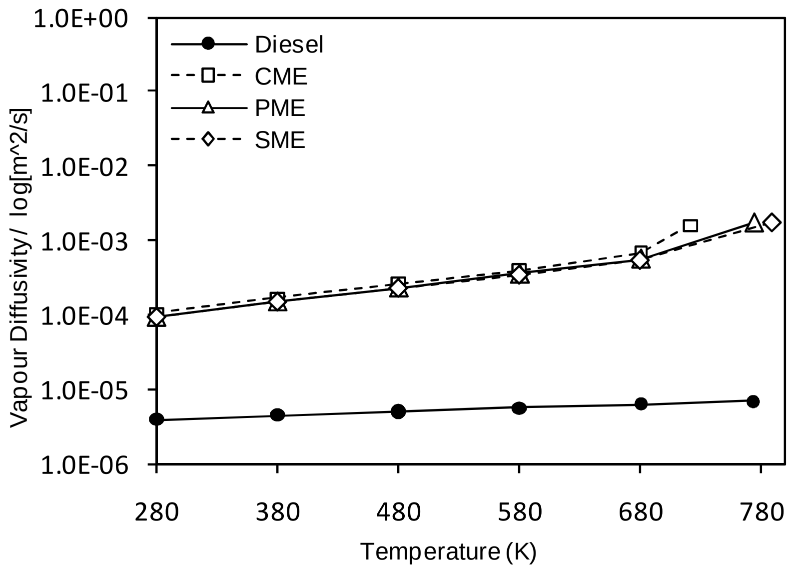
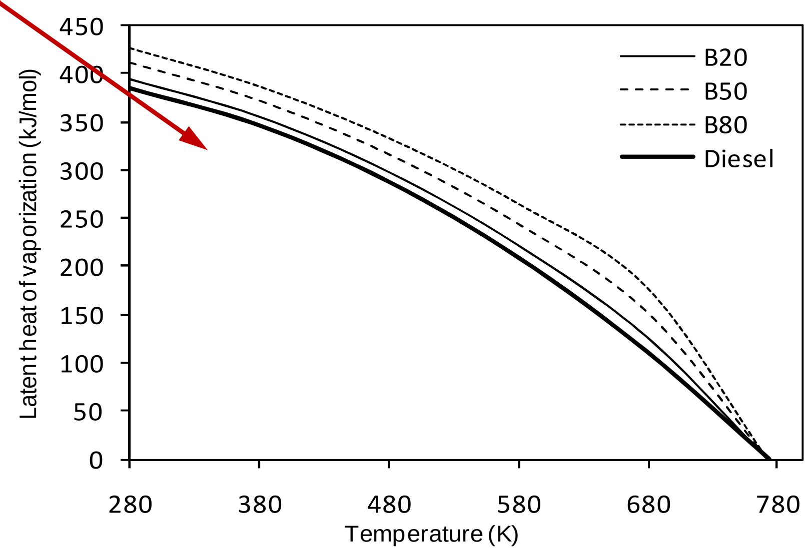




Some examples of the PME blends (B0 –B100) as compared to diesel for illustration





Biodiesel Thermo-physical & Transport Properties Implementations in OpenFOAM

```
        //- Construct null
        PME2()

            TValues_(6, 0.0),
                  dataValues_(6, 0.0),
                  rho_
                  (
                        "rho",
                        "Temperature",
                        "density",
                        (TValues_),
                        (dataValues_)
                  ),

{

                  scalarField& rhoX = rho_.x();

                  rhoX[0] = 280;
                  rhoX[1] = 380;
                  rhoX[2] = 480;
                  rhoX[3] = 580;
                  rhoX[4] = 680;
                  rhoX[5] = 780;

                  scalarField& rhoY = rho_.y();

                  rhoY[0] = 887.95;
                  rhoY[1] = 750.33;
                  rhoY[2] = 618.03;
                  rhoY[3] = 488.81;
                  rhoY[4] = 355.08;
                  rhoY[5] = 134.91;
```

- **Snippets of properties implemented in OpenFOAM fuel library**

Interpolate function were utilised to estimate fuel properties at different temperatures

Experimental Setup (Nottingham Research Engine)

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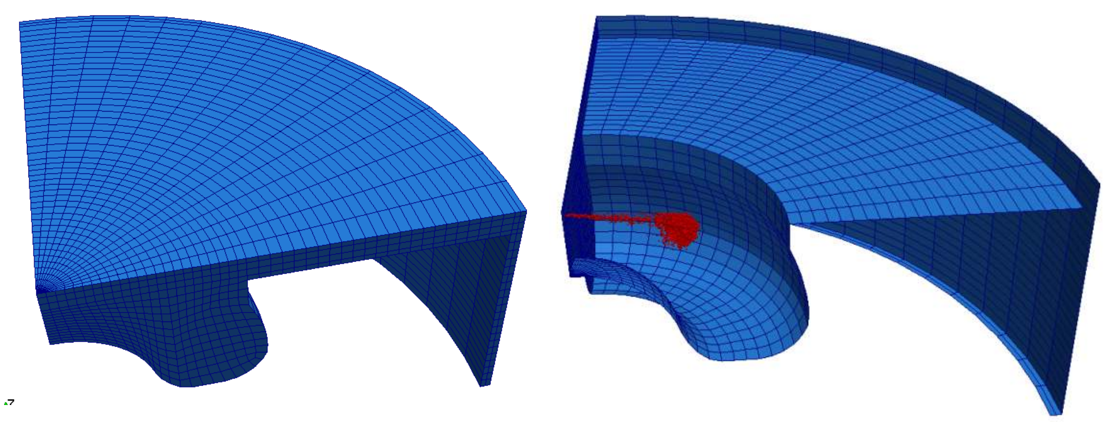
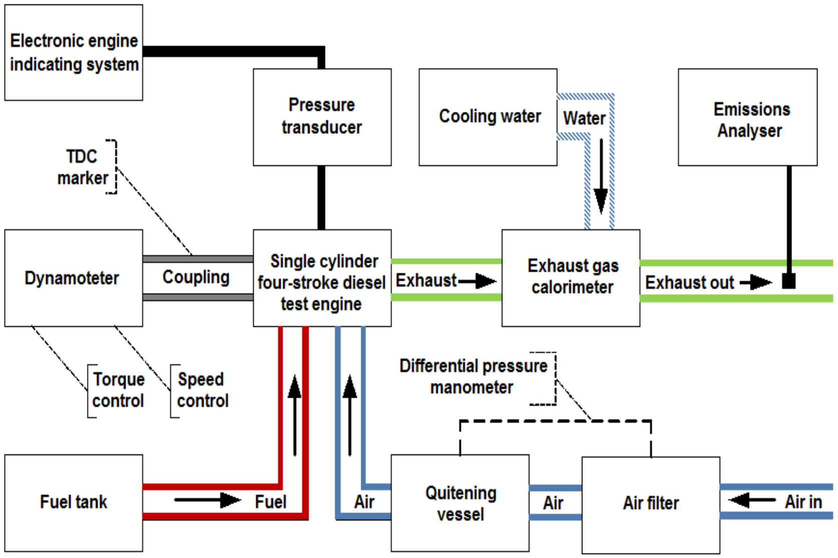
Nottingham Research Engine Specifications	
Engine Type	Light-Duty Diesel
Piston Type	Bowl-in-piston
Displacement Volume per-cylinder	$347 cm^3$
Compression Ratio	19 : 1
Stroke	69 mm
Bore	80 mm
Connecting Rod Length	114.5 mm
Intake Valve Closing (IVC)	-140^o ATDC
Exhaust Valve Opening (EVO)	140^o ATDC
Engine Speed	1500 – 3500 rev/min

- Experimental engine consists of 4-hole injector at 90^o apart
- A 90^o 3D-model of the combustion chamber is generated
- The mesh set with 1 injector hole at 45^o from X and Y axis.
- Dynamic mesh with cell size of 1mm



