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CFD Simulation of a DME Fuelled CI Engine

Gaurav Mittal, Jasmeet Kalra

Abstract: ***A computational study is conducted for a DME fuelled CI engine of 373.3 cm^{3}displacement and 17.8 compression ratio at moderate load with detailed chemistry. Due to the symmetry of the cylinder, the simulations are conducted on a sector of the cylinder, from the closing of intake valve to the opening of exhaust valve. In the pilot injection strategy employed, 10% of the total fuel is injected during the pilot injection and the balance in the main injection at 5^0 BTDC. The computational model is first validated using the experimental data. Results show two-stage ignition characteristic for the DME injected in the pilot injection.***

Keywords: DME, CFD simulation, pilot injection

I. INTRODUCTION

Dimethyl Ether (DME) is recognized as a clean alternative to petroleum derived diesel fuel. With DME there is no particulate matter (PM) formation due to the lack of C-C direct bond. In compression ignition engines, DME performance may be superior to diesel and engine operation is less noisy. Its high vapour pressure leads to reduction in wall-wetting [1]. A high cetane number of around 55 and a low boiling temperature of -25 ºC provides rapid mixing, decreased ignition delay, and outstanding cold starting characteristics. The potential of DME fuelled CI engines has been explored by a number of researchers, for example [1-9]. Use of multiple injections, in which more than one injections are employed every cycle, have been shown to be a potential means for mitigating emission of pollutants from CI engines. In a pilot injection, less than 10% fuel is injected in the first injection. Pilot and split injection can be effective in concurrently reducing soot and $NO_x$from CI engines. By using DME in CI engines there is no soot formation, and by using multiple injection strategy, NO_x formation can potentially be reduced.In this work, combustion inside a DME fuelled CI engine is studied computationally. In the following, the computational specifications are provided, followed by a discussion of results.

II. COMPUTATIONAL SPECIFICATIONS AND VALIDATION

The computational model was developed using the Converge CFD code. Simulations employed RNG k−ε turbulence model and KH-RTspray models. O'Rourke collision model was employed for droplet collision, whereas Frossling model was used for evaporation. The drop/wall interactions were modelled using the wall film model.

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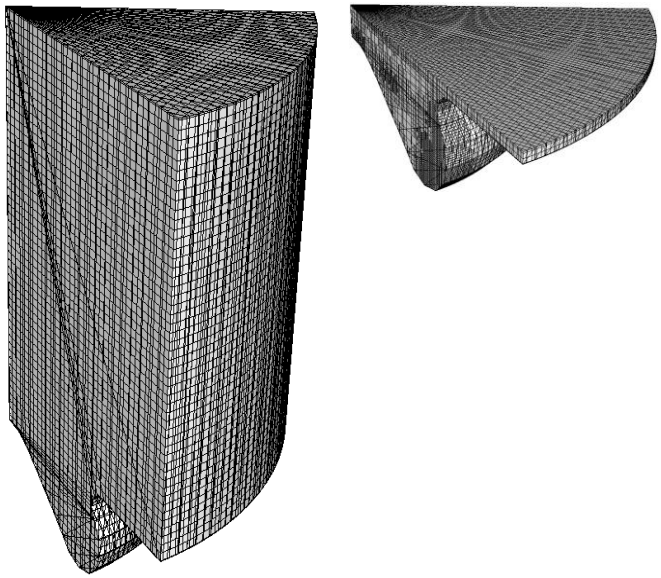
***** Correspondence Author (s)
Gaurav Mittal, Department of Mechanical Engineering, Graphic Era Deemed to be University, Dehradun, India. E-mail: gauravmittal@geu.ac.in
Jasmeet Kalra, Department of Mechanical Engineering, Graphic Era Hill University, Dehradun, India

Experimental and numerical studies of Kim et al. [1,2] were selected for computational validation. The engine had a bore of 75 mm, stroke of 84.5 mm, compression ratio of 17.8, and 6 hole injector with 0.128 mm hole diameter. IVC and EVO occurred at 128^{0}BTDC172^0 ATDC respectively. For validation, an engine running at 1500 rpm and swirl ratio of 1.63 was modelled. DME injection pressure was 50 MPa. Mass of the fuel injected into each injector per cycle was 1.33 mg.

