Implementation of CMC in a 0-D Single-Zone Model of a Diesel HCCI Engine

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Abstract

Homogeneous charge compression ignition (HCCI) engines use a new mode of combustion where, in principle, there is no spark plug or fuel injector to initiate the combustion. The combustion is self-ignited once the mixture has reached its chemical activation energy. Thus, the combustion is fully controlled by the chemical kinetics mechanism. A zero-dimensional (0-D) single-zone (homogeneous) model was used to study the combustion behaviour, where the model is able to reduce the computing time. A Conditional Moment Closure (CMC) model was then implemented in this 0-D environment to account for the turbulent mixing effects in the combustion chamber. The results show that the use of CMC in a 0-D environment improves on the results from the homogeneous model by eliminating the characteristics of short combustion duration and high peak pressure of the homogeneous model. The model is also in a good agreement with experiment and thus can be used for further analysis.

Keywords: CMC, Diesel HCCI, zero-dimensional,0-D, single-zone, homogeneous

1. Introduction

Homogenous Charge Compression Ignition (HCCI) engine research has received worldwide attention due to its advantages in reducing emissions levels, such as NOx and soot [1, 2]. The engine has the potential to be used in a hybrid configuration (combination of two or more power sources), which can reduce the emissions levels further [3]. In principle, the engine has no spark plug or fuel injector to initiate the combustion [4]. Instead, the combustion is self-ignited once the mixture has reached its chemical activation energy [5]. Thus, the engine is fully controlled by the chemical kinetics mechanism [6].

Simulations are undertaken to reduce research costs while maintaining good productivity because of their cost efficiency compared to experiment. For engine research, a zero-dimensional (0-D) model is known for its advantage in reducing computational time compared with a multidimensional Computational Fluid Dynamics (CFD) approach. However, the 0-D model has the limitation of shorter combustion duration and rapid pressure rise compared to experiment [7, 8]. CFD on the other hand yields more accurate results at the expense of computational resources [9, 10]. In short, CFD could be used for an in-depth fundamental study, while a 0-D model offers versatility in a reduced simulation time.

Conditional Moment Closure (CMC) [11] is a model for the mixing in the combustion chamber at modest computational cost. The use of CMC in a 0-D engine simulation is relatively new in the literature, where most of the CMC studies use the CFD approach [12-14]. Kwon et al. [15] studied the use of CMC in a 0-D model of diesel engine. The diesel was direct-injected and the spray was modelled with a multi-zone spray penetration model. They reported that the result of the in-cylinder pressure trace was in reasonably good agreement with the experiment, showing that the CMC model could be used in a 0-D simulation.

The approach used in this paper is slightly different, where the engine used is a HCCI engine with fuel being injected in the inlet manifold instead of direct-injected. Thus, there is no spray model to be used in the combustion chamber, following the HCCI combustion principle. This study aims to validate the use of the CMC model in a 0-D HCCI engine simulation before progressing to a parametric study.

2. Model Formulation

The 0-D model in this paper is for an open system, initially developed by Assanis and Heywood [16]. However, the model uses chemical kinetics to solve the chemical reactions during combustion, while Assanis and Heywood [16] used a pre-defined ignition model without chemical reactions. The approach used here also uses a different heat transfer model; the equations used in the 0-D model are detailed elsewhere [17]. The 0-D model is then coupled together with the CMC model.

2.1 Conditional Moment Closure Model

The CMC transport equations solve the conditional means of reactive scalars and temperature. The reactive scalar is chosen to be Y_i, which is the mass fraction of species i. In the CMC model, this is

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conditioned on the conserved scalar Z, which is the mixture fraction:

$$Q_i \equiv \langle Y_i | \eta = Z \rangle \tag{1}$$

where η is the sample space variable for the mixture fraction Z.