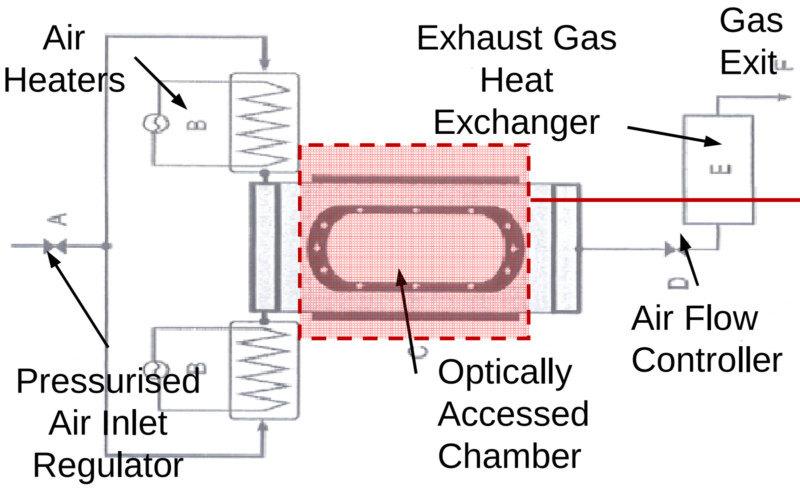
EXPERIMENT SETUP



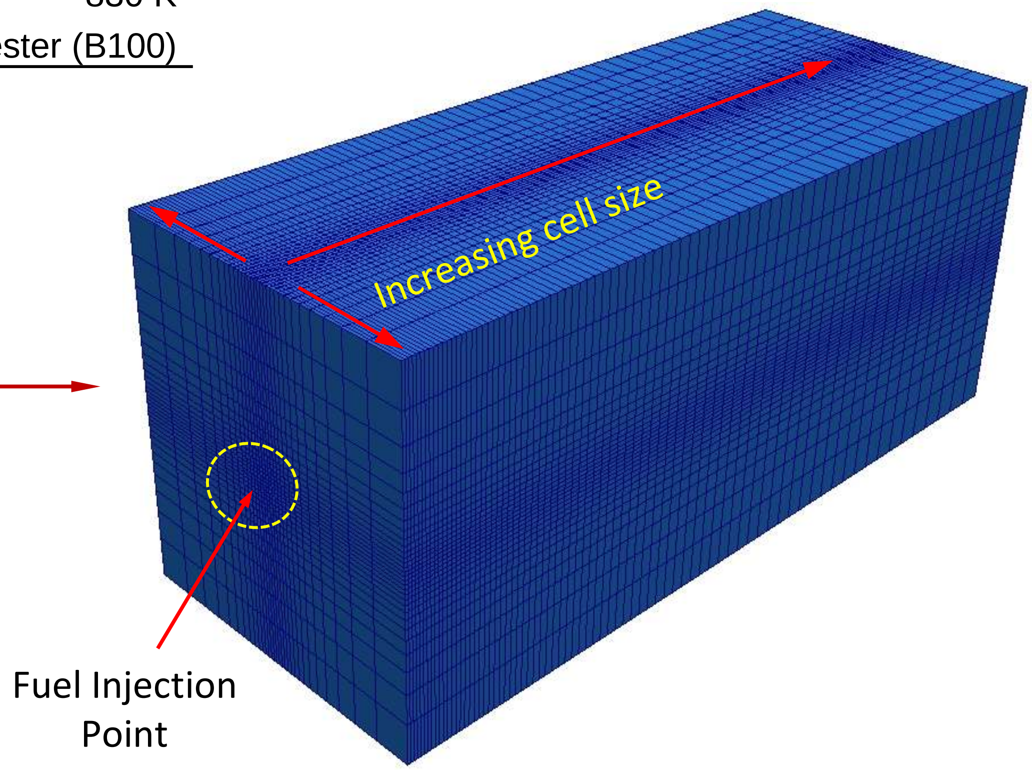
Experimental Setup (Chalmers HP/HT Rig)

Chalmers High Pressure/High Temperature Rig	
Type	Constant Volume
Volume	2.0 l
Injection Period	3.5 ms
Injection Pressure	1200 bar
Fuel Temperature	313.15 K
Chamber Pressure (constant)	50 bar
Chamber Initial Temperature	830 K
Fuel of Interest	Diesel(B0), Palm methyl-ester (B100)

- Cell size increased from 0.25 to 2 mm
- Chamber size fit to (60 x 60 x 150) mm
- Chamber air density maintained to match experimental condition at 20.89 kg/m^3



Raul *et al.* (SAE 2008-01-1393)



Utilised OpenFOAM ICE-Lib (Polimi) Models

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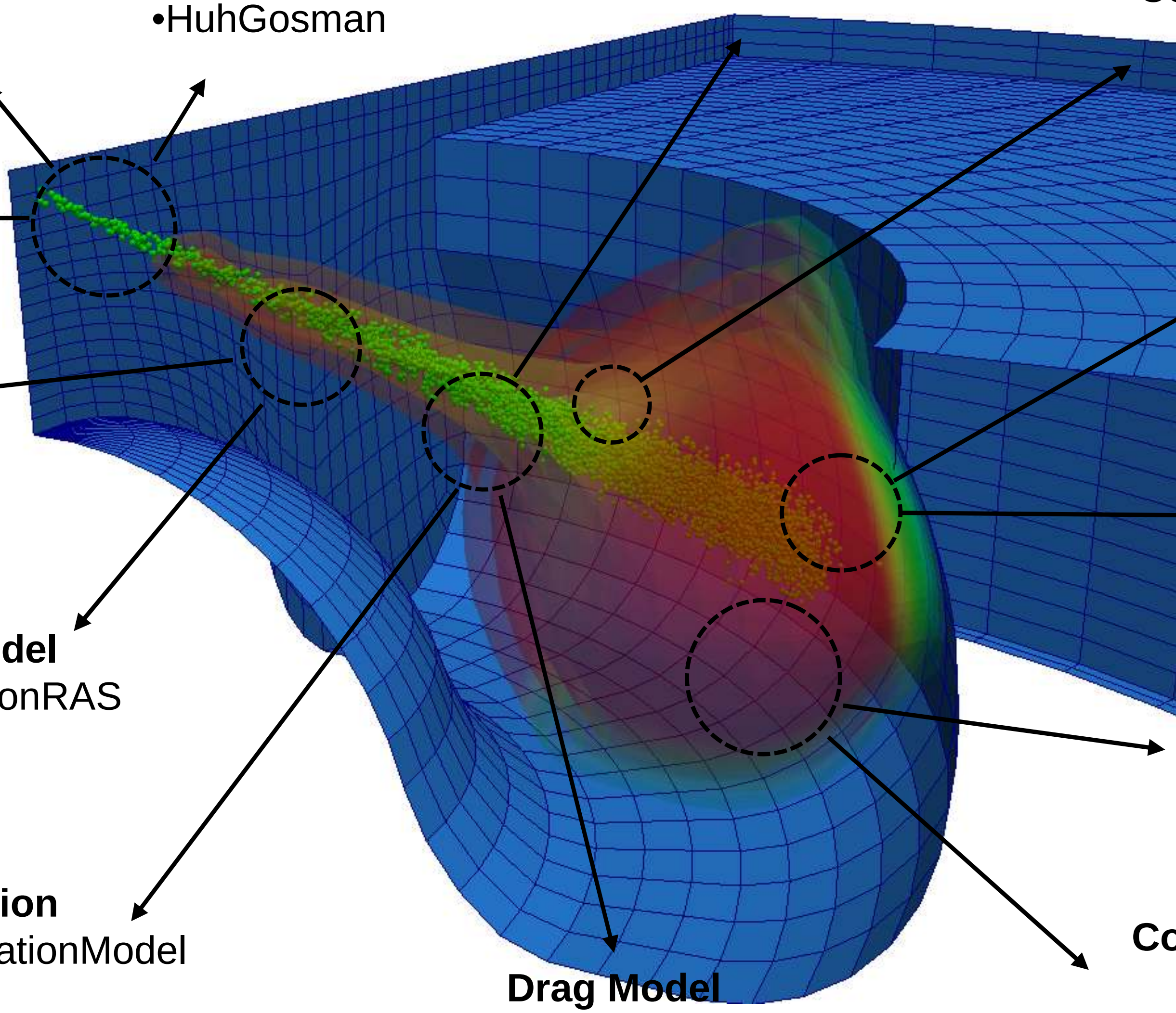