As there are six injection nozzles or holes, the engine can be divided into six sectors, each of 60^0. Due to the symmetry of the combustion chamber, the CFD simulations were conducted on a 60^0 sector mesh. Simulations were run from IVC to EVO. The CFD code used a structured Cartesian grid having a base cell of 1.0 mm. Adaptive mesh refinements in the region of large gradients and fixed embedding in the spray region were also employed. The kinetic model for DME by Zhao et al. [10]was employed for the present study. It has 55 species and 290 reactions and has been well validated over a broad range of temperatures and pressures relevant to engines.

The engine sector along with the mesh is shown in Figure 1. The initial gas temperature inside the cylinder at intake valve closure (IVC) was 320 K and initial pressure was 1.07825 atm. The temperature at piston, head, and cylinder walls was specified as 550 K, 520 K and 430 K respectively. Based on [1,2] the start of pilot injection timing was selected as 20^0 BTDC for validation. The duration of injection was estimated from the spray penetration curve or injection rate curve [1,2].

The results from the validation study are compared against the experimental data from [1,2] in Figure 2. An excellent agreement is noted between the experiment and simulation during the compression and expansion stroke as well as in the peak pressure and combustion phasing. Since the chemical kinetic mechanism used here was already comprehensively validated, the agreement in the engine pressure traces may be taken as a sufficient evidence of the suitability of the present engine model for predictive simulations.



a. 87.9^0 BTDC **b. 0.0056^0 ATDC**

Figure 1 – Computational mesh

III. RESULTS

In the pilot injection strategy, only 10% of fuel was supplied during the first pulse of injection at 40^{0}BTDC and the balance 90% during the main injection at 5^{0}BTDC. The numerical conditions are specified in Table 1. Engine specifications have already been detailed.

Table 1 - Numerical conditions of DME fuelled engine

Engine speed (rpm)	1500
Initial temperature (K)	320
Initial pressure (atm)	1.74
Injection pressure (MPa)	60
Mass of fuel injected(mg/cycle)	26
Injection fuel temperature (K)	300

Figure 3 shows pressure curve of a reactive cycle as well as the motored pressure trace. The difference between the two pressure traces indicates the extent of energy released from combustion. From the pressure traces, it is evident that there is significant heat release from the pilot injection even before the onset of the primary injection. The heat release rate curve is shown in Figure 4. The initial peak in the heat release is around 15^0 BTDC, followed by a lower peak before the main injection. Both of these peaks are due to combustion of the pilot injection. Combustion of the main injection is noted only after TDC. An important aspect is to understand the manner in which the combustion of the pilot charge modifies the in-cylinder temperature and concentration at the instant of main injection.

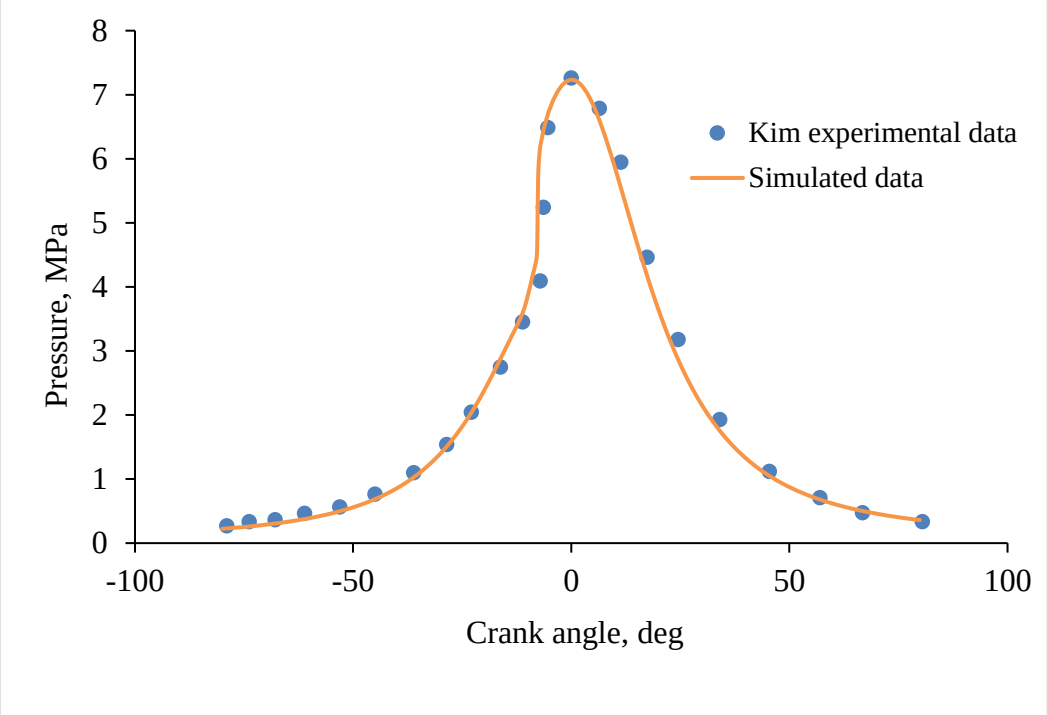


Figure 2 –Comparison of simulation with experimental result from [1,2].