A homogenous CMC, also called 0-D CMC model was used in the study. The combustion chamber is modelled as an Incompletely Stirred Reactor (ISR) [15] with varying Probability Density Function (PDF). By using volume integration and flux divergence theorem, the conservative CMC equation of ISR for the *i*th species mass fraction and enthalpy reduces to

$$\frac{\partial Q_i P_z \rho_\eta}{\partial t} + \frac{(Q - Q_{in})\dot{m}_{in} P_{in}^*}{\rho V} = P_z \langle N|\eta \rangle \frac{\partial^2 Q_i}{\partial \eta^2} + P_z \langle \dot{\omega}|\eta \rangle \tag{2}$$

$$\frac{\partial Q_h P_z \rho_\eta}{\partial t} + \frac{\left(Q - Q_{in}\right)\dot{m}_{in} P_{in}^*}{\rho V} = P_z \rho_\eta \langle N|\eta \rangle \frac{\partial^2 Q_h}{\partial \eta^2} + P_z \rho_\eta \left\langle \frac{1}{\rho_\eta} \frac{\partial p}{\partial t} \middle| \eta \right\rangle - P_z \rho_\eta \left(h_c (Q_T - T_w) \frac{A_w}{m} \right) \tag{3}$$

where ρ_η is the conditional density, V is the volume, $\dot{m}_{in}$ is the mass flow rate into the system, Q_{in} is the inlet reactive scalar and P_{in}^* is the inlet averaged PDF. The first and second terms on the LHS of (2) and (3) are the transient and flux, respectively. The first term on the RHS of (2) represents the diffusion in conserved scalar space affected by scalar dissipation rate, N, and the last term is the conditional expectation of the chemical source term, $\dot{\omega}$. The mass flow rate $\dot{m}_{in}$ in (2) and (3) is a function of time depending on the inlet valve opening and closing. The pressure rate of change, $\partial p/\partial t$ in (3) is important in engine simulation due to varying in-cylinder pressure across the crank angle (CA) step [13]. A heat loss term is introduced in the enthalpy equation: Q_T is the conditional temperature, T_w is the wall temperature, A_w is the total cylinder wall area and m is the total mass of the mixture in the chamber.

In HCCI engines, the heat loss due to radiation is neglected because its effect is very small [18, 19]. The convective heat loss is used to model the heat loss via the cylinder wall. The heat transfer coefficient, h_c is modelled by the modified Woschni correlation [19], as given by

$$h_c = \propto_{scaling} B^{-0.2} p^{0.8} T^{-0.73} (v_{tuned})^{0.8} \tag{4}$$

where $\propto_{scaling}$ is the scaling factor used to match the experimental data, which is 194.7 [20]. B is the bore and v_{tuned} is the characteristic velocity, given by

$$v_{tuned} = C_1 \overline{S_p} + \frac{C_2}{6} \frac{V_d T_r}{p_r V_r} (p - p_{mot}) \tag{5}$$

C_1 and C_2 are constants which are 2.28 and 0.00324, respectively. $\overline{S_p}$ is the mean piston speed, V_d is the displacement volume, T_r, p_r and V_r are the temperature, pressure and volume at the reference point and p_{mot} is the motoring pressure (pressure without combustion).

The conditional scalar dissipation rate in (2) and (3) is modelled using the Amplitude Mapping Closure (AMC) [21] as

$$\langle N|\eta \rangle = \frac{\bar{\chi} G(\eta)}{2 \int_0^1 G(\eta) P_z(\eta) d\eta} \tag{6}$$

$$G(\eta) = \exp(-2[\mathrm{erf}^{-1}(2\eta - 1)]^2) \tag{7}$$

where erf is the error function and $P_z(\eta)$ is the mixture-fraction PDF. The mean scalar dissipation rate, $\bar{\chi}$, is modelled by

$$\bar{\chi} = C_D \frac{\varepsilon}{k} \widetilde{Z''^2} \tag{8}$$

A simplified k-ε model for 0-D simulation [22] is used to model the turbulence dissipation rate, ε, and turbulence kinetic energy k in (8). $\widetilde{Z''^2}$ is the mixture fraction variance and C_D is a constant, selected to be 1.5 as the best match of the simulation results with experiment. The PDF of the mixture fraction P_z is modelled using a presumed β-function PDF. Then, the mean mass fraction of the *i*th species is obtained as

$$\overline{Y_i} = \int_0^1 Q_i(\eta)\, P_z(\eta) d\eta \tag{9}$$

2.2 Interfacing of CMC and 0-D Model

A 0-D model is used to solve the energy equation formulated with the CA as the independent variable instead of time [17]. The CMC model is used to transport the conditional species mass fraction and enthalpy to obtain the mean values for feedback to the energy equation. The program was coded such that the ordinary differential equation (ODE) obtained from the energy and CMC equations were solved using a stiff solver. The interfacing between 0-D and CMC models is shown in Fig. 1.

