Modelling of Methanol Combustion in a Direct Injection Compression Ignition Engine using an Accelerated Stochastic Fields Method

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Modelling of methanol combustion in a direct injection compression ignition engine using an accelerated stochastic fields method

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Abstract

Methanol combustion in a direct injection compression ignition (DICI) engine is studied using experiments and a novel approach based on Eulerian stochastic fields (ESF) method accelerated by the chemistry coordinate mapping (CCM) technique. This method is capable of handling all modes of combustion from auto-ignition to premixed flames and non-premixed flames in a mixture where they can potentially co-exist. Two operating conditions, namely, a HCCI and a partially premixed charged (PPC) operating modes are studied. It is shown that even in the PPC case, where the start of injection is near the top dead center (TDC), the start of ignition is well after the end of injection. As a result, combustion of methanol under both the HCCI and the PPC conditions involve strong auto-ignition contribution. In the PPC case, however, there are strong evidences of the presence of fuel-lean premixed flames in stratified mixtures. It is conformed the turbulence-chemistry interaction in the PPC case does have significant effects on the prediction of the onset of ignition, as well as on the progress of combustion to the later stages.

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Keywords: Eulerian stochastic field method; chemistry coodriante mappting; methnol; direct injection

1. Introduction

Methanol, CH_3OH, is the simplest alcohol and is potentially a renewable alternative for fossil fuel in the transport sector due to its environmental performance, low cost and large amount of feedstocks [1]. Currently methanol is used in shipping and also in automotive applications in China [2,3]. Methanol works very well in spark ignition (SI) engines due to its high octane rating and high heat of vaporization. Several studies showed that by using methanol the efficiency of SI engines can be improved compared to the gasoline operation. Operation in compression ignition (CI) engines is much less common. Apparently,

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operating with the high octane rating needs major changes to conventional CI engines to ignite the fuel. Caterpillar used a special injection ring pattern and glow-plug assistance to achieve year around operation with standard compression ratio diesel engines. Another approach is to use dual-fuel where direct injection of diesel is used to ignite the charge. Wärtsilä's concept of using separate direct injection of methanol and diesel while others use port injection of methanol and direct injection of diesel [4].

Whatever the injection and the operating strategy would be, the combustion of methanol spray may be very different from that of combustion of the conventional fossil based diesel fuels in the same operating strategy. There are at least two major controlling factors that can potentially shift the combustion of methanol spray from a classical diffusion controlled diesel flame to a partially premixed to premixed reacting system where ignition, premixed reaction front and diffusion flame can potentially co-exist and interact with each other. These factors are: its very high octane number; and its very large heat of evaporation.

Jangi et al. [5] have recently investigated the effect of fuel octane number on the structure of diesel spray combustion. They found that as the fuel octane number increases the combustion departs from classical diffusion controlled combustion to a more partially premixed and even premixed combustion, and significant heat release of combustion is come from auto-ignition and premixed flame rather than diffusion controlled flame front. This can be pronounced in the case of methanol combustion where its larger heat of evaporation cools down the surrounding gases, and prolongs the ignition delay time, which in turn enhances the mixing prior to the onset of auto-ignition, and thus promotes a premixed type of combustion. Motivated by this observation, a general purposed CFD modelling framework based on the Eulerian Stochastic Fields (ESF) is applied to study methanol combustion in direct injection compression ignition engines. Engine experiments are carried out and together with the CFD modelling the fundamental characteristics of methanol combustion is studied under HCCI and PPC operating conditions.