Validations of Fuel Thermo-physical & Transport Properties Using OpenFOAM

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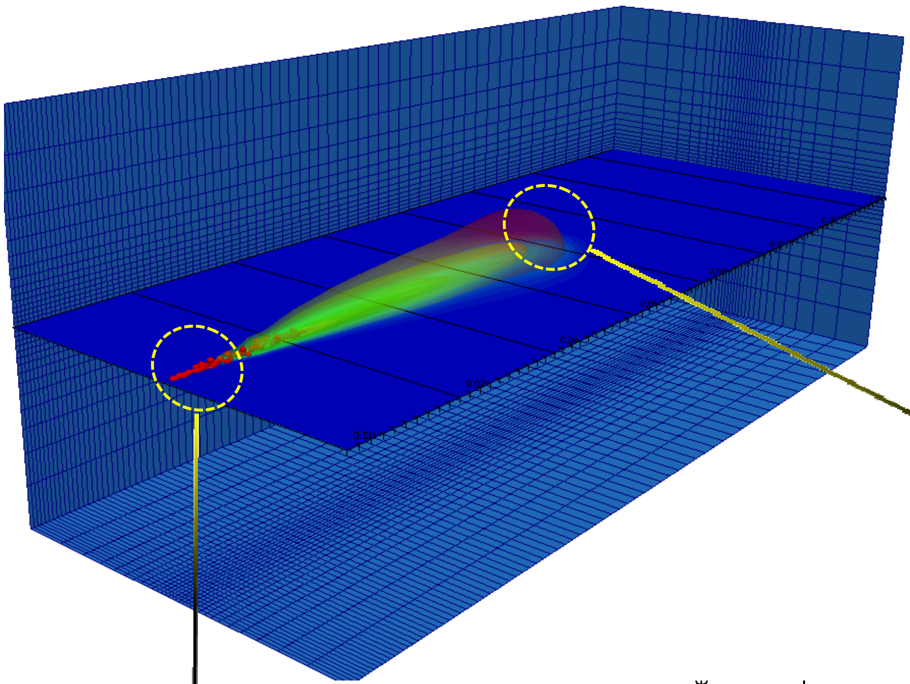
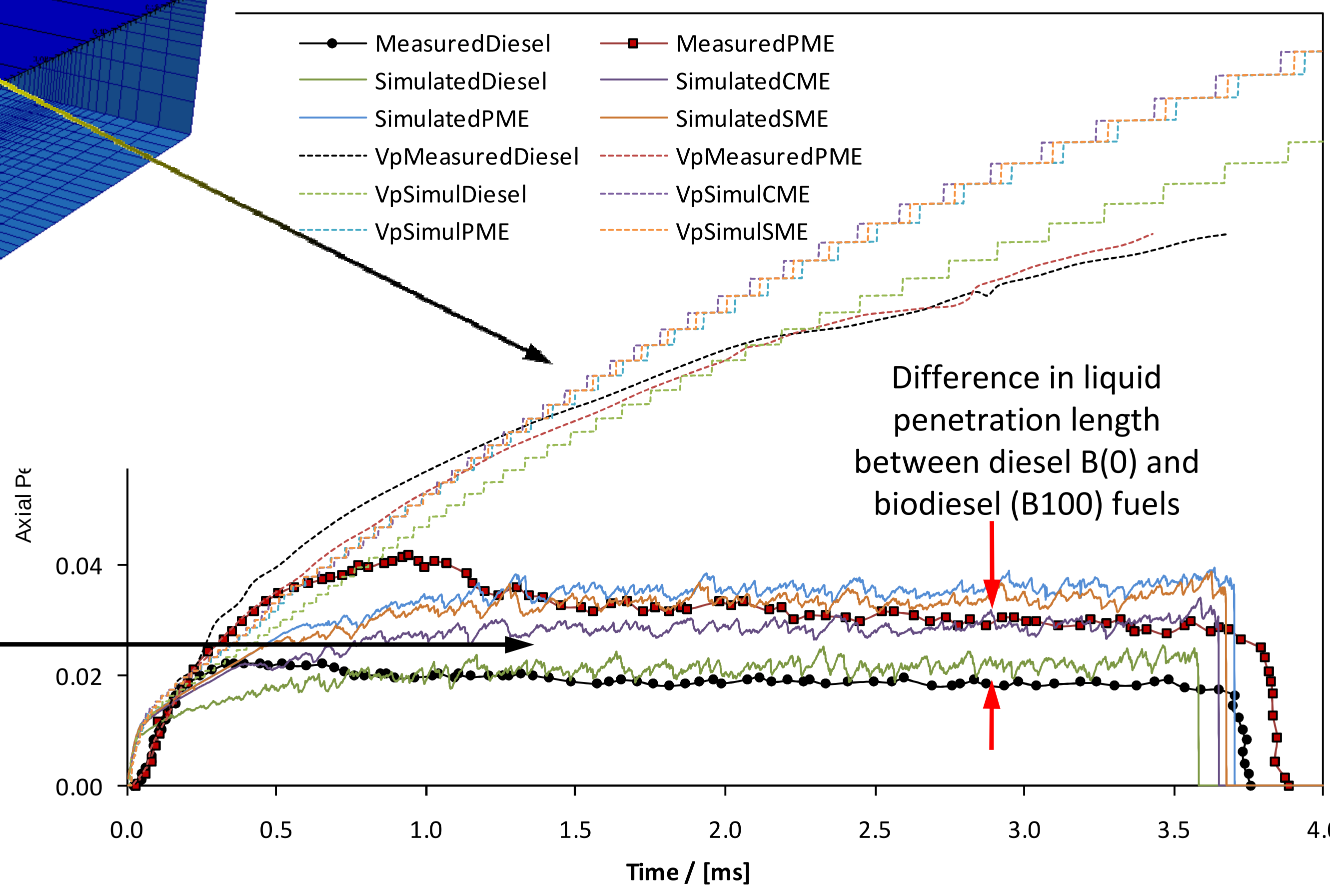
- The simulated spray structure matches with experimental data with good accuracy
- Fuel spray structure could be simulated using the developed fuel properties





The thermo-physical and transport properties validated against experimental liquid & vapour **axial penetration length**

Validations of Fuel Thermo-physical & Transport Properties Using OpenFOAM

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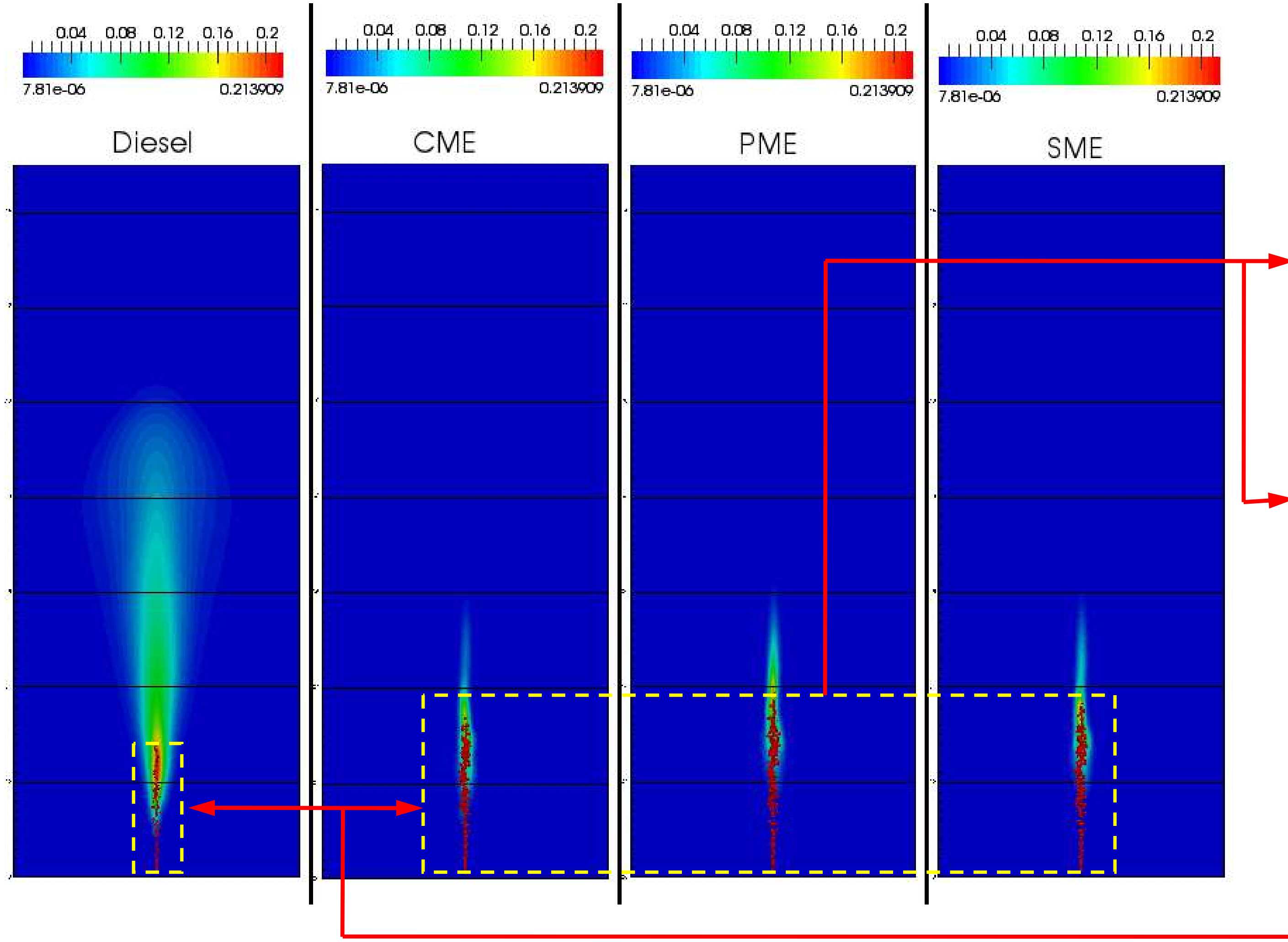
➢ Illustration of the four fuel species distribution contour plot



