**Keywords: CFD, Simulation, Combustion, Methanol, Dual Fuel**

# Development of dual fuel methanol engine using CFD techniques for PFI and HPDI injection strategies

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## Abstract

The shipping industry plays a significant role in the global economy, responsible for 90% of world commerce. Moreover, it also accounts for 2 to 3% of global $CO_2$ emissions. There is increasing pressure on the marine sector to reduce its carbon footprint, and the net $CO_2$ emissions should reach zero by the end of 2050. The usage of carbon-free fuels such as hydrogen and ammonia are under development and not fully mature yet. Methanol can be a carbon-neutral fuel when produced using green hydrogen and captured $CO_2$, thus bringing the net $CO_2$ emissions to zero. It can act as a transition fuel due to easy handling and existing infrastructure for bunkering. Since the ship engines are in operation for up to 40 years, $CO_2$ neutrality should be achieved for the existing engines in the fleet, as replacing old engines with new ones is uneconomical. Therefore, the retrofit solutions can be an effective and economical way to reduce the net GHG emissions of the maritime industry. Furthermore, when it comes to new engine concepts fueled with methanol, their performance is of utmost importance.

MAN-ES has been working on the development of dual-fuel methanol engines for retrofit solutions and newbuilds. The retrofit solution for the existing engine is achieved by incorporating minor modifications in the intake port and other engine components. The methanol injectors are installed in the intake port, called port fuel injection (PFI), operated at low injection pressure. This reduces not only GHG emissions but also costs for customer. Another approach to bring the methanol into cylinder is the high-pressure direct injection (HPDI) technique, in which methanol is burned in diffusion combustion manner. Pilot fuel is used for igniting methanol in both port fuel and direct injection conditions.

CFD technique can be employed to evaluate the preliminary design of injector and cylinder components and their influence on mixture formation and combustion for PFI and HPDI conditions. Since it is used for the design analysis, it is vital to validate the CFD simulation method. Two experimental configurations are considered for validation, and the results obtained are presented in this paper. The first set of HPDI measurements was conducted at TUM using a Rapid Compression and Expansion Machine (RCEM), and the second at WTZ using PFI methanol injection on a 32/44DF single-cylinder engine (SCE).

The first part presents the CFD simulation results of the RCEM for spray characteristics and methanol combustion. The high-pressure methanol injection is modeled using Huh and Reitz-Diwakar breakup model: The predicted spray angle, penetration length, and shape are compared against experimental data. Two modeling approaches, Extended Coherent Flamelet Model (EFCM) and detailed chemistry were investigated for simulating diesel-ignited methanol combustion. The results of the combustion process are in good agreement with the RCEM experimental data for the variation of methanol injection timing and the interaction angle between the methanol and diesel spray.

In the second part of the paper, the simulation results of the SCE engine for PFI methanol injection are presented for the variation of engine load and air/fuel ratio. The CFD results gave insights into methanol evaporation in the intake port, and mixture formation in the cylinder, which is vital for combustion stability and emissions. The simulation methods for HPDI and PFI methanol combustion will be further employed to facilitate the development of MAN's methanol engines for reducing GHG emissions.

# 1. Introduction

The shipping industry plays a significant role in the global economy, responsible for 90% of world commerce. Moreover, it also accounts for 2 to 3% of global $CO_2$ emissions. There is increasing pressure on the marine sector to reduce its carbon footprint, and the net $CO_2$ emissions should reach zero by the end of 2050 as enforced by the International Maritime Organisation (IMO). To achieve the future emission requirement, the ship engine manufacturers are focusing on using alternative fuels and drive concepts in the maritime sector. The usage of carbon-free fuels such as hydrogen and ammonia are under development and not fully mature yet. Methanol can be a carbon-neutral fuel when produced using green hydrogen and captured $CO_2$ or biomass, thus bringing the net $CO_2$ emissions to zero [1].

Methanol is considered as one of the most favourable alternative fuels due to its renewability, cost, and its combustion characteristics due to the presence of the hydroxyl group. As it has a single carbon atom, it cannot easily form particulate matter from long-chain hydrocarbons when compared to other alcohols. It has a high-octane rating and, thus has higher knock resistance and can be used at high compression ratios [2]. However, for CI engines, usage of methanol can be challenging due to its low Cetane number and latent heat of vaporization which is four times than that of diesel. Due to this high ignition temperature and being in liquid at standard temperature pressure (STP), methanol is safer to store, and transport. Considering all the mentioned properties of methanol, easy handling, and existing infrastructure for bunkering, it can act as a transition fuel before moving into carbon-free fuels in the future. Since the ship engines are in operation for up to 40 years, $CO_2$ neutrality should be achieved for the existing engines in the fleet, as replacing old engines with new ones is uneconomical. Therefore, the retrofit solutions can be an effective and economical way to reduce the net GHG emissions of the maritime industry. Furthermore, when it comes to new engine concepts fuelled with methanol, their performance is of utmost importance.

MAN Energy Solutions SE has been working on the development of carbon-free and carbon-neutral fuel engines, such as dual-fuel methanol/diesel engines for retrofit solutions and newbuilds [3]. Different fuel admission and combustion concepts were evaluated based on ease of retrofit, costs, time to market, and performance. PFI and HPDI injection strategies are considered for fuel injection that leads to premixed Otto-like and Diesel-like diffusion combustions respectively [4] [5]. The retrofit solution for the existing engine is achieved by incorporating minor modifications in the intake port and other engine components. The methanol injectors are installed in the intake port, called port fuel injection (PFI), operated at low injection pressure. This reduces not only GHG emissions but also costs for customers. Another approach to bringing the methanol into a cylinder is the high-pressure direct injection (HPDI) technique, in which methanol is burned in a diffusion combustion manner. Pilot fuel ignites methanol in both port fuel and direct injection conditions. The PFI technique will be implemented in MAN's 48/60 and 51/60 engine platforms and for the 21/30 genset engines. Moreover, the HPDI methanol injection method will be introduced in new builds and retrofit solutions to the newly developed 32/44 and 49/60 engine platforms [5].

CFD technique can be employed to evaluate the preliminary design of injector and cylinder components and their influence on mixture formation and combustion for PFI and HPDI conditions. Since it is used for the design analysis, it is vital to validate the CFD simulation method. Two experimental configurations are considered for validation, and the results obtained are presented in this paper. The first set of HPDI measurements was conducted at TUM using a Rapid Compression

and Expansion Machine (RCEM), and the second at WTZ using PFI methanol injection on a 32/44DF single-cylinder engine (SCE).

## 2. Experimental Setup and Data

### 2.1. Rapid Compression and Expansion Machine (RCEM)

For the HPDI methanol-diesel combustion, experiments were carried out using a RCEM setup by Scharl et al. [6], the obtained measurement data are used for the current CFD validation. The RCEM is a pneumatically driven engine that mimics the stroke motion of an internal combustion engine, particularly in the top dead center (TDC) area, and thus permits investigations under engine conditions. Figure 1 shows the schematic overview of RCEM with piston, fuel injectors, and optical measuring equipment.

