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Combustion Modeling in RCCI Engines with a Hybrid Characteristic Time Combustion and Closed Reactor Model*

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Abstract: This study proposed a hybrid model consisting of a characteristic time combustion (CTC) model and a closed reactor model for the combustion modelling with detailed chemistry in RCCI engines. In the light of the basic idea of the CTC model of achieving chemical equilibrium in high temperature, this hybrid model uses the CTC model to solve the species conversion and heat release in the diffusion flame. Except for the diffusion flame, the auto-ignition in RCCI combustion is computed by a closed reactor model with the CHEMKIN library by assuming that the computational cells are closed reactors. The border of the transition between the CTC model and closed reactor model is determined by two criteria, a critical temperature and a critical Damköhler number. On the formulation of this hybrid model, emphasis is placed on coupling detailed chemistry into this hybrid model. A CEQ solver for species equilibrium