Biodiesel fuel tends to have SIMILAR spray and evaporation structure, but NOT SAME

The dissimilarities can be clearly seen in fuel evaporation simulation without combustion

Biodiesels (B100) have longer spray penetration length due to higher viscosity and surface tension

Effects of Fuel Thermo-physical & Transport Properties (Fuel Type Comparison)

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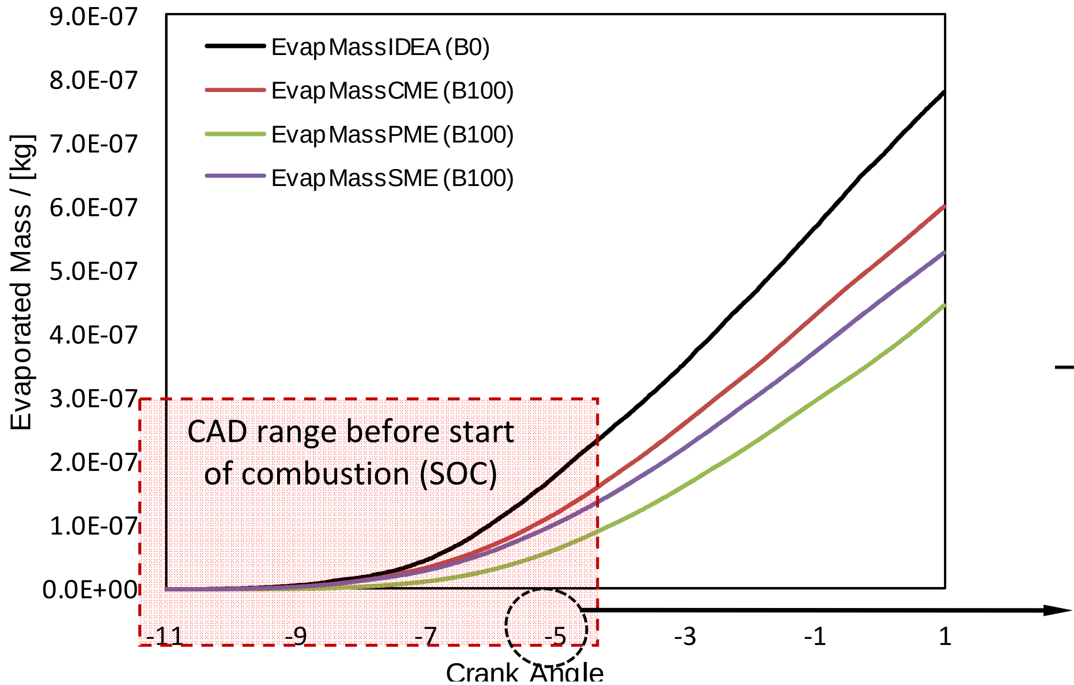

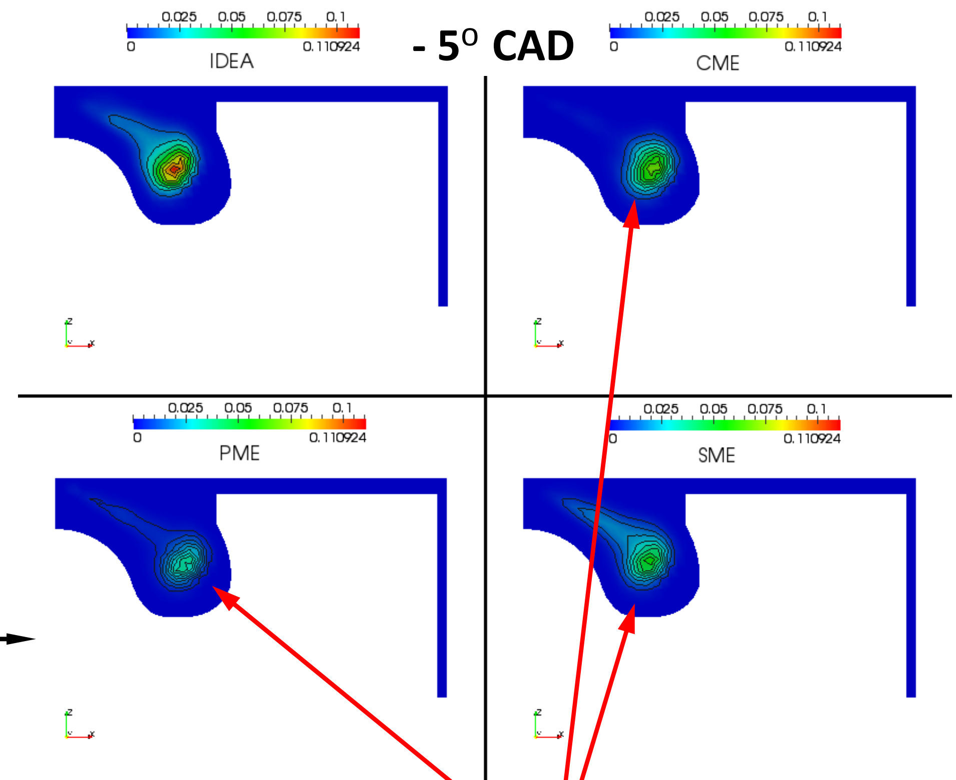

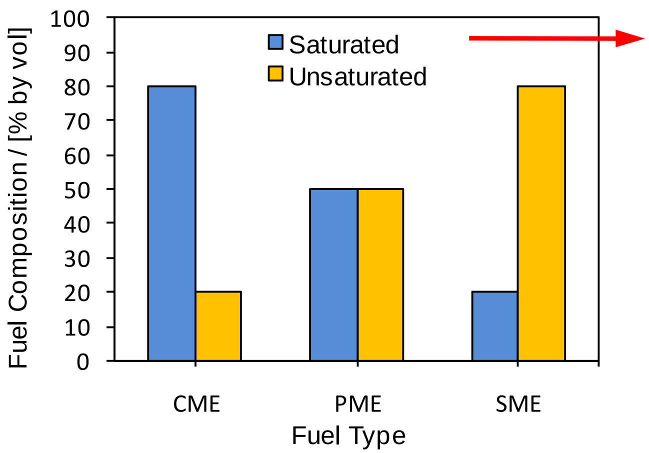

% of Unsaturation

SME > PME > CME

% of individual composition that makes up SME and PME

Rate of Evaporation:

Diesel (IDEA) > CME > **SME > PME**

Mass of fuel injected equal for all fuel

Effects of Fuel Thermo-physical & Transport Properties (Fuel Type Comparison)