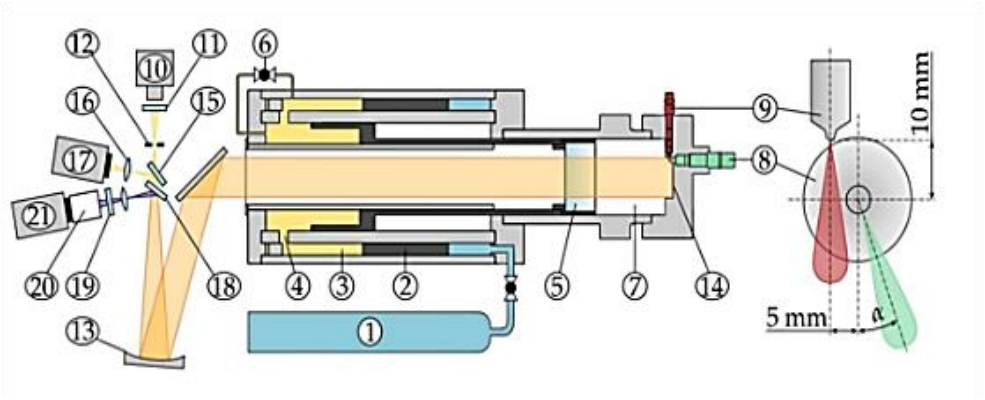


*Figure 1: RCEM experimental setup with optical measurement (left), engine (middle) and injector arrangement (right). Components: (1) compressed air bottles, (2) driving piston, (3) hydraulic oil, (4) orifice holes, (5) working piston, (6) bypass valve, (7) combustion chamber, (8) methanol injector, (9) diesel injector, (10) arc lamp, (11) UV filter*

For each experiment, air in the cylinder is compressed from its initial state to the required final pressure and temperature at the top dead center (TDC). Two operating conditions such as OP1 and OP4 are considered for the spray validation in which the final pressures are 75 and 125 bar as shown in Table 1. Around TDC, diesel and methanol are injected via the injectors with variable arrangement. The diesel injector (9) is a single-hole injector while the methanol injector (8) is a double-hole injector with an angle of 30° between the individual holes. The diesel injector is the pilot injector with an axially mounted nozzle with a diameter of 0.2 mm, which is designed for injections in small quantities. This is arranged at right angles to the methanol injector, which has a radial nozzle diameter of 0.94 mm so that the jets lie in an interaction plane orthogonal to the cylinder axis.

*Table 1: Overview of pressure and temperature at initial and final conditions (before TDC) in RCEM*

| | P_Initial (bar) | T_Initial (K) | P_Final (bar) | T_Final (K) | Inert - Spray Data | HDPI – DF Combustion Data |
|---|---|---|---|---|---|---|
| OP1 | 2.37 | 296 | 75 ±1.5 | 780±8 | at 75 bar | |
| OP4 | 2.16 | 296 | 125±2 | 920±10 | at 125 bar | Spray Interaction angle (+7.5° / +22.5°) Injection timing (+0.5 ms, -0.5 ms) |

The methanol injector can be rotated by an angle $\alpha$ relative to the diesel injector. Together with an electronic control system for the injections this design allows any variation in the spatial and temporal interaction of both fuels. Investigation of methanol spray has been carried out for OP1 and OP4 in which the RCEM was filled with inert gas without oxygen and pilot diesel. In addition, a series of ignition and combustion tests were conducted for OP4, carried out at full-load engine operation. The mass of injected pilot diesel in combustion test is 5 mg and the injection duration is 0.5 ms. Also, 254 mg of methanol was injected as the main fuel for the injection duration of 2.7 ms, and the injection profiles are shown in Figure 2. Two ranges of relative injection timings of +0.5 ms (diesel injected first) and -0.5 ms (methanol injected first) were varied. The interaction angle $\alpha$ is measured for the far side of the spray and is varied between two positions as shown in Figure 2: +7.5 (interaction with both the sprays), +22.5° (strong interaction with near side spray). The CFD simulations were carried out for evaluating spray and combustion characteristics and the results were validated using these measurement points.

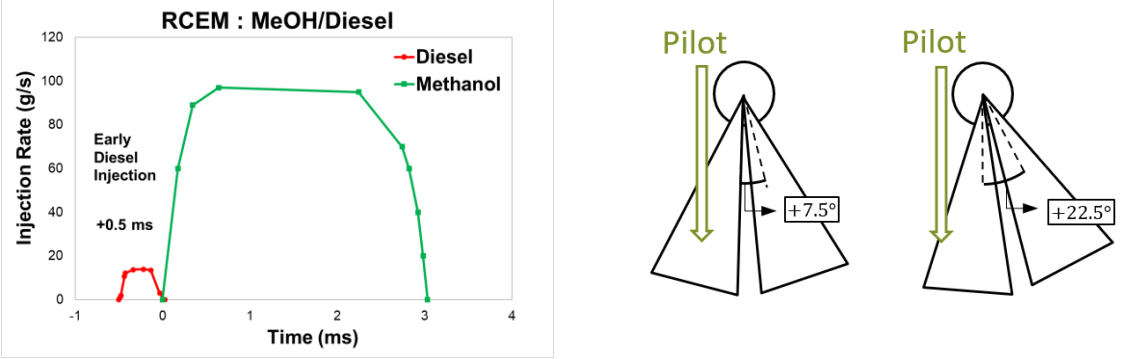


*Figure 2: Injection profiles for diesel and methanol (left) and spray interaction angles of +7.5 ° and +22.5 ° between pilot-diesel and methanol (right)*

The simulation geometry and mesh of the RCEM combustion chamber including the methanol and diesel injectors are shown in Figure 3. A global mesh size of 3 mm is assigned for the combustion chamber. Two levels of grid refinements were applied for better prediction of diesel and ammonia sprays. For turbulence modeling, the RNG k-epsilon model is used. The primary and secondary droplet breakups are modeled using Huh atomization and the Reitz-Diwakar models. Similarly, combustion is modeled using complex chemistry and EFCM-CLEH approaches. The CFD simulations are conducted using STAR-CCM+ 2210 [7].

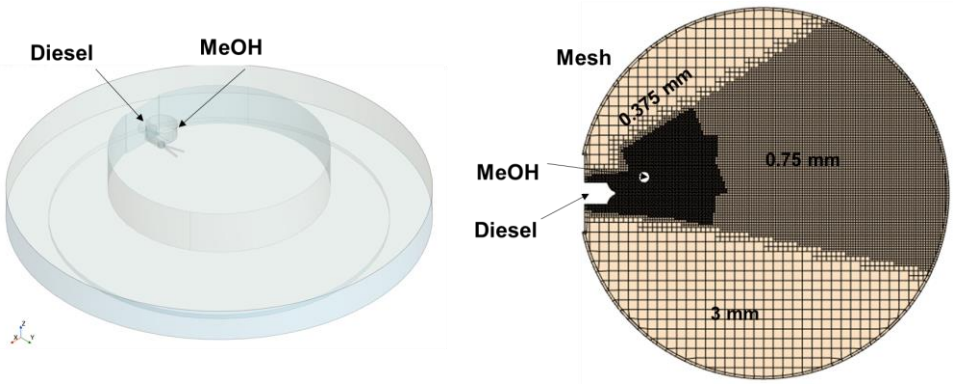


*Figure 3: Simulation model of RCEM with single hole diesel injector and 2-hole methanol injectors (left), Simulation mesh for the cut sections through diesel injector plane (right), mesh size of 3 mm and two levels of refinement.*

## 2.2. Single Cylinder Engine (SCE) Testbed

The Dual fuel combustion experiments of methanol and diesel pilot fuel were carried out in WTZ using the MAN 32/44DF-M which features a 320 mm bore diameter, and 440 mm stroke length. The single-cylinder engine uses a PFI injection strategy with two methanol injectors integrated into the intake ports through a retrofit solution, which provides an easy way to convert existing engines to dual-fuel operation mode without major design changes. The position and orientation of the methanol injector are important as they dictate the ease of installation and mixture formation in the cylinder. In the present test bench, the injectors were installed and directed towards their respective intake valves. Methanol is supplied continuously at a low pressure of 15 bar. Figure 4 shows the methanol conditioning unit and the single cylinder engine (SCE) test bench of 32/44DF-M.

*Figure 4: Methanol conditioning unit (left) and the MAN-32/44DF-M SCE Engine test bench (right) at WTZ, Roßlau*

The methanol-air mixture enters through the two intake valves into the cylinder. A high-pressure diesel injector sits at the head of the cylinder and injects a small amount of pilot diesel directly into the cylinder. Experiments are performed with varying intake air temperature, methanol start of injection (SOI), and two operating conditions. The simulation geometry and mesh of the SCE MAN 32/44DF-M engine is shown in Figure 5. Additional two-level mesh refinements are applied downstream of the methanol injector and cylinder head. Engine load points of 50% and 85% are considered with the intake

air temperature of 65 °C and 45 °C respectively. The methanol is injected at 45° CA and 30° CA after the intake valve opening for 50% and 85% loads respectively. The PFI methanol spray is defined using droplet size distribution and cone angle, and the breakup is modeled using the Reitz-Diwakar model.