The 0-D model calculated all the in-cylinder parameters including the turbulence at each CA step. Then the turbulent quantities were used to solve the CMC equations, where the Cantera [23] chemical kinetics package was used to provide the chemical properties and reactions mechanisms. Equations (2) and (3) were solved using implicit finite difference method. To ensure the stability of the code, a Courant–Friedrichs–Lewy (CFL) criterion for the diffusion term was checked at each CA step, with CFL $\leq 1/6$ in order to minimize the truncation error [24].

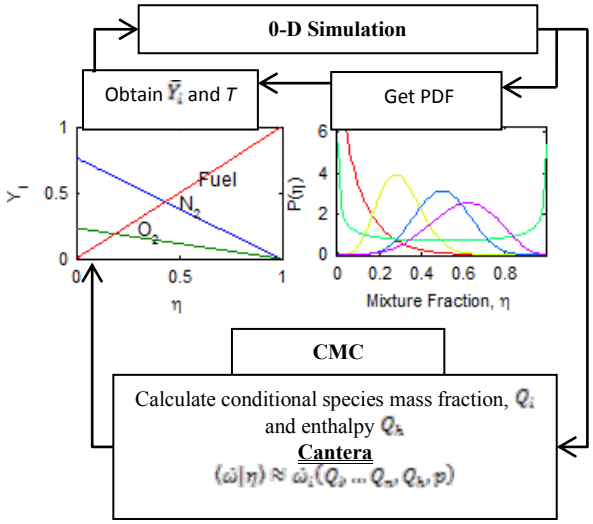

Figure 1 Interfacing between 0-D and CMC models.

3. Results and Analysis

The model was validated against experimental data and 0-D model from Guo et al. [25], where the HCCI engine was run by using *n*-heptane as the fuel with port fuel injection. The *n*-heptane reduced mechanism [26] with 160 species and 770 elementary reactions was chosen as a surrogate fuel because the chemical properties (e.g. cetane number) are similar to conventional diesel. Furthermore, *n*-heptane as a diesel surrogate has been widely used by many researchers [27, 28]. The engine parameters used in this simulation are shown in Table 1.

Table 1 Engine parameters used in the simulation [25]

Cylinder bore	82.55 mm
Stroke	114.3 mm
Connecting rod length	254 mm
Compression ratio	10
Engine speed	900 rpm
Inlet pressure	95 kPa
Inlet valve open (IVO)	10° CA ATDC
Inlet valve closed (IVC)	36° CA ABDC
Exhaust valve open (EVO)	40° CA BBDC
Exhaust valve closed (EVC)	5° CA ATDC

The simulation result is compared with the experimental data in Fig. 2. For 0-D model, the intake air temperature was set 20K higher than the actual to account for the mixing effects [25]. Another study also stated that the intake temperature for a single-zone model has to be increased up to 30K, while up to about 10K for a multi-zone model [29]. In the study for the 0-D model only [17], the intake temperature was increased to 333K for the intake temperature of 313K.

The result in Fig. 2 shows that both 0-D models predict higher in-cylinder pressure compared to the experiment, with the 0-D model from Guo et al. [25] over-predicting by more. In a diesel HCCI engine, the fuel has a characteristic of two-stage ignition, which is low temperature reaction (LTR) (also called the cool flame phenomenon) and high temperature reaction (HTR) [30, 31]. LTR for the 0-D models occurred at a temperature below the auto-ignition temperature and was advanced by about 10° CA compared to the experiment.

CMC with 0-D model on the other hand, is in good agreement with the experiment. The model predicted the LTR and HTR points close to the experiment. However, the model predicts lower in-cylinder peak pressure. This behaviour is similar to that observed when modelling a 0-D CMC in a diesel engine, where the result was improved when implementing CMC in a multi-dimensional simulation (Fig. 3) [14].