2. Mathematical model: PDF-CCM

In this study spray is modelled using Eulerian-Lagrangian method. The gas phase is described in Eulerian framework with the unsteady Reynolds-averaged Navier Stocks (URANS) equations. The liquid phase is presumed to be a discrete phase consisting of individual parcels and treated using Lagrangian particle tracking (LPT). OpenFOAM is used for numerical solution of the governing equations. The PDF method that is used here employs the Eulerian stochastic fields' (ESF) method [6]. In the ESF method, turbulent reactive flows are represented by N_F number of stochastic fields. The transport equation for the nth stochastic field is:

$$\bar{\rho} d\phi_\alpha^n = -\bar{\rho}\tilde{u}_i \frac{\partial \phi_\alpha^n}{\partial x_i} dt + \bar{\rho} S_\alpha^r(\boldsymbol{\phi}^n) dt + \bar{\rho} S_\alpha^s(\boldsymbol{\phi}^n) dt + \frac{\partial}{\partial x_i}(\Gamma_t \frac{\partial \phi_\alpha^n}{\partial x_i}) dt - \frac{1}{2}\bar{\rho} C_\phi (\phi_\alpha^n - \tilde{\phi}_\alpha)\omega_t dt + \bar{\rho}\sqrt{2\frac{\Gamma_t}{\bar{\rho}}}\frac{\partial \phi_\alpha^n}{\partial x_i} dW_i^n \qquad (1)$$

The above equation implies invoking the gradient transport hypothesis for approximating transport by turbulent velocity fluctuations. Here $\Gamma_t = \mu/\sigma + \mu_t/\sigma_t$ is the effective turbulence diffusion coefficient, μ_t is turbulent viscosity, and σ_t is turbulent Schmidt or Prandtl number. $S_\alpha^r dt$ is the change in ϕ_α^n due to chemical reactions and $S_\alpha^s dt$ is the change in ϕ_α^n due to spray. The term involves C_φ is the molecular mixing which is modelled by Interaction with Exchange to the Mean (IEM) model and ω_t in this term is the turbulent frequency obtained from $\omega_t = \varepsilon/k$ with k and ε being the turbulent kinetic energy dissipation rate. The dW_i^n represents the Wiener process vector that is spatially uniform but different for each field. Here, dW_i^n is approximated by the time-step increment $\sqrt{dt}\eta^n$ and η^n is a $(-1,1)$ dichotomic random number. The mean and moments of each variable α can be approximated from the ensemble of N_F stochastic fields.

An operator splitting strategy is used to integrate the chemical source terms, e.g., $\int_{t_0}^{t_0+dt} S_\alpha^r(\boldsymbol{\phi}^n)dt$. A potentially more efficient way to evaluate the chemical source terms would be to first identify and cluster all cells in all stochastic fields that have similar thermodynamic states into phase space zones, and then perform the integration once for all of the fields in the zone. This approach is known as clustering [7], or sometimes is referred to as an agglomeration [8] technique. The CCM approach as proposed in [5,9] is adopted for clustering. In principle, the CCM phase space consists of a subset of the composition space. The mapping of the n^{th} field with composition $\boldsymbol{\phi}^n(Y_1,\ldots,Y_{N_S},h)$ to the discretized phase space can be considered as a mapping between the CFD cell index (i,j,k) in n^{th} field to the zone index in the discretized phase space. In our previous study with transported PDF method for partially premixed lifted jet flames [9] as well as spray combustion with various fuels [5], we have shown that computational cells at a given time can be mapped into a phase space (T,ξ,χ,Y_{fuel}). Here, ξ is the elemental based mass fraction, χ is the scalar dissipation rate. The same strategy is adopted here; a mapping is carried out into (T,ξ,χ,Y_{fuel}) space. The sensitivity of the results to various extensions of the phase-space dimensionality, e.g., mapping to higher dimension $(T,\xi,\chi,Y_1,\ldots,Y_{N_S})$ can be found in our previous works [5,9] and references therein. In this study we use Bilger's mixture fraction ξ as one of phase space coordinates. The Bilger's mixture fraction for the n^{th} field, ξ^n, is