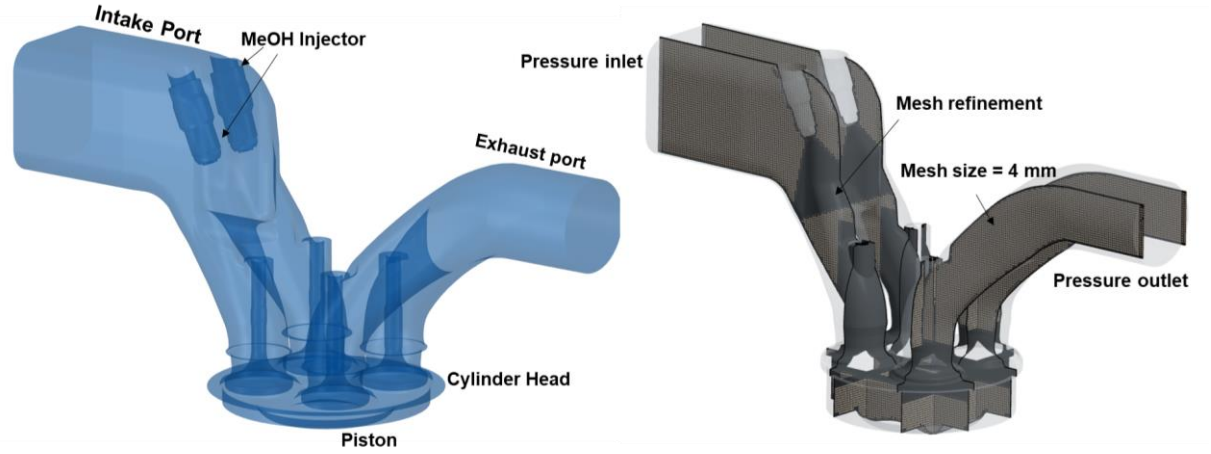


*Figure 5: Simulation model of MAN-32/44DF-M SCE with two methanol injectors in intake port*

# 3. Modelling and Simulation Approach

## 3.1. Spray Modelling

The liquid fuel droplets are introduced in the form of Lagrangian parcels, and the primary and secondary droplet breakups are modelled using the Huh atomization model and Reitz-Diwakar breakup model respectively. When a droplet is injected and the critical Weber number ($We_{crit}$) is reached, the represented droplets undergo an atomization process immediately after they leave the nozzle. In the model of Huh et al., two main factors are considered responsible for spray atomization: gas inertia and turbulence stresses generated within the nozzle. For the secondary breakup the Reitz-Diwakar model was chosen. It accounts for two different breakup regimes, 'bag'-breakup and 'stripping'-breakup. Bag breakup is caused by the droplet expanding into the low-pressure wake region behind it until it disintegrates. It is assumed to be possible when We > $We_{crit}$. The stable diameter is obtained when We= $We_{crit}$. The characteristic time scale for this breakup regime is derived to be:

$$\tau_b = \frac{C_{b2} d}{4} \sqrt{\frac{\rho_l d}{\sigma}} \quad \text{We} > \text{Wecrit} \tag{1}$$

In the stripping breakup regime, new droplets are stripped from the droplet surface by the shear forces. It is assumed to occur when We > max ($2C_{S1}Re^{0.5}$, $We_{crit}$). The timescale for this breakup regime is:

$$\tau_s = \frac{C_{s2}}{2} \sqrt{\frac{\rho_l}{\rho}} \frac{d}{|v_s|} \tag{2}$$

## 3.2. Combustion Modelling

During combustion, hundreds of reactions occur between different species resulting in new species at different rates. A reaction mechanism represents these reactions as a sequence of elementary reactions and the kinetics of the starting materials and intermediates as a function of thermodynamic conditions over a wide range. Utilizing the reaction mechanism, the combustion can be modelled by species

transport equation and a chemistry solver to solve the source terms. To achieve this, the simulation tool provides a tabulated and detailed approach for combustion modelling.

### Complex Chemistry (CC)

The complex chemistry approach solves thousands of chemical reactions among various species in each computational cell in addition to continuity, momentum, and energy transport equations. The chemical reaction mechanism, thermal, and transport properties of reaction mechanisms in Chemkin format are coupled to the solver. The species transport equation is:

$$\frac{\partial}{\partial t}\rho Y_i + \frac{\partial}{\partial x_j}\left(\rho u_j Y_i + F_{k,j}\right) = \omega_i \tag{3}$$

where $Y_i$ is the mass fraction and $\omega_i$ is the rate of production of species $i$, and $F_{k,j}$ is the diffusion flux component.

The species transport is solved with an explicit reaction source term $\omega_i$ for the $i$th species:

$$\omega_i = \rho f\left(\frac{Y_i^* - Y_i}{\tau}\right) \tag{4}$$

Simulations with detailed chemistry method results in a high computational effort, which is many times higher than that of the tabulated combustion models.

### Tabulated Chemistry

To reduce computational time, the reactions representative of different thermodynamic conditions can be precomputed, and the relevant quantities can be tabulated. In the simulation tool, the Extended Coherent Flame Models (ECFM) model has been implemented which is a type of laminar flamelet model, where the turbulent flame is assumed to be composed of many thin laminar flamelet structures that are locally one-dimensional. Assuming this one-dimensional model, the reaction products can be precomputed and stored in lookup tables. The ECFM model is applicable in the region of the corrugated flames regime (Da = 1) represented in the Borghi Diagram. ECFM models are further modified to ECFM-3Z (three zones) and ECFM–CLEH (Chemical rates Limited by Equilibrium of Enthalpy) to model partially premixed combustion. In ECFM 3Z and ECFM-CLEH models, each computation cell is divided into three zones: unmixed air, mixed air, and fuel, and unmixed fuel zone. The zones are further divided into unburnt gas (u) and burnt gas zones (b). The amount of unburnt and burnt gases in the mixed zone is given by the progress variable $\bar{c}$. $\bar{c}$ is zero when it is a fresh-unburned mixture and one when all the fuel in the mixed zone has been burned.

In the ECFM-CLEH model, mean reaction rates are calculated based on four different combustion modes, such as auto-ignition (AI), premixed (PM), diffusion (DIFF), and post-oxidation (PSTOX). For example, the mean turbulent reaction rate in the premixed model is calculated using the flame surface density (Σ), and the laminar fuel consumption per unit surface ($w_L$). $w_L$ is calculated from the unburned gas mixture density $\rho\left(Z_{f|PM} - Y_{f|PM}^{eq}\right)$ and laminar burning velocity ($U_l$). The required intrinsic properties of mixture, such as ignition delay time (IDT) of the fuel-air mixture and unstretched laminar burning velocity ($U_l$) is calculated for the variation of mixture temperature, pressure, equivalence ratio, concentration of each fuel, and exhaust gas concentration in fresh mixture. The IDT and $U_l$ tables are used for predicting the reaction rate and thereby the net heat release rate in each combustion mode and they are created using different chemical reaction mechanisms.

### Chemical Mechanism

Reaction mechanisms play a vital role in the prediction of single or dual-fuel combustion in both detailed and tabulated chemistry approaches. Three different reaction mechanisms have been considered for the investigation. The first mechanism (Mech1) is from Xu et al. [8] with 69 species and 389 reactions, that was developed and validated for hydrocarbon fuels and later extended for ammonia combustion. The second mechanism (Mech2) is a blended reaction mechanism of Curran et al. [9] and Ulrike et al. [10] which has 224 species and 1204 reactions that has not yet been published. The third mechanism (Mech3) is a comprehensive mechanism for n-heptane combustion by Sieser et al. [11] with 160 species and 1540 reactions. For the detailed chemistry simulation, the reaction mechanisms in CHEMKIN format can be incorporated for calculating the reaction rates. And for tabulated chemistry, the required IDT, $U_l$, and equilibrium tables are generated using all three reaction mechanisms.