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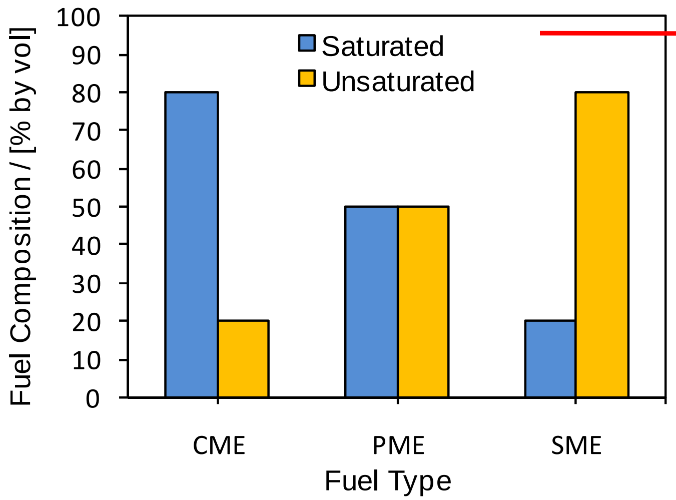
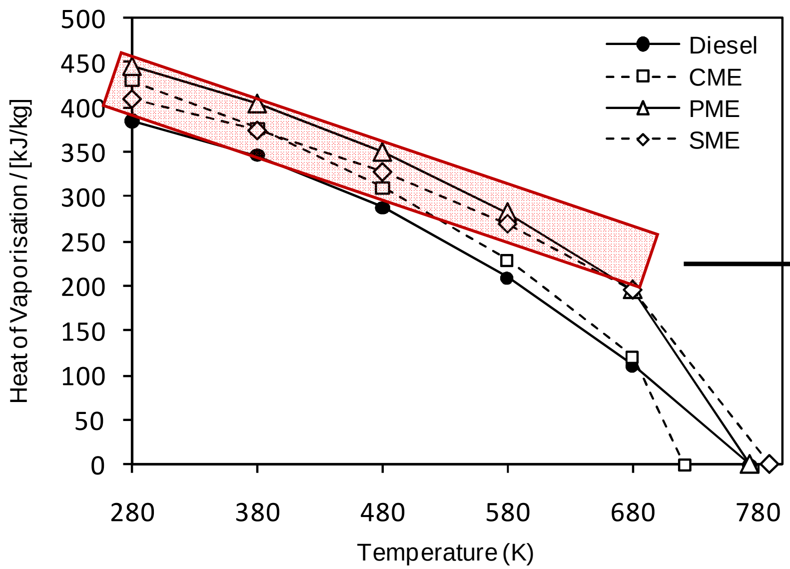


% of Unsaturation
SME > PME > CME

Rate of Evaporation:
Diesel (IDEA) > CME > **SME > PME**
Mass of fuel injected equal for all fuel

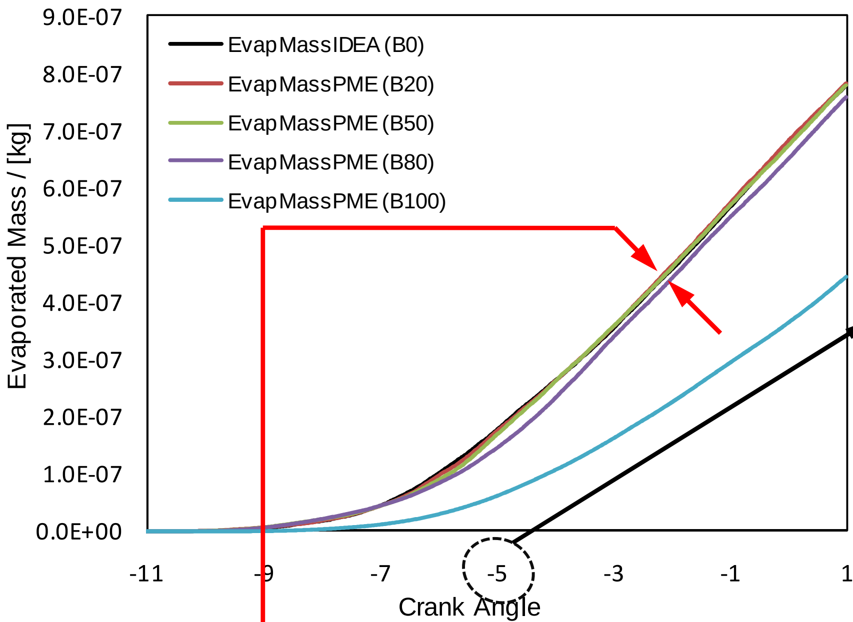
Suggests the importance of % individual composition that makes up SME and PME

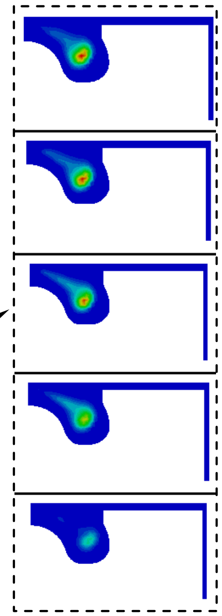
SME can be evaporated significantly faster

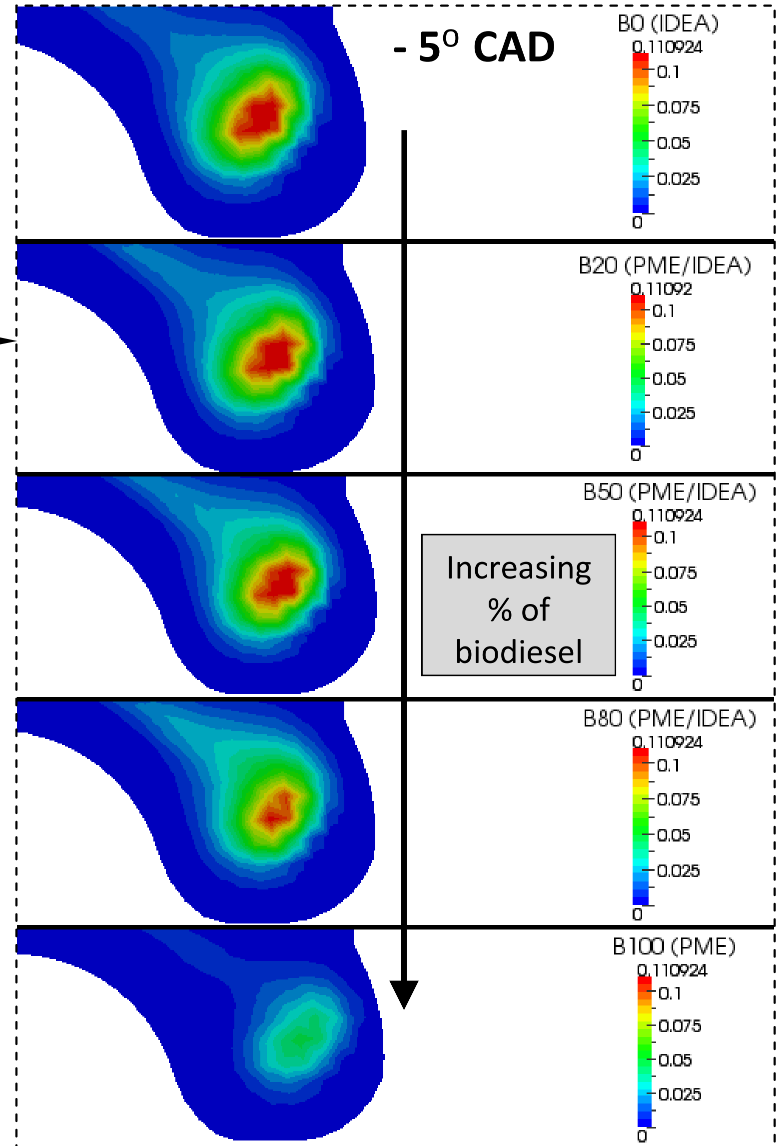


Heat of Vaporisation:
From T = 280 – 650 K
SME < PME

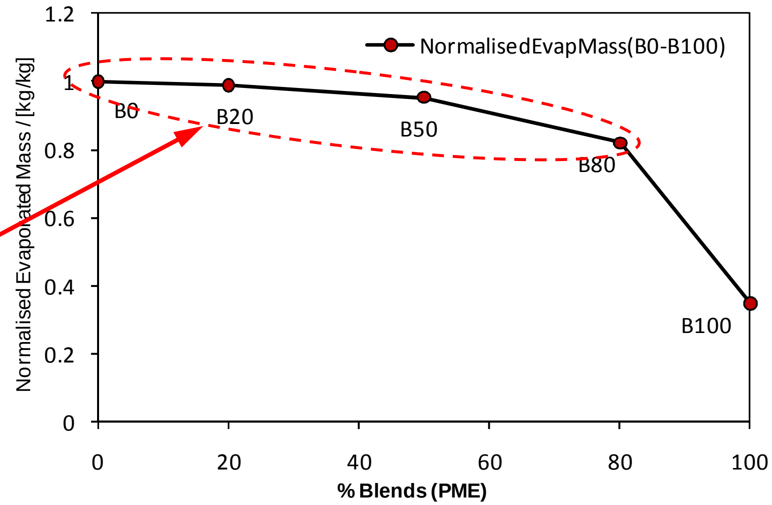
Effects of Fuel Thermo-physical & Transport Properties (Palm B0-B100)