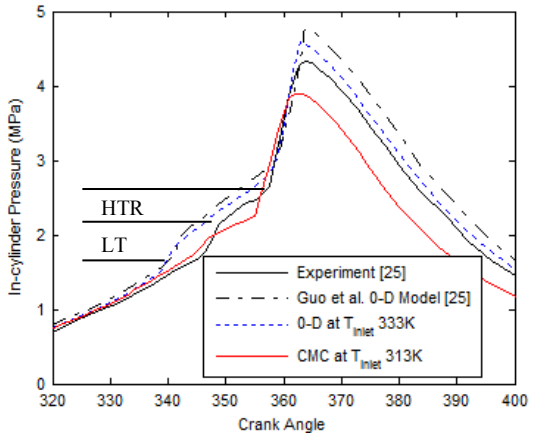

Figure 2 Comparison of the in-cylinder pressure between experiment [25], 0-D from Guo et al. [25], 0-D in this study and CMC with 0-D.

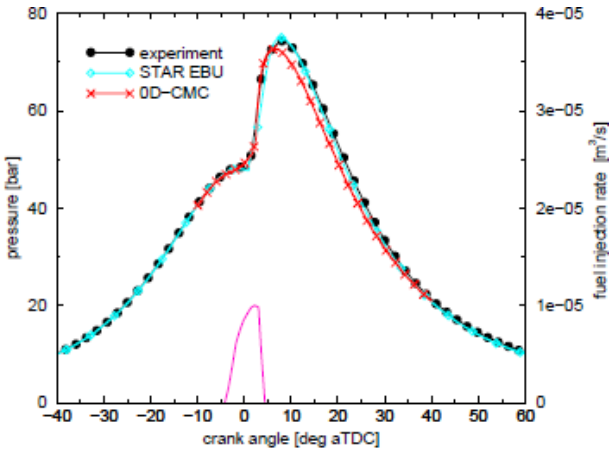

Figure 3 0-D CMC and a multi-dimensional simulation (STAR EBU) compared with experiment [14]

The advantage of using CMC in 0-D mode in this study is that the model does not require the increase in intake air temperature that a 0-D model needs. Instead, the model uses the actual experimental intake temperature, which is 313K. The result shown in Fig. 2 was using the intake temperature of 313K for CMC compared to 333K for 0-D alone, where both of them yield almost a similar HTR point.

To test the sensitivity of the intake temperature, Fig. 4 shows the CMC model with the same intake temperature as the 0-D, which is 333K: the combustion is advanced by about 10˚ CA. This is expected from actual engine operation: combustion is advanced when

the intake temperature increases. The 0-D model on the other hand, predicted that auto-ignition failed to occur when the intake temperature was set to be the same as the experimental data. Thus, it is necessary to fine tune the intake temperature before the 0-D model can be used, while the CMC model can be used without any artificial alteration of the input parameters.

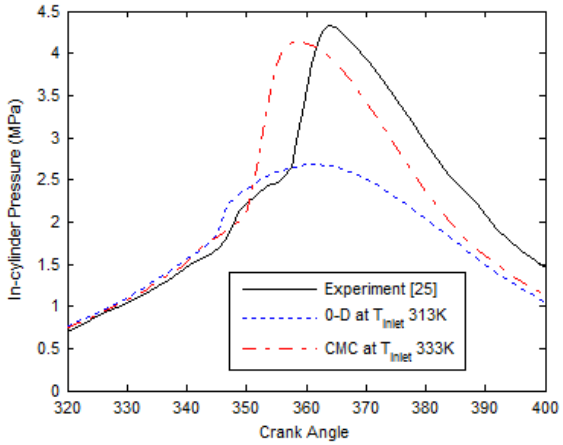

Figure 4 Combustion behaviours when the intake temperature was changed for both models.

4. Conclusion

This paper has discussed the use of CMC in a 0-D model of a diesel HCCI engine. Both the 0-D and CMC models are in good agreement with the experiment. 0-D model over-predicts the in-cylinder pressure, while CMC under-predicts it. The 0-D model also advanced the LTR by about 10˚CA, where the CMC predicts the timing well. The CMC model has the advantage by using the actual intake temperature, while predicting HTR point well, compared to the 0-D model where the intake temperature has to be increased to account for the mixing effects. Because the CMC model in a 0-D simulation predicts the timing of key events with a known under-prediction of pressure, this model can be used for further analysis.

5. References

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