## 4. CFD Simulation Results: RCEM-HPDI

Scharl et al. [6] conducted spray measurements at OP1 and OP4 conditions, in which the cylinder of RCEM was filled with inert gas, without oxygen and pilot diesel. In the inert spray experiments, only methanol was injected for a relative angle of +7.5°, and the data was used for spray model validation.

### 4.1. HPDI: Spray Validation

Since the HPDI combustion highly depends on fuel droplet breakup, air entrainment, and fuel-air mixing, accurate prediction of spray is essential. The properties of methanol are different from the conventional hydrocarbon fuels, the spray breakup model parameters set should be determined for methanol. For this spray investigation, three parameters such as Reitz-Diwakar stripping breakup time scale coefficient $C_{s2}$, discharge coefficient for injector $C_d$, and injector nozzle length $L$ are varied for OP4. The obtained spray simulation results have been compared with the measured vapor penetration length, spray angle, and spray shape. In the simulation, an iso-surface of methanol vapor is created for 0.1% mass fraction to compare the spray shapes.

After varying multiple combinations of three spray parameters, one parameter set has better predicted the spray characteristics of methanol at 125 bar cylinder pressure (OP4). Using the same parameter set, for OP1 spray has been simulated. As illustrated in Figure 6, the measured and simulated vapor penetration lengths are in good agreement with specific set up spray model parameters for OP1 and OP4. Moreover, the comparison of shadowgraph images of methanol spray with iso-surfaces obtained from the simulation are closely matching, including the hot island zone in the middle of the spray. The spray angles are quantitively calculated and compared, and they are 35° for OP4 and 40° for OP1.

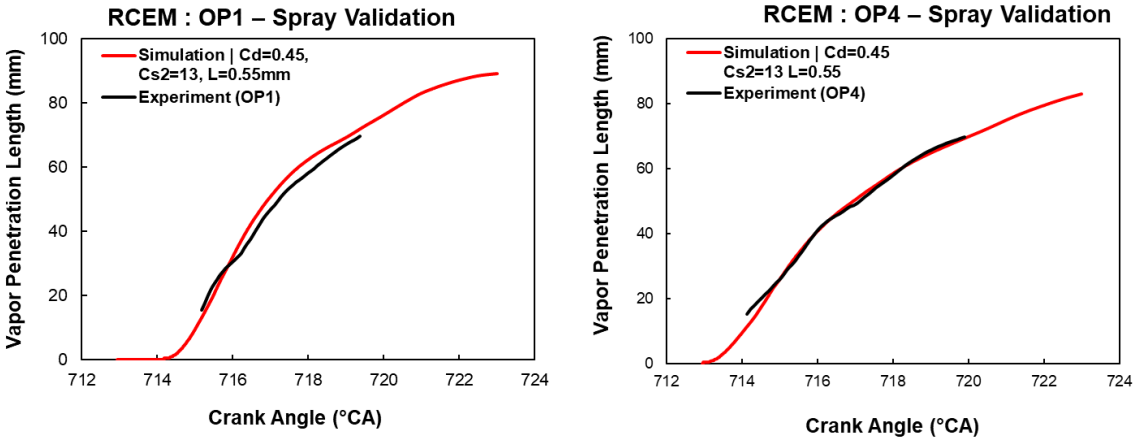


*Figure 6: Simulated vapor penetration length at OP1 and OP4 conditions*

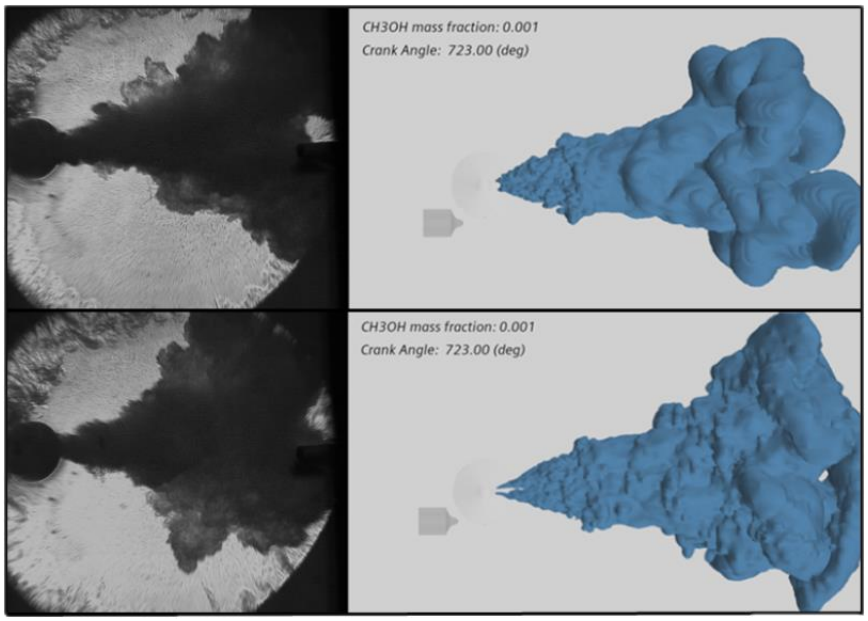


*Figure 7: Shadowgraph images of methanol spray (left) at OP1 (top) and OP4 (bottom) with 0.1% methanol mass fraction from simulation (right)*

## 4.2. HPDI: Combustion Simulation Results

In this section, simulation results of methanol-diesel combustion at OP4 for the variation of reaction mechanisms (Mech1, Mech2, Mech3) and combustion modelling (complex chemistry, ECFM-CLEH) approaches using the available experimental data as given in Table 1, for the variation of spray interaction angles (+7.5° and +22.5°) and injection timings (+0.5 ms and -0.5 ms) are presented. For the combustion simulation, the determined spray parameter set has been used.

### Reaction Mechanism Variation using CC: Mech1 / Mech2 / Mech3

Figure 8 illustrates the different stages of diesel-ignited methanol combustion using the "Mech1" mechanism, spray interaction angle of +7.5°, and methanol injection timing of +0.5 ms. At first, pilot-diesel is injected into the cylinder, which is then evaporated and combusted forming the hot plume of burned products in the center of the cylinder. The injected methanol from two nozzle holes penetrates through the hot gas, thus enhancing evaporation, and igniting the methanol-air mixture. This

phenomenon can be observed on the near side of the methanol spray where the $CO_2$ and OH radicals formed on the outer regions of the spray at t = 0.652 ms (716.8° CA). Due to the continuous injection of methanol, the gas temperature in the inner region of the plume drops due to methanol evaporation and mixing, thus changing the flame shape, and drifting the flame position towards the cylinder wall. The concentration of $CO_2$ and OH radicals at t = 1.763 ms (720° CA) reveals the position of the combustion, i.e., mainly on the outer regions of the methanol spray. Since the RCEM wall temperatures were relatively lower than the gas temperature, the methanol flame at the front got quenched, leading to the flame propagation only in the radial direction. The methanol flame is anchored at a certain distance from the methanol injector and remains identical throughout the injection duration. The temperature contours of the simulation align closely well with the experimental combined SG/OH*-CL images. This alignment suggests a strong overall predictive capability of the CFD model.