$$\xi^n = \frac{0.5(J_H^n - J_{H,o}^n)/W_H + 2(J_C^n - J_{C,o}^n)/W_C - (J_O^n - J_{O,o}^n)/W_O}{0.5(J_H^n - J_{H,f}^n)/W_H + 2(J_C^n - J_{C,f}^n)/W_C - (J_O^n - J_{O,f}^n)/W_O}, \quad (2)$$

where J_H, J_C and J_O are element mass fractions of hydrogen, carbon oxygen elements, respectively. W_H, W_C and W_O are atomic weights and subscripts "*o*" and "*f*" indicate the oxidizer and fuel streams, respectively. Elemental based scalar dissipation rate in the n^{th} field is

$$\chi^n = 2(\overline{D} + \frac{\mu_t}{Sc_t})\nabla\xi^n \cdot \nabla\xi^n. \quad (3)$$

Discretizing the phase space in the χ coordinate with uniform $\Delta\chi$ is not efficient; $\exp(-\chi)$ is used as the phase-space variable, instead. This is equivalent to disceretizing phase space in the χ coordinate with a non-uniform grid. For all other phase space variables, a uniform grid is employed.

3. Results and discussions

The simulation results presented here are based on a metal engine experiments. It is a heavy-duty CI engine, which was modified from a Scania D13 six cylinders engine with five of the cylinders deactivated. The bore size was 130 mm and the stroke 160 mm. The piston used, was a modified straight wall bowl piston and the geometric compression ratio was 15:1. The load range of these experiments was approximately 1.5-9.2 IMEPg using neat methanol with 200 ppm of infineum lubricant oil. Details of the engine specifications can be found in [10]. Simulation results are presented for two cases: case I with very early start of injection at -140 crank angle degree (CAD) after top-dead-center (ATDC); and case II with start of injection at -17.5 ATDC. The nozzle in both cases had 8 holes with a size of 0.135 mm, and the total injected fuel mass for case I was 164 mg/cycle and for case II 193 mg/cycle. The intake pressure and in both cases were 2.25 bar and 410 K. Both cases have injection duration of approximately 10 CAD with an engine RMP of 1200. In this way, case I was designed to replicate homogeneous charge compression ignition (HCCI) operating condition whereas case II was designed to mimic the combustion of methanol relevant to the injection timing in advanced diesel engines.

2.1 Early injection: HCCI operating condition

Figure 1 shows the time history of the in-cylinder charges temperature for case I with SOI of -140 ATDC. For this case the ESF method and an alternative well-stirred reactor combustion model (which is ESF with one stochastic field and no Wiener term in Eq. 1) give similar results and both agree well with the experiments. For this operating condition, it can be seen that the temperature of the in-cylinder gases remains lower than 800 K until -25 ATDC. The mixture in this temperature range is virtually chemically inactive. On the other hand, the early injection provides a sufficient time for the evaporation and mixing of the injected fuel with the ambient gases. This case is regarded as a HCCI case.

To examine the fuel/air mixing process, the volume averaged equivalence ratio of the in-cylinder gases as well as the root-mean-square of spatial fluctuations (a measure of mixture inhomogeneity) are shown in Fig. 2. It can be seen that after the start of injection, the equivalence ratio and its fluctuation are both rapidly increasing. This is due to the evaporation of the injected fuel. After the end of injection, at -130 ATDC, the equivalence ratio maintains its increasing trend until -60 ATDC. This implies the liquid droplets will still present in the domain for almost 70 CAD after the end of injection before they are entirely evaporated.

The spatial fluctuation, which is a measure of the inhomogeneity of the composition of the gases, also shown in this figure, is governed by the competition between two processes: the evaporation, which is in favour of creating the inhomogeneity; and turbulence mixing which is acting to diminish the inhomogeneity. Results imply that during the injection and for 5 CAD after the end of injection the evaporation is stronger than the mixing rate. However, shortly after the end of injection the evaporation process became less important as it is evident in the decrease of the slope of the equivalence ratio profile. When the evaporation is almost finished at around -75 ATDC, the inhomogeneity in the composition is quickly vanished within 30 CAD. This is reflected in the composition and temperature of in-cylinder gases (not shown) as they become almost homogeneous everywhere in the domain.