The reason for the two distinct heat release curves for pilot injection is temporal separation of the first and second stage heat release. The concentrations of formaldehyde, DME, and CO are shown in Figure 5. The concentrations in Figure 5 are scaled for clarity. From these plots, it is clear that the first peak in heat release at 15^0 BTDC is due to the first stage ignition of the pilot injection. During this phase, significant amount of formaldehyde is produced due to low temperature reactions involving peroxidation. Furthermore, the rise in maximum temperature at this time is small and the peak temperature remains less than 1000 K even after the first peak in heat release. Following the first stage ignition, the peak temperature reaches 2500 K at around 11^0 BTDC, which is followed by a second, smaller peak in the heat release. This indicates that the second peak in heat release is due to the second stage or hot ignition during which combustion in the part of the domain goes to completion.

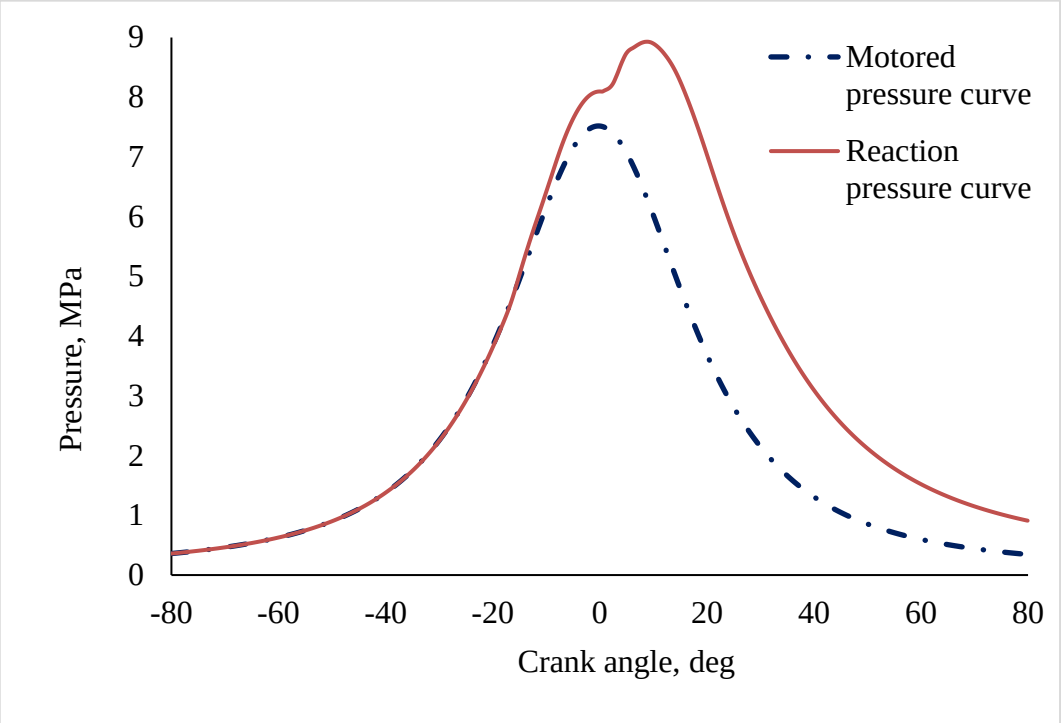


Figure 3 – Pressure curves

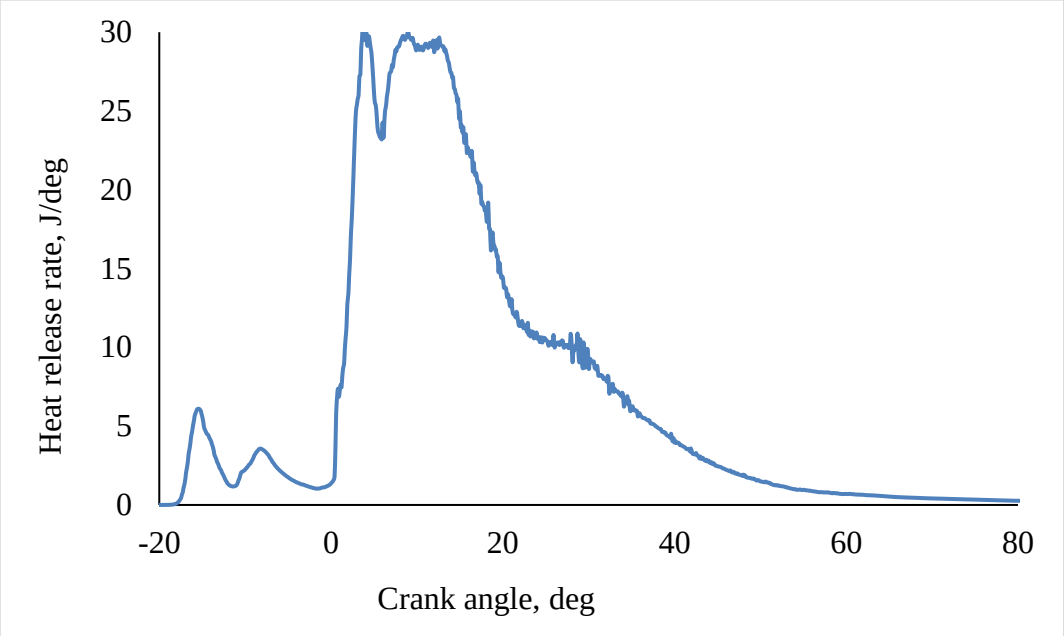


Figure 4 - Heat release rate for pilot injection at 40^0 BTDC and main injection at 5^0 BTDC

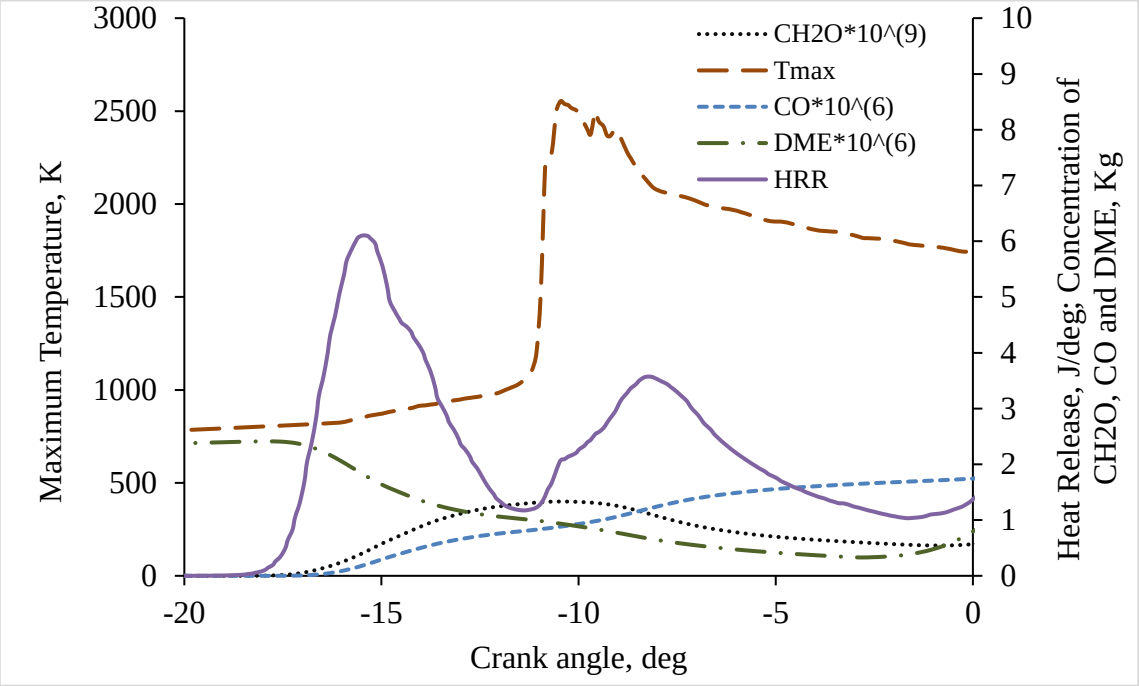
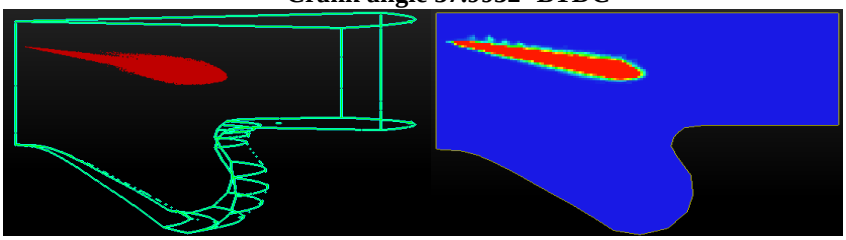