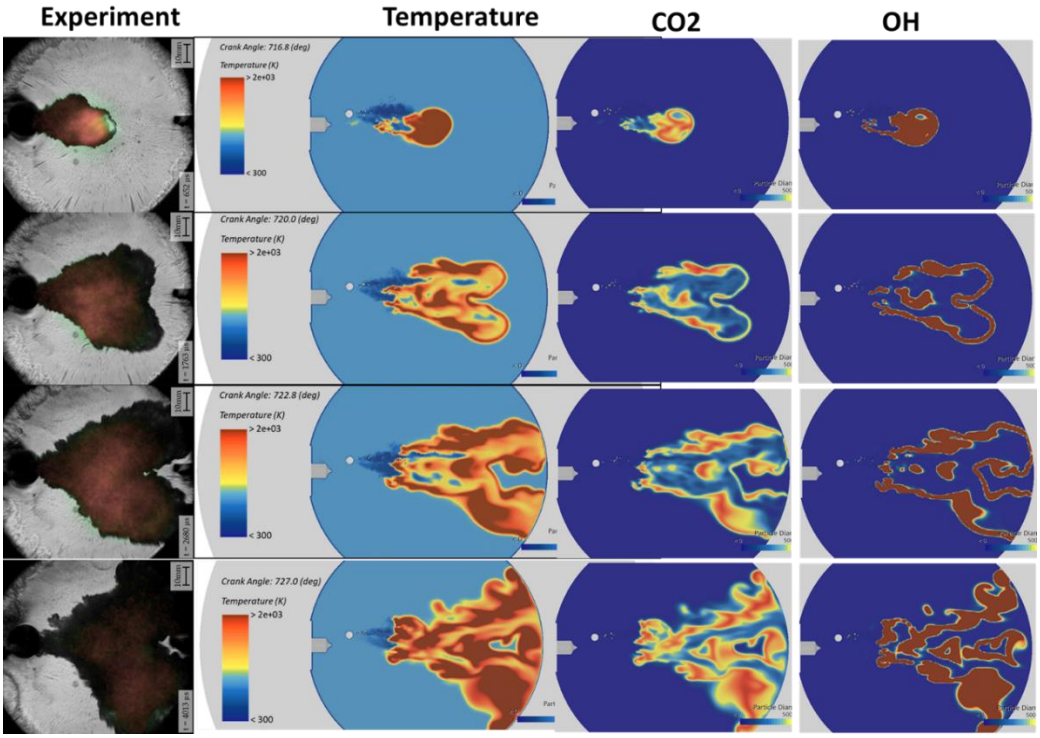


*Figure 8: Combined shadowgraph (SG) and OH*-Chemiluminescence (CL) images (Experiment) and simulated temperature, $CO_2$, and OH contours for spray interaction angles of +7.5°, injection timings of +0.5 ms, and Mech1*

In Figure 9, the heat release rates of the experiment and simulation for early diesel (+0.5 ms) and early methanol (-0.5 ms) injection results are presented. In the case of early diesel injection, it can be observed that three reaction mechanisms show nearly identical combustion characteristics. However, the Mech2 predicts diesel combustion more accurately. Mech1 and Mech3 have some delay in diesel ignition by up to 1.5° CA. For early methanol injection (-0.5 ms), diesel combustion starts relatively later, and the premixed combustion peaks are overpredicted by Mech3. The difference between the experiment and simulation after 720°CA occurs when the flame touches the wall as shown in Figure 9. In the experiment, the heat loss to the RCEM wall is calculated based on the temperature gradient. It could be possible that the calculated heat loss is relatively higher in the experiment compared to the simulations. Overall, Mech1 and Mech2 show good agreement with the experimental data for both early diesel and early methanol injection conditions.

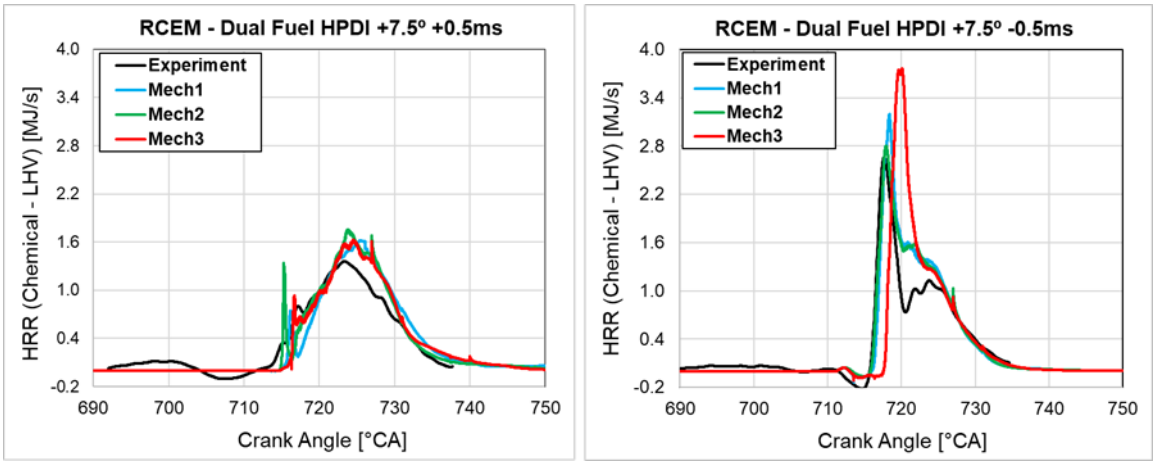


*Figure 9: Experimental and Simulated HRR for spray interaction angles of +7.5° and injection timings of +0.5 ms and -0.5 ms for three reaction mechanisms*

**Combustion modelling - CC / ECFM-CLEH : Early methanol Injection (-0.5 ms)**

Combustion simulations have been performed for OP4 conditions using complex chemistry (CC) and EFCM-CLEH modelling approaches. Using the Mech1 reaction mechanism the IDT, $U_l$, and equilibrium tables were generated for the ECFM-CLEH model and used in the combustion simulation. The results for the spray interaction angle of +7.5° with early diesel injection (+0.5 ms) and early methanol injection (-0.5 ms) are presented in this section. Figure 10 depicts the combustion phenomenon that occurs in early methanol injection condition (-0.5 ms). At t = 1.499 ms (716° CA), injected methanol during the early phase of injection is evaporated and forms an ignitable mixture in the cylinder. The pilot diesel ignition arises in the outer regions of the methanol spray which ignites the premixed methanol air mixture at the near end of the diesel nozzle, thus causing more heat release in a short duration. Furthermore, the methanol flame propagates further to combust the methanol from the second nozzle. After the premixed combustion at t = 3.852 ms (721° CA), the methanol burns in a diffusive combustion mode. Comparing the temperature contours between CC and ECFM-CLEH in Figure 10, one can observe that the CC model can predict the earlier diesel ignition and premixed methanol combustion well compared to the ECFM-CLEH model.

The quantitative comparison of HRR in Figure 11 concludes that the EFCM-CLEH model shows small deviation at the early phase of injection, mainly on diesel ignition. However, the difference becomes smaller at the late phase of methanol injection, followed by combustion and heat release. Overall, both complex chemistry and ECFM-CLEH combustion modelling approaches could predict well the full diffusion combustion and a combination of premixed and diffusion modes and their predictions are in good agreement with the experimental data. Since all the reactions that exist in the mechanism have to be solved for each cell in a complex chemistry method, the computational time for one simulation is 6 times longer compared to that of the ECFM-CLEH model.