Suggests the strong influence of IDEA fuel (Diesel) up to 80% biodiesel mixture (B80)



Development & Applications of Generic Reduced Biodiesel Fuel Surrogate Combustion Kinetics

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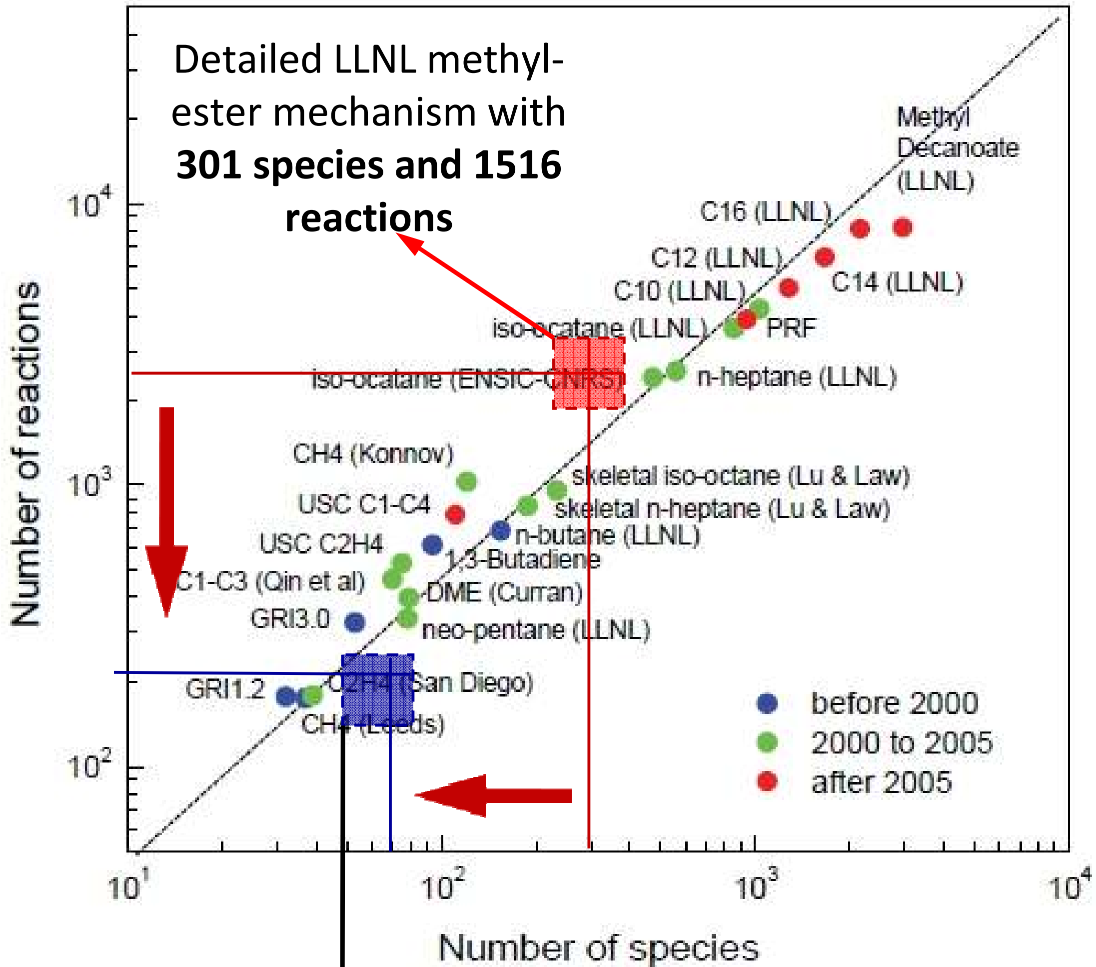
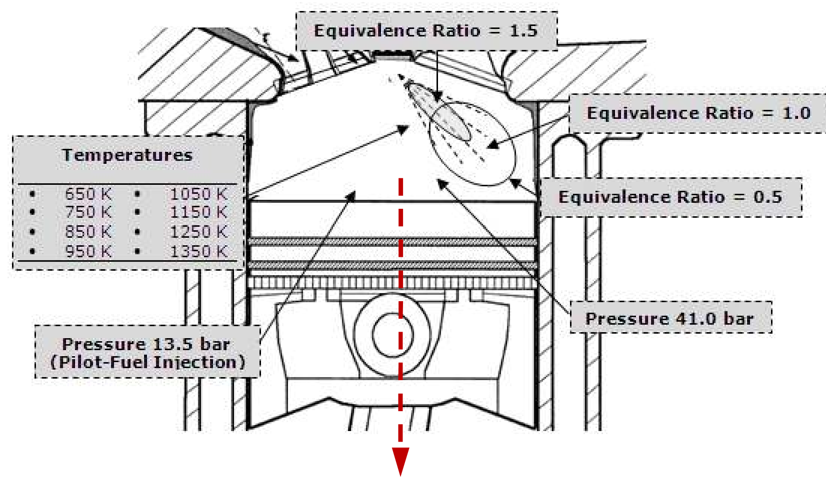


Adapted from C.K Law et al. [AIAA 2008-969]

Reduced mechanism **77 species 212 reactions**

Motivation

- Computational resources (time & cost)
- Lack of widely available biodiesel mechanism validated for Palm, Coconut and Soy methyl-esters
- To investigate the combustion and emission characteristics of Palm, Soy and Coconut biodiesel fuels.



- Reduced and validated for 48 shock-tube conditions (STC) during entire mechanism reduction process with comparison the detailed mechanism

0-D (PSR) Validations of Generic Reduced Biodiesel Fuel Surrogate Combustion Kinetics

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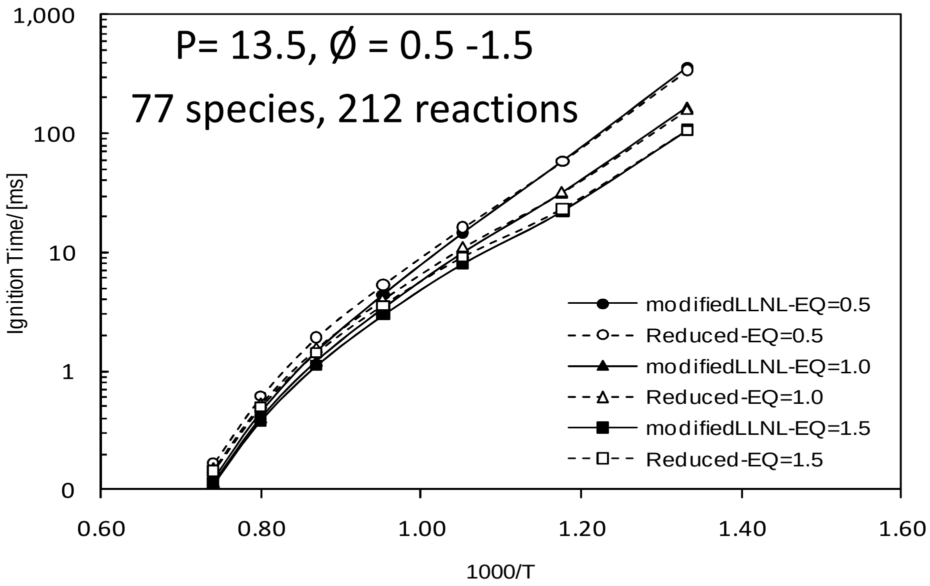