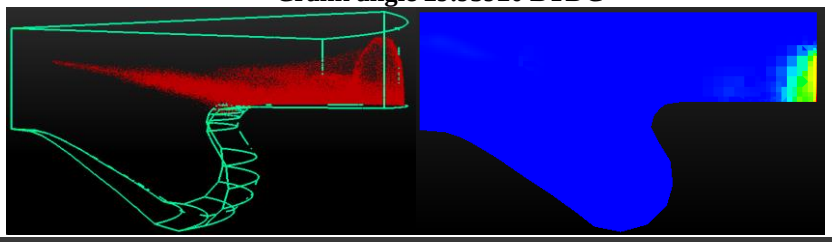
Figure 5 – HRR, formaldehyde, CO, DME concentrations and maximum temperature

The second stage ignition is, however, highly non-uniform and occurs only in part of the domain. This is based on the observation that the concentration of CO remains significant as well as formaldehyde persists. Persistence of these species is a clear indication that some regions in the domain are over-mixed and do not allow for the second stage ignition to occur. It has important implications for emissions as the CO and HC in the over-mixed region, which did not undergo hot ignition, might not burn even during the main injection and may lead to engine out CO and HC emissions.

Crank angle 37.9932^0 BTDC



Crank angle 29.95920 BTDC



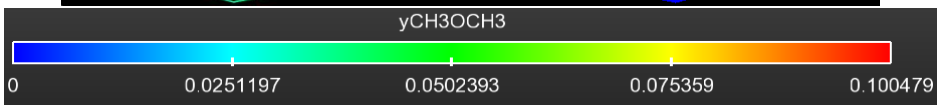


Figure 6 - Spray penetration and spray vaporization in the cylinder after the pilot injection at 400 BTDC

The heat release following main injection, Figure 4, is typical of diesel combustion where a premixed burning phase is followed by the mixing controlled combustion as spray continues. The premixed burning phase here, however, has only one peak as the cylinder temperature is high and the first stage and hot ignition are not temporally separated.Spray penetration and DME vapour mass fractions following pilot injection and main injection are shown in Figures6 and 7, respectively. The pilot injection is targeted in the squish region. The larger and colder droplets are closer to the injector. As they travel away from the injector, they are broken down and evaporated due to the rise in the temperature by absorption of heat and finally the fuel gets converted from liquid state to gaseous state.

In Figure 6, DME vapours are observed only close to the wall. This is, however, misleading because the mass fraction shown is only in the plane of injection;

whereas, DME vapours are convected in the direction of swirl. Before the main injection, all the fuel injected during pilot injection mixes completely with the gas present in the cylinder. Main injection starts at 5^0 BTDC.

The main injection is targeted in the bowl where it burns as also noted by temperature fields shown in Figure 8. Since the first injection is targeted in the squish, which may not be ideal, additional studies could be conducted by changing the spray umbrella angle.

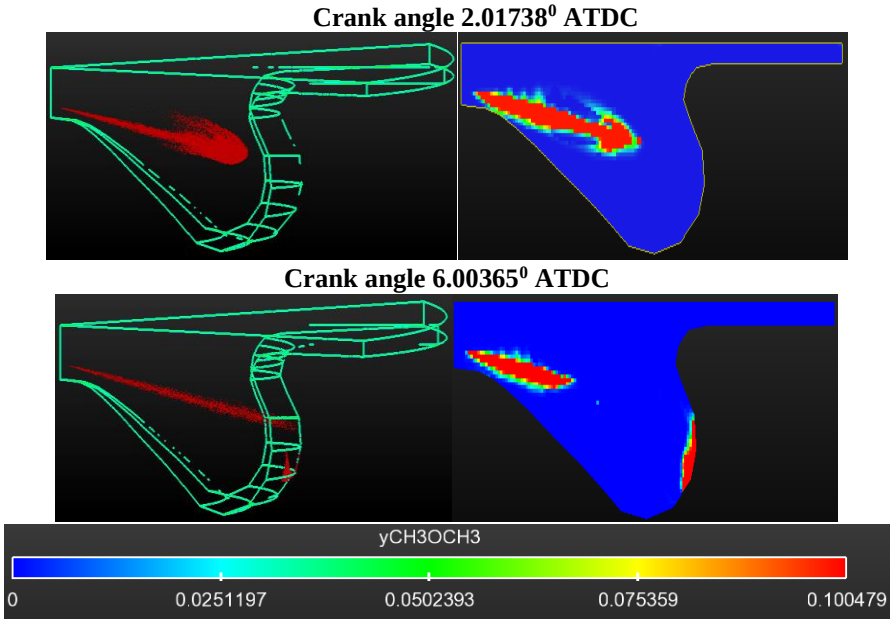
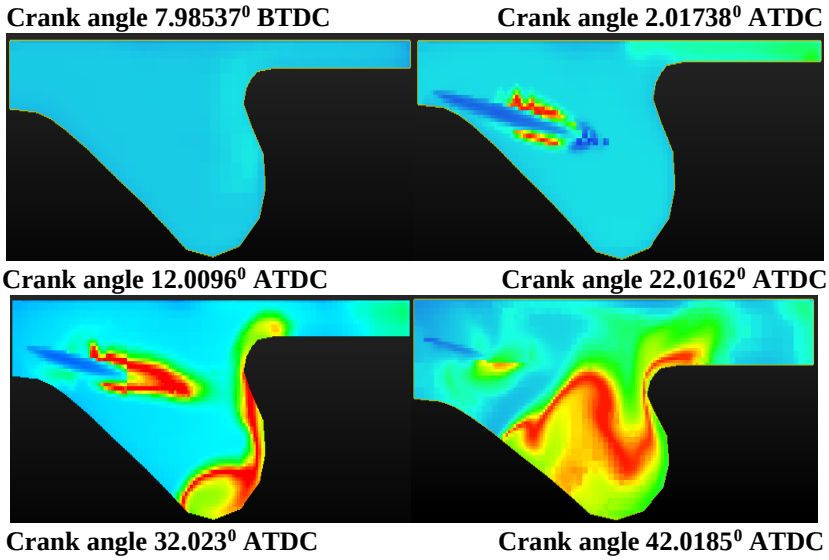


Figure 7 - Spray penetration and vaporization inside the cylinder after the main injection.

IV. CONCLUDING REMARKS

DME fuelled CI engine was studied computationally after validating with experimental data. Simulation was conducted for a pilot injection strategy in which 10% fuel was injected as pilot and 90% as main injection. Simulations show distinct two-stage ignition of pilot fuel. However, pilot injection at 40^0 BTDC leads to some over-mixed regions in which the hot ignition does not go to completion. This observation has implications for CO and HC formation. In addition, the pilot injection occurred in the squish region. Further studies should be conducted by varying the timing of pilot injection as well as the injector umbrella angle to optimize efficiency and minimize pollutants.



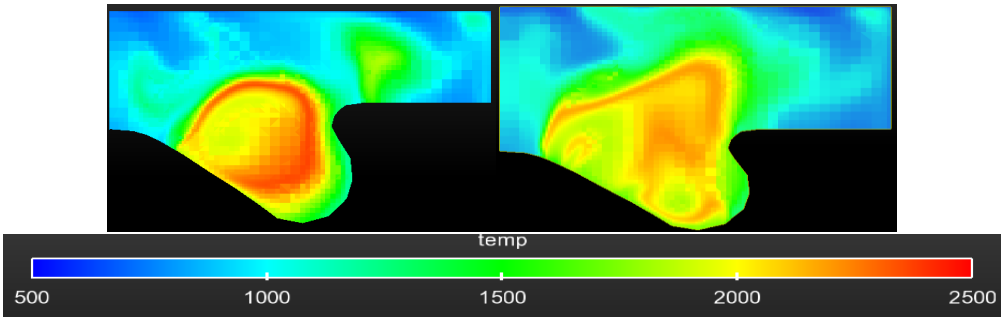


Figure 8 – Temperature distribution (K) inside the cylinder after pilot injection

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