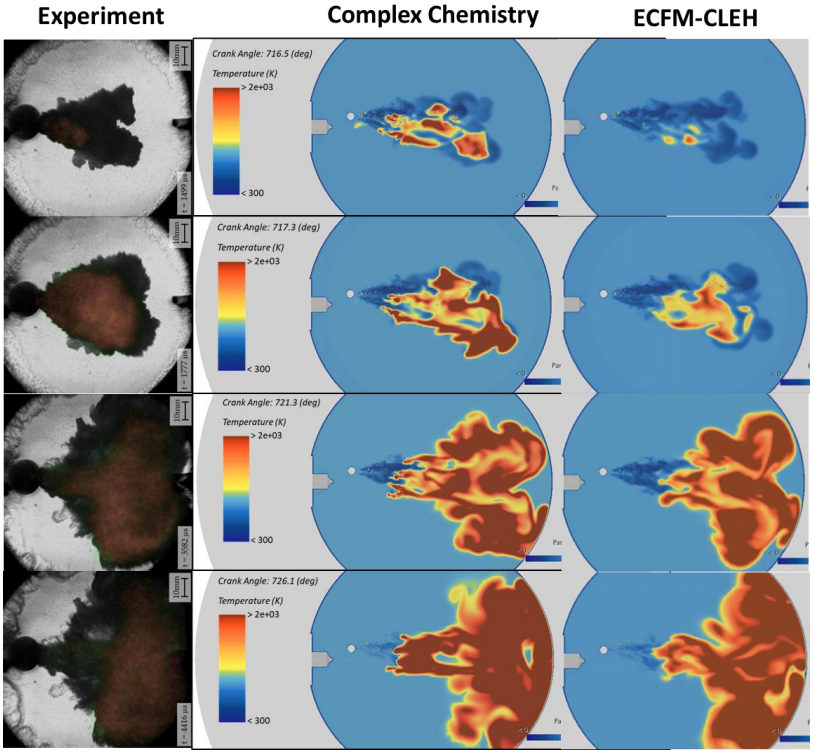


*Figure 10: Combined shadowgraph (SG) and OH*-CL images (Exp.) and temperature contours of Complex-Chemistry and ECFM-CLEH simulations at OP4 with +7.5° spray interaction angle, early methanol injection (-0.5 ms)*

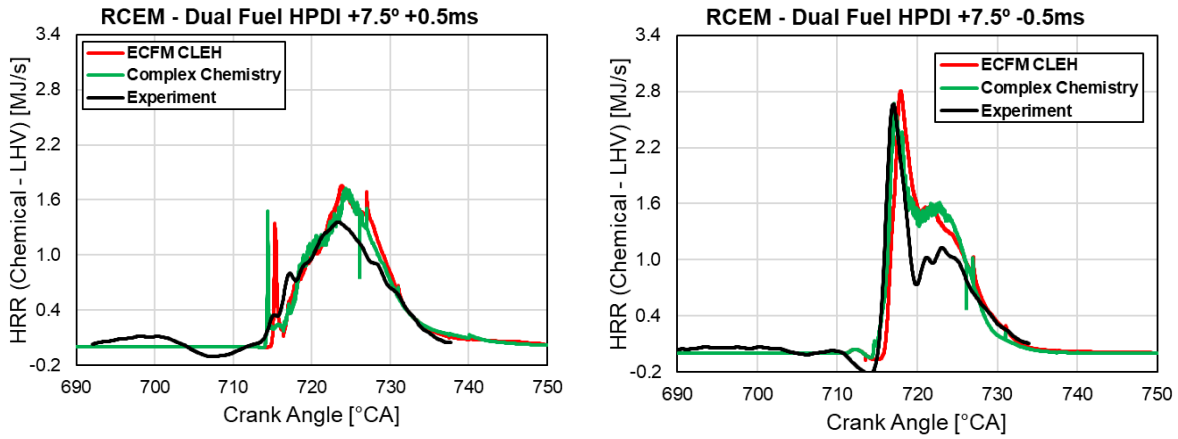


*Figure 11: Experimental and Simulated HRR for spray interaction angles of +7.5° and injection timings of +0.5 ms and -0.5 ms for EFCM-CLEH and complex chemistry combustion modelling techniques*

### Diesel/Methanol spray interaction angle variation: 22.5 °

In a two/more needle multi-hole injector, the interaction between individual diesel and methanol sprays plays a major role in diesel ignition and methanol combustion. So, the simulation methodology has been further validated using the measurement data for the 22.5° interaction angle and early diesel injection (+0.5 ms). Figure 12 illustrates the early diesel injection, followed by the ignition of methanol and its combustion. At t = 0.986 ms (714° CA), the diesel ignites the methanol mixture at the near side of the methanol spray. And the developed flame propagates into methanol released from the nozzle hole located at the far end of the diesel injector, thus causing lower HRR compared to that of observed in

+7.5°. The methanol flame drifts towards the wall during injection and the methanol flame stabilizes at the downstream of injector. From the comparison of OH*-CL and temperature contours at various timings, one can conclude that methanol combustion is well predicted in both the early and late stages of methanol injection.

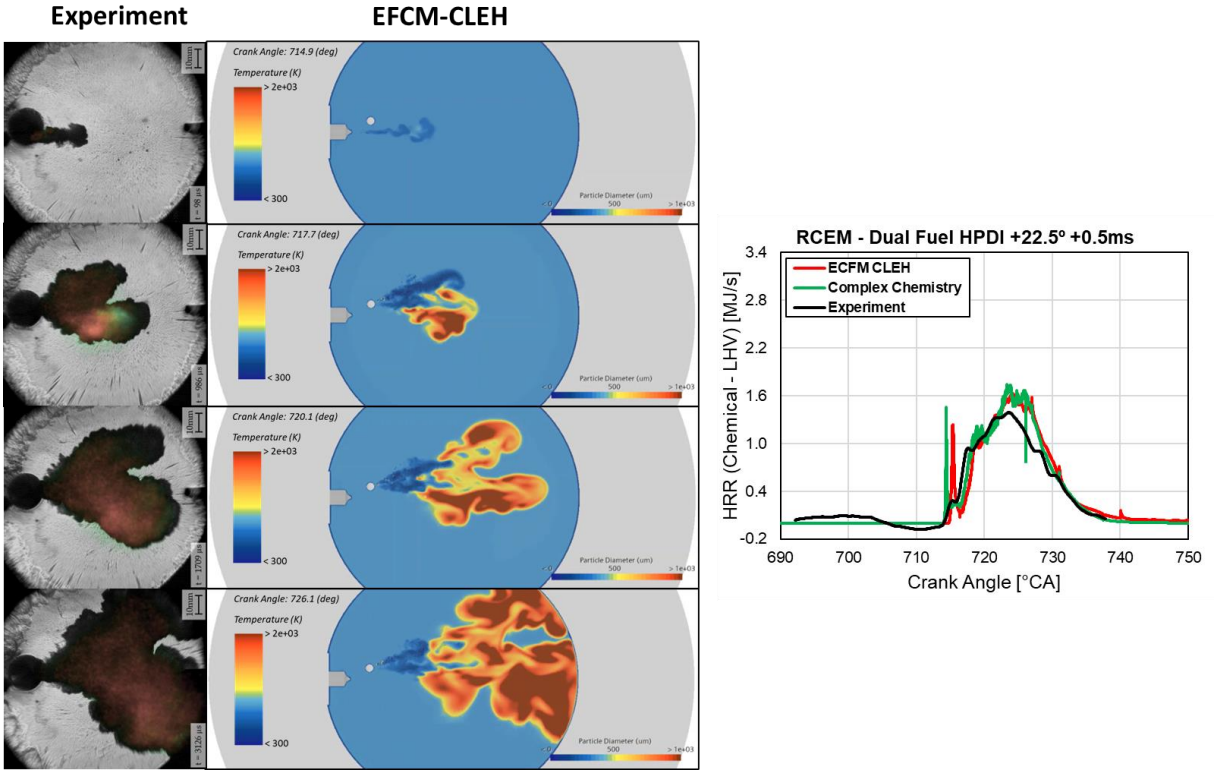


*Figure 12: OH*-Chemiluminescence (CL) images (Exp.) and temperature contours of ECFM-CLEH simulations at OP4 with +22.5° spray interaction angle and +0.5 ms injection timing (left) and the heat release rates comparison (right)*

## 5. CFD Simulation Results: Port Fuel Injection (PFI)

Retrofits of existing fleet engines can be realized by injecting methanol in the intake port, thereby a portion of the methanol is evaporated and mixed with air at the intake port. The remaining evaporation and mixing occur in the cylinder during the intake and compression stroke. The premixed methanol-air mixture is ignited by the diesel pilot fuel. Furthermore, the methanol injection, evaporation, and mixture formation play a significant role in the emission and performance behaviours of an Otto-cycle methanol engine. Achieving good methanol-air mixing in the cylinder depends on many parameters such as injector design and its position in the intake port, injection timing, and intake air conditions. The influence of injector position on mixing has been discussed in [5]. In this investigation, CFD simulations have been carried out to evaluate evaporation and mixing characteristics at two engine load points of 50% and 85% for the variation of injection timings and their results are presented in this section.