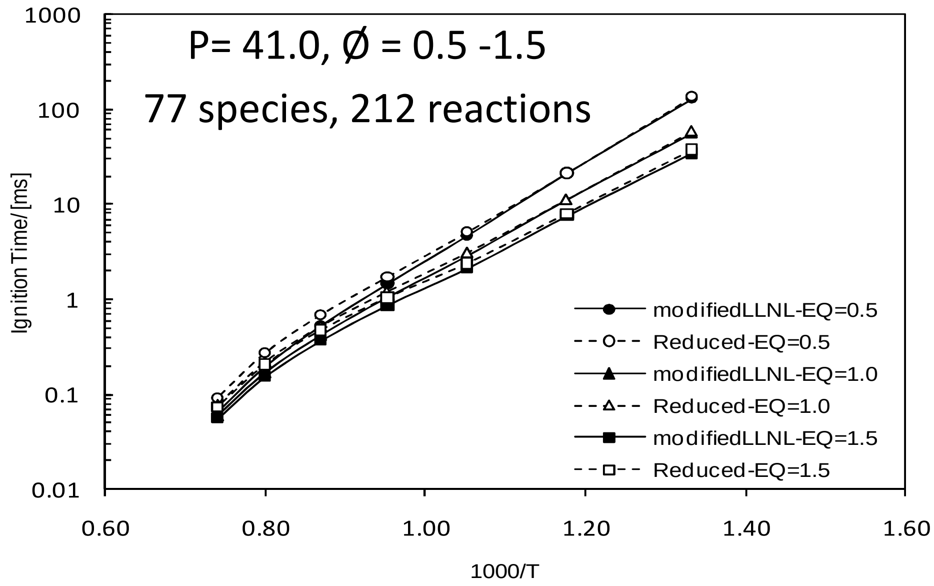

Gas Phase (PSR) Validations at 48-STC

- Error in ID less than 13 % during 0-D reductions process as compared to LLNL mechanism
- Combine with modified skeletal n-heptane mechanism to match energy content and C/H/O ratio
- ID shown here based on Nottingham Research Engine calibrations

3-D CFD Validations of Reduced Biodiesel Fuel Surrogate Combustion Kinetics Using OpenFOAM

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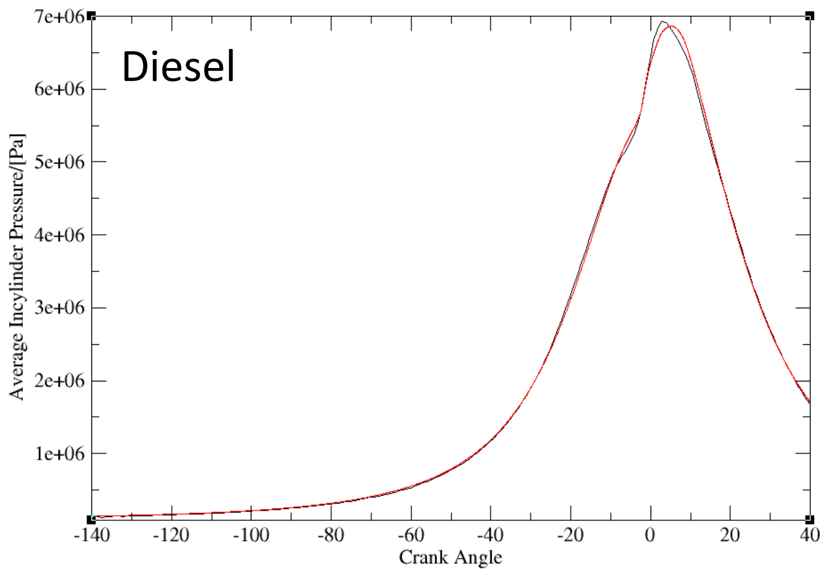
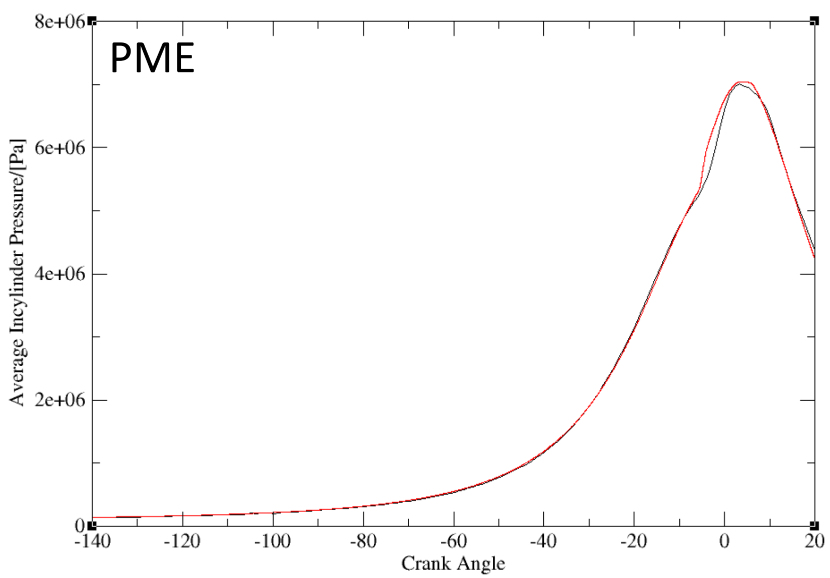
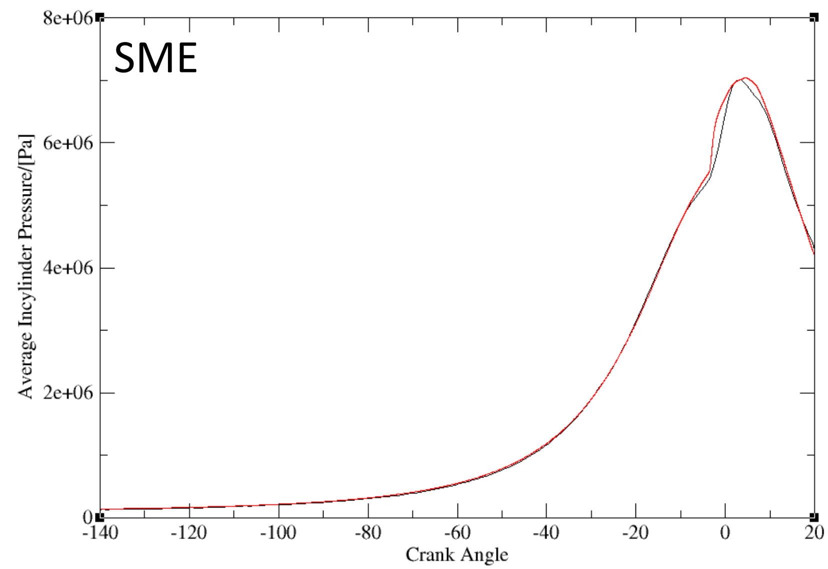


- Pressure trace comparison for engine conditions at 2000 rpm and power 1.5kW
- The simulated spray combustion matches with experimental data with good accuracy
- Future test will be conducted on constant fuel mass and constant ID to study the combustion an emission characteristics for CME, PME and SME



Legend
Measured
Simulatied



Combustion and Emission Characteristics of Palm, Soy and Coconut (B100) Biodiesel Fuels