2.2 Late injection: PCCI operating condition

Shown in Fig. 3 is the pressure trace in case II. Symbols in this figure are from experiments; the solid line is the simulation results with ESF method and with 48 stochastic fields whereas the dashed-dotted line is the simulation results using the well-stirred reactor (WSR) model. The simulations using the ESF method agree very well with the experiments, while the WSR model predicts a much slow ignition. Obviously, the results in case II are very sensitive to the combustion sub-model, which implies in case II (the PPC case) the impact of turbulence-chemistry interaction in the modelling is significant. We further analysis the results and elaborate on this idea.

The rapidly increasing of the pressure right after the onset of ignition at around TDC implies the methanol combustion in DICI engine is far different from combustion of conventional diesel fuel under similar operating condition. This feature is very similar to that of the pressure trace in the HCCI operating mode and indicates significant contribution of auto-ignition to the total heat release rate from combustion, even with an SOI of -17.5 ATDC of case II. There are two reasons behind this combustion behaviour: the first is the large evaporation heat of methanol compared with that of the fossil based diesel fuel; the second is the very high octane number of methanol of around 120 compared with that of diesel fuel with an octane number of 40-60. Both these effects delayed the onset of auto-ignition. As it can be seen in Fig. 3, the onset of ignition for this case has been retarded approximately to around TDC, which is more than 7 CAD after the end of injection. Note that the ignition dwell in the classical diesel engine is negative (ignition start before the end of injection).

The positive 7 CAD dwell is a rather long delay, and provides enough time for premixing before high temperature combustion starts. This is best seen in Fig. 4, where snapshots of temperature and mixture fraction distribution at four instances have been shown.

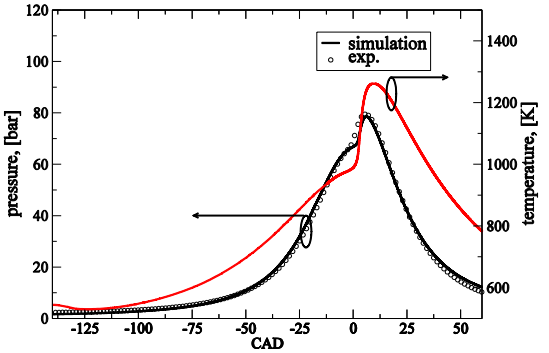

Figure 1. Pressure trace and in cylinder gases temperature for case I.

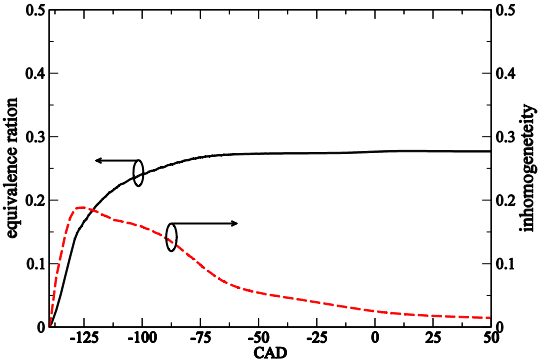

Figure 2. Inhomogeneity and its fluctuations in case I.

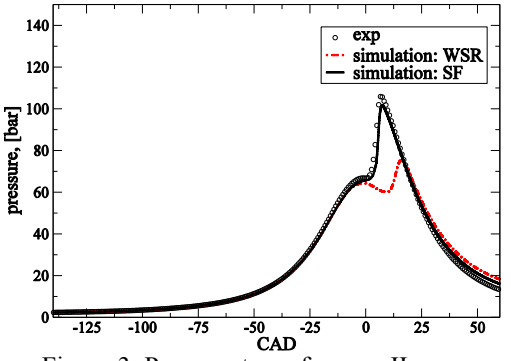

Figure 3. Pressure trace for case II.