### 5.1. Spray and Mixing Characteristics

The simulation CAD model and mesh, that are shown in Figure 5 are used for the CFD analysis. The measured experimental data is used as initial and boundary conditions for the cylinder, intake, and exhaust ports. The injected methanol mass for both engine operating conditions corresponds to 95% of the total energy. The injection profile is defined with an initial ramp-up curve and ramp-down curve

with a constant profile in the middle. The chosen injection duration allows enough time for most of the liquid droplets to flow into the cylinder. Thus, reduces the stored methanol in intake port and its slip during valve overlap. The start of injection (SOI) of methanol, for 50% and 85% loads are IVO+45° CA, and IVO+30° CA respectively. Figure 13 shows the methanol injection from two injectors and liquid droplet distribution in the air at the intake port. At downstream of the methanol injector, the droplets start to break up and evaporate, thereby vapor is even formed at the tip of the injector. The methanol vapour and liquid droplets are flowing on the right side, this is to avoid the methanol droplet and liner collision in the cylinder. Three stages of droplet breakup were observed, i.e., immediately after the injection, in the intake port, and above the intake valve head where the gas reaches high velocity. The temperature contours in Figure 14 indicate that the gas temperature drops by up to 40 K locally due to methanol evaporation, and the low-temperature gas shows the flow path of liquid droplets. Since the injection pressure of methanol is low, conditions of intake air play a vital role in droplet breakup and evaporation.

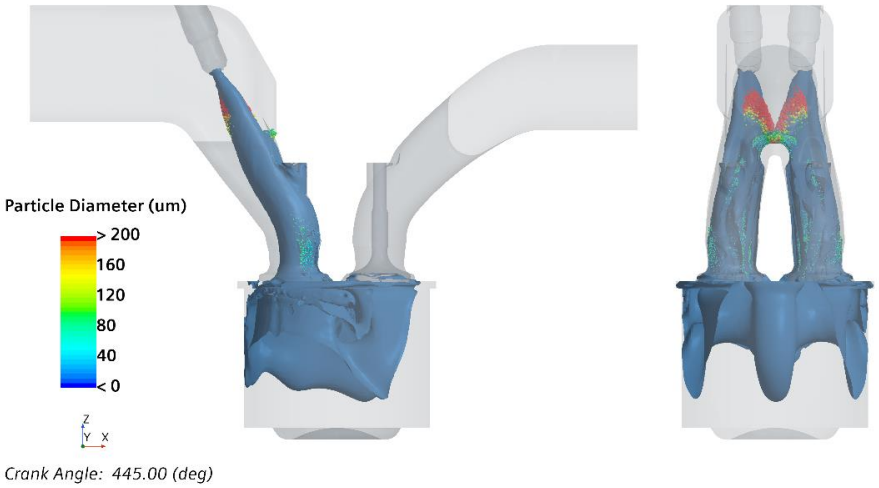


*Figure 13: Iso surface of methanol vapor, mass fraction between 0.1 and 10% and methanol droplets during injection for engine load P = 50%, SOI_Methanol = IVO + 45° CA*

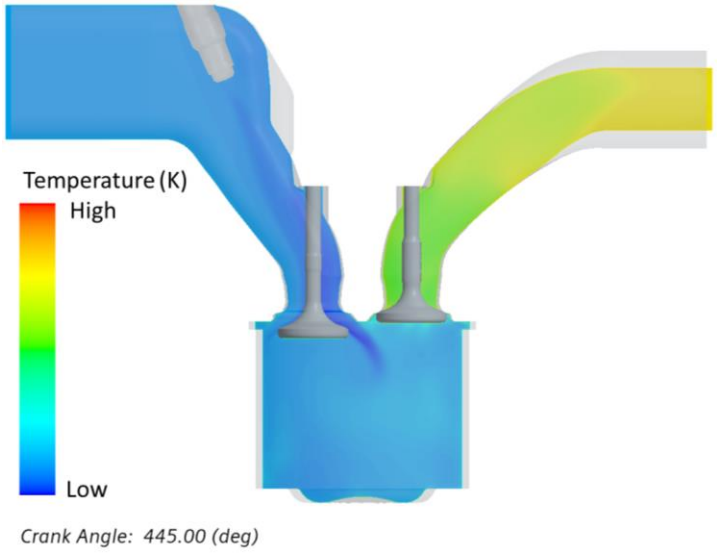


*Figure 14: Contours of gas temperature during methanol injection for engine load P = 50%*

The mass of methanol evaporated in the intake port is less than 20% and the remaining evaporation occurs in the cylinder. The methanol-air mixing is prominently dominated by the flow distribution and how the methanol vapour interacts with the intake air. Figure 15 depicts how the methanol vapour and its droplets flow in the cylinder for engine load of 85% and for SOI_Methanol of IVO+30° CA. One portion of the methanol vapour passes through the front section of the intake valve hit the piston directly below the exhaust valves. The remaining liquid droplets and vapour flow along the liner and mix with the air. As shown in Figure 16, most of the evaporation occurs during the intake phase of the engine cycle due to high turbulent flow in intake port and cylinder which enhances droplet breakup and mixing. During the compression phase, the remaining droplets are converted into vapour before TDC. The higher intake air temperature at 50% load facilitates methanol evaporation, thereby lowering the mass of liquid droplet at the end of compression. The contours and histogram of the air-fuel ratio in Figure 17 and Figure 18 indicate that slightly better mixing is observed in 50% load conditions compared to 85%. This could be due to slightly higher intake air temperature and later methanol injection timings, thus, enhancing droplet breakup, evaporation, and mixing. Overall, the mixing quality in both conditions is good, though there is a small deviation in the local concentrations. Finally, the comparison of the simulated pressure is well aligned with the measurement data, and the temperature shows a minor deviation at TDC which was further improved while using liquid film models in the simulation.

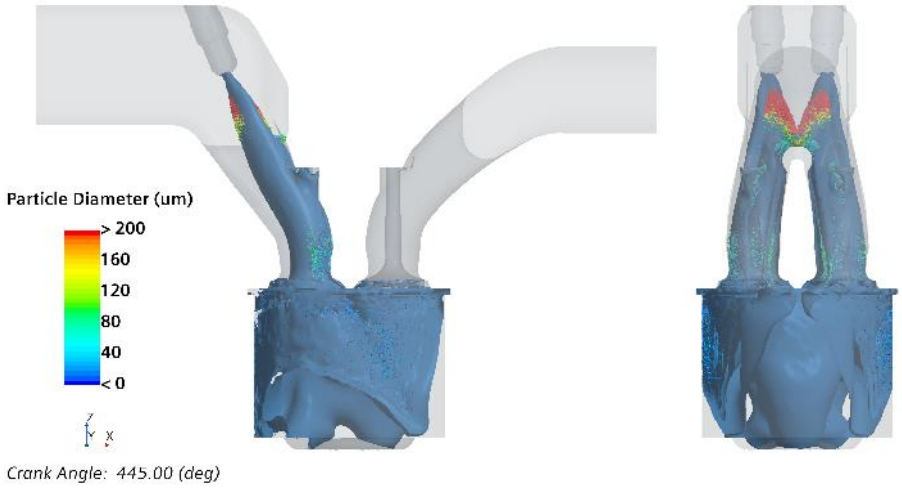


*Figure 15: Iso surface of methanol vapor, mass fraction between 0.1 and 10% and methanol droplets during injection for engine load P = 85%, SOI_Methanol = IVO + 30° CA*

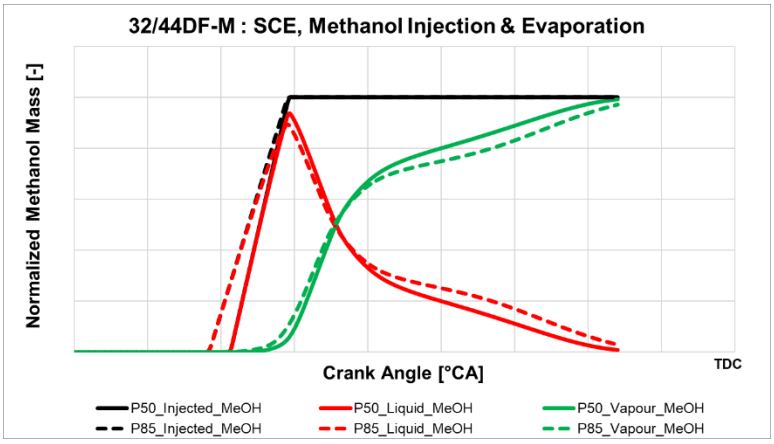


*Figure 16: Methanol mass injected, in vapor phase after evaporation and the remaining mass in liquid phase*

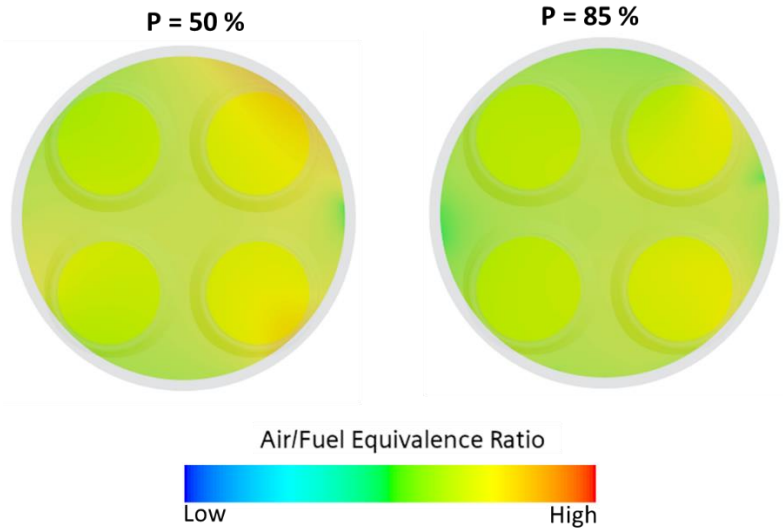


*Figure 17: Contours of air/fuel equivalence ratio for engine load 50% (left) and 85% (right)*

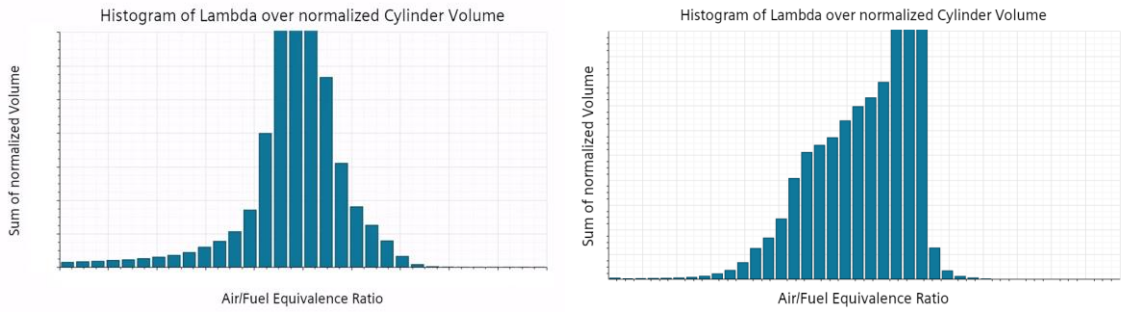


*Figure 18: Histogram of air/fuel equivalence ratio vs norm. cylinder volume for engine load 50% (left) and 85% (right)*

## 6. Conclusion

MAN Energy Solutions SE has been working on the development of carbon-free and carbon-neutral fuel engines, such as dual-fuel methanol engines for retrofit solutions and newbuilds. PFI and HPDI injection strategies are considered for fuel injection that leads to premixed Otto-like and Diesel-like diffusion combustion respectively. The PFI technique will be implemented in MAN's 48/60 and 51/60

engine platforms as well as for the 21/30 genset engines. Besides, the HPDI methanol injection method will be introduced in new builds and retrofit solutions to the newly developed 32/44 and 49/60 engine platforms.

In this CFD investigation, spray validation has been carried out using RCEM setup for 50 bar and 125 bar cylinder pressure conditions. The simulated spray shape, spray cone angle, penetration length, are in good agreement with the experimental data for certain Reitz-Diwakar model parameter sets. The combustion simulation results for the early diesel injection (+0.5 ms) case show that the diesel combustion products ignite methanol. Most of the combustion occurs in diffusive mode on the outer regions of spray where OH and $CO_2$ concentrations are higher. For early methanol injection (-0.5 ms), methanol forms a combustible mixture, thus releasing high heat release due to premixed combustion, followed by a diffusive combustion due to slow evaporation and mixture formation. Methanol could be ignited by the pilot for diverging sprays with +22.5° angle between diesel-methanol sprays and the combustion characteristics are nearly identical to that of predicted in +7.5°. This indicates that the methanol ignition could be secured even for diverging spray with low interaction between methanol and diesel sprays.

The predictions of Mech1 and Mech2 are aligned with the experimental data while using complex chemistry and ECFM-CLEH modelling approaches for all the simulated conditions. Mech3 shows delayed diesel ignition and faster methanol combustion, which is largely deviating from the heat release rate for both early diesel and early methanol injection conditions. Overall, the simulated temperature contours which depict the diesel and methanol flames, match well with the combined SG/OH*-CL images from the experiments, indicating a good overall predictive capability of the CFD methodology for HPDI dual fuel methanol-diesel combustion.

The PFI simulations carried out for 32/44DF-M SCE engine setup for load points 50% and 85% indicate that the intake air temperature is reduced by up to 40 K due to methanol evaporation. For the simulated conditions, less than 20% of the injected methanol is evaporated in the intake port and the remaining 80% occurs in the cylinder during intake and compression stroke. During the intake phase, a sharp increase of methanol vapour mass in the cylinder was observed due to better interaction between droplet and air. Around 40% of the droplets evaporated in the cylinder during compression phase. At the BDC, the gas temperature is low, and the movement of air is slower than that of observed in intake port. Thus, reduces the evaporation rate. At the later phase of compression, increase in gas temperature enhances the droplet evaporation. The predicted mixing quality for 50% load is better compared to 80% owing to higher intake air temperature and earlier methanol ignition timings. Using this simulation approach, the evaluation of injector design, its position, and injection timing has been completed for 51/60DF-M and 21/31DF-M engines. The combustion simulation of dual fuel premixed methanol combustion ignited by pilot diesel is currently ongoing. The developed simulation methods for HPDI and PFI methanol combustion will be further employed to facilitate the development of MAN's methanol engines for reducing GHG emissions.

## Abbreviations and acronyms

| | |
|---|---|
| GHG | Greenhouse gas |
| IMO | Internation maritime organisation |
| CC | Complex chemistry |

| | |
|---|---|
| ECFM-3Z | Extended coherent flamelet Model – 3 Zone |
| ECFM-CLEH | Extended coherent flamelet model – Combustion limited by equilibrium enthalpy |
| RCEM | Rapid compression and expansion machine |
| HPDI | High Pressure Direct injection |
| MeOH | Methanol |
| PFI | Port fuel injection |
| OH*-CL | OH*- Chemiluminescence |
| SG | Shadowgraphy |
| IVO | Intake valve open |
| TDC | Top dead center |
| BDC | Bottom dead center |

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