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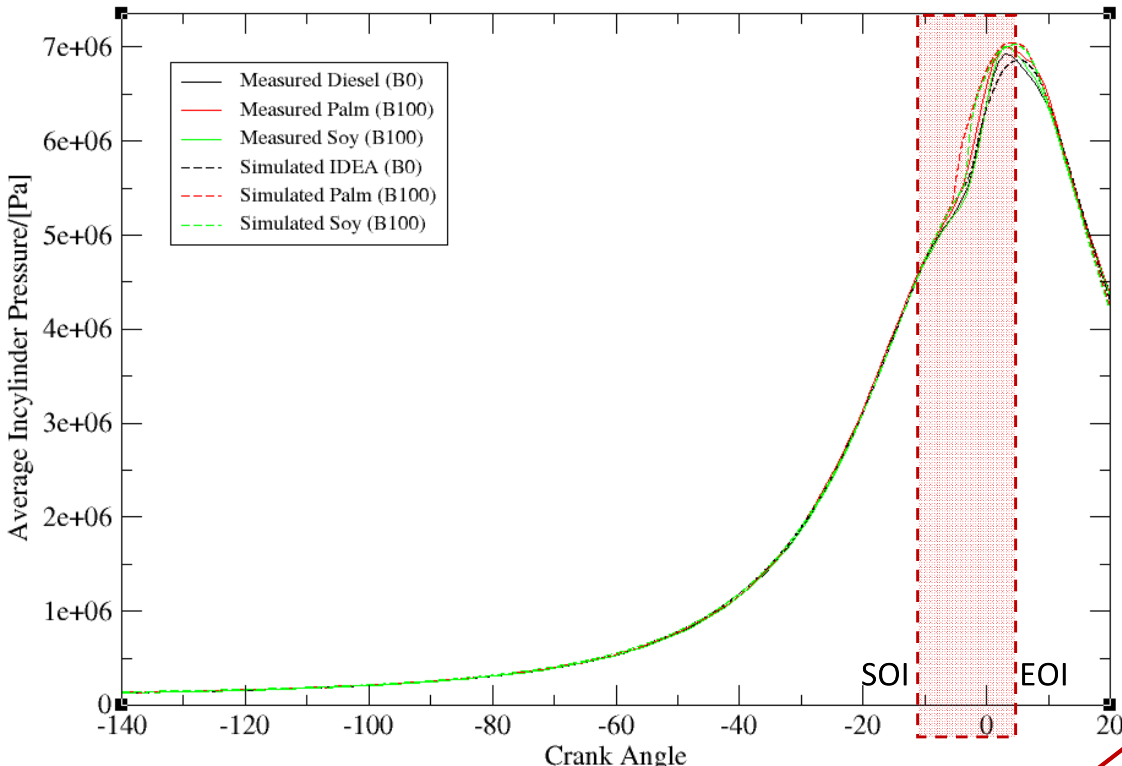
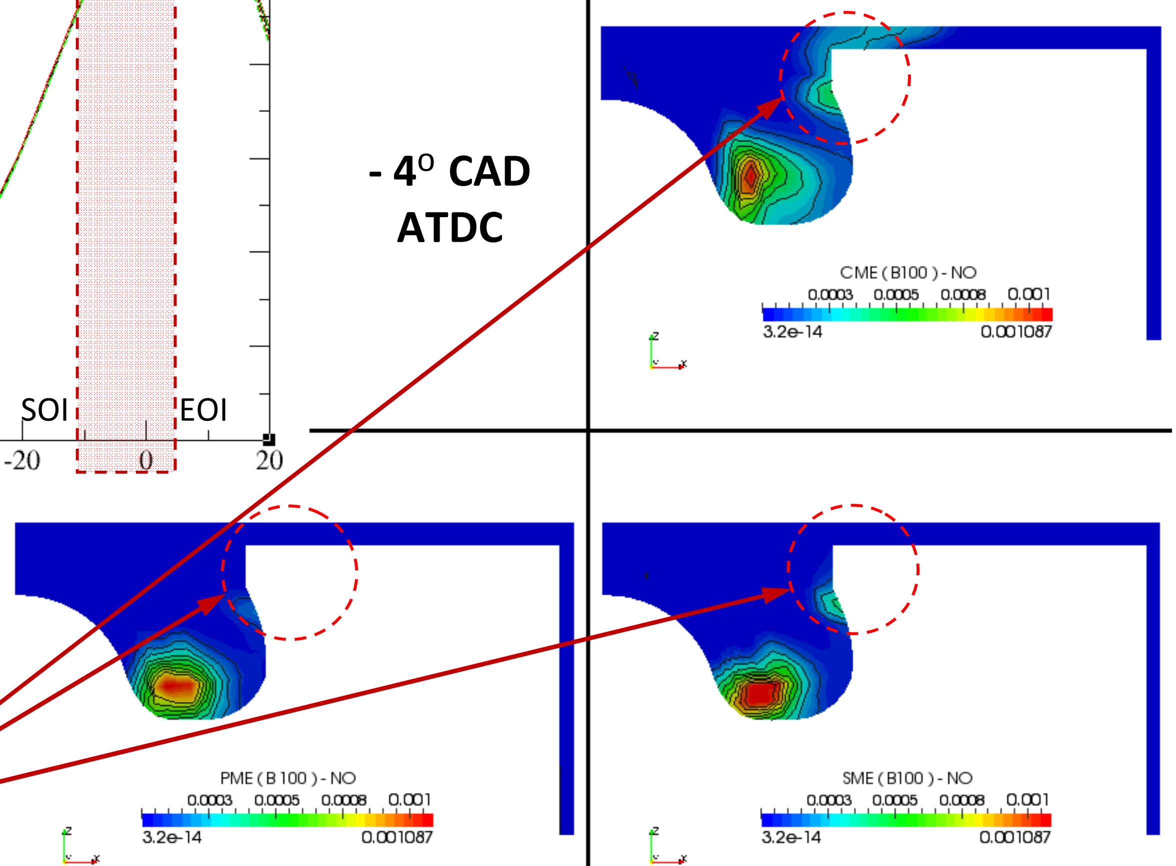


- NO plot for engine conditions at 2000rpm and 1.5 kW of power.
- Start of injection (SOI) and end of injection (EOI) for all cases are the same



Change in fuel type leads to change in NO distributions

Combustion and Emission Characteristics of Palm, Soy and Coconut (B100) Biodiesel Fuels

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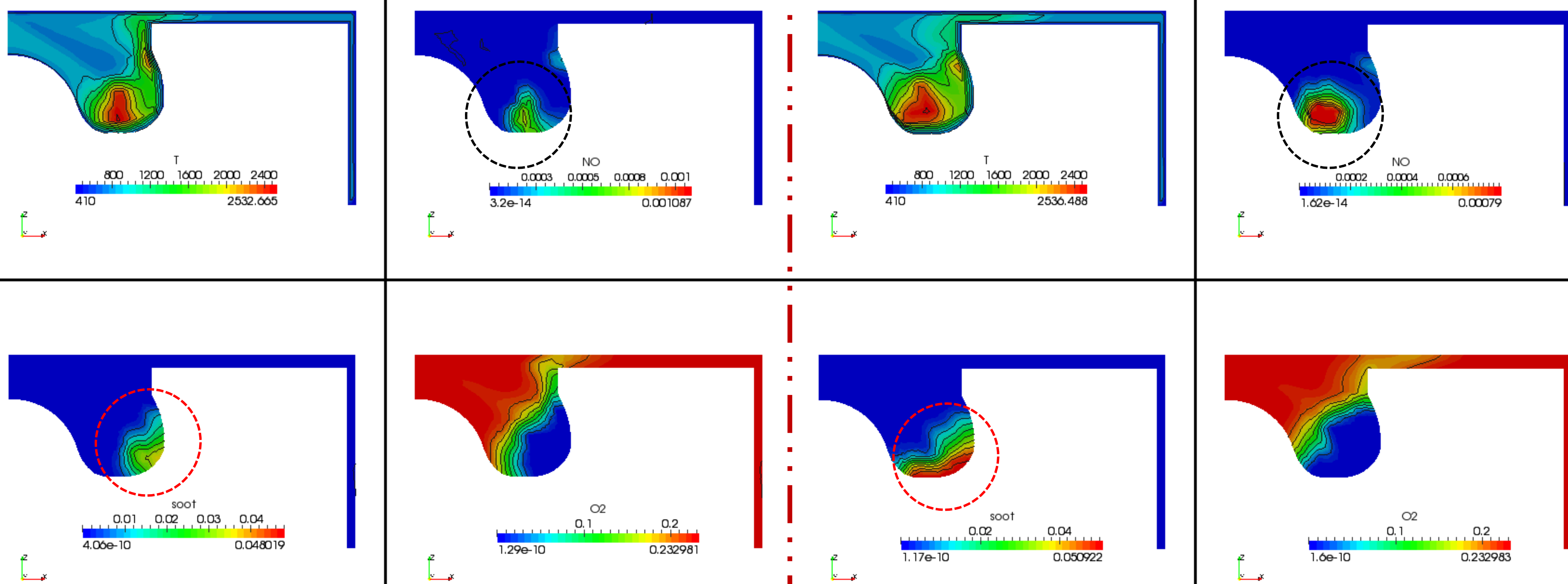
SME **- 4^{o} CAD ATDC** **PME**



NO mass fraction at -4^{o} CAD ATDC
SME > PME

Soot mass fraction at -4^{o} CAD ATDC
SME > PME

- Similar to trend observed in experimental studies
- Three possibilities for the observed trend :
- ✓ Mass of fuel injected (SME > PME)
- ✓ Ignition Delay (SME > PME)
- ✓ Level of usaturation in the fuel (SME > PME)

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Conclusions

- Main objectives of development and implementations of biodiesel fuel properties and combustion kinetics were achieved
- As for preliminary validations, good level of agreement was achieved between computed and measured data for both fuel properties and combustion kinetics
- Effects of fuel properties and chemical kinetics could be isolated using CFD studies to better understand the combustion and emission characteristics of biodiesel fuel in CI engines

Acknowledgments

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THANK YOU

Contact email: harun.ismail@nottingham.edu.my

Internal Combustion Engine Group
Energy, Fuel and Power Technology Research Division
Department of Mechanical, Materials and Manufacturing Engineering
University of Nottingham (Malaysia Campus)