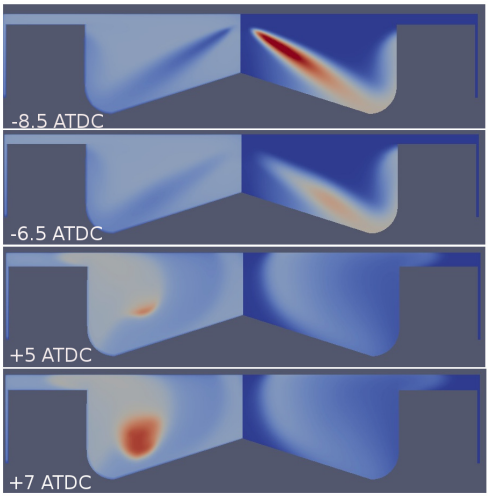

Figure 4. Snapshot of temperature (on the left-hand-side), and mixture fraction (on the right-hand-side) distribution near TDC for case II. The blue-red colour range for temperature is 500-2200 K and in mixture fraction 0-0.25.

In Fig. 4, and at CAD, the left-hand-side is temperature and the right-hand-side is mixture fraction distribution. Particularly, only 1 CAD after the end of injection, at -6.5 ATDC, the fuel-rich region has been substantially shrunken. This is attributed to the mixing rate enhancement after the end of injection, which and has been observed experimentally by others in optical engine experiments, cf., Cartier et al. 2011 [11]. More important is the distribution of mixture fraction before the onset of auto-ignition around +5 ATDC. As it can be seen, the mixture has become rather premixed almost everywhere in the domain. The detailed analysis of the results showed stratified premixed gases with a mixture fraction variation in the range of 0-0.11 at +5 ATDC. Considering the stoichiometric mixture fraction for methanol/air mixture of 0.135, is can be concluded that before the onset of auto-ignition the mixture everywhere is the domain has an equivalent ratio of smaller than unity and is fuel-lean.

Results show that combustion mode, even in case II with a late start of injection of -17.5 ATDC, is auto-ignition to premixed flame propagation in stratified fuel-lean mixtures. Obviously, such combustion mode is different form that is observed in the classical diesel engines operating with diesel fuels in which the combustion is dominated by non-premixed diffusion controlled flame. This finding is of great importance both from practical point of view, as well as from theoretical and modelling aspects of combustion science.

4. Conclusions

An accelerated Eulerian stochastic fields (ESF) method was formulated and applied to simulate combustion of methanol in DICI and under different operating conditions. Different operating conditions were achieved by adjusting different start of injection. Results showed that very early injection with an SOI of -140 ATDC leads to an HCCI combustion mode where auto-ignition is the dominating phenomenon. However, with a SOI of -17.5 ATDC the combustion process exhibits very different trend. In these conditions, although the pressure trace exhibits very similarity to the HCCI case, which implies significant contribution of heat release form auto-ignition, however, the simulation results was very sensitive to the inclusion of the turbulent-chemistry interaction in the modelling. This feature is not seen in HCCI mode. Although the start of ignition for this case was also well after the end of injection, yet, the in-cylinder gas cannot be modelled as a perfectly homogeneous mixture and turbulence-chemistry interaction appears to play an important role. It was shown that methanol combustion has a tendency of combusting in a mixed mode of both auto-ignition and premixed reaction front propagation, which is significantly different from diesel fuelled PPC engine under similar operation conditions. The consequence is a rather high pressure-rise-rate in methanol engine as compared with diesel engine.

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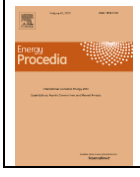

Biography

Mehdi Jangi earned his PhD from Tohoku University in Japan. He then moved to Sweden and worked as a senior researcher in Lund University from 2009-2015. He joined Murdoch University in Perth, Australia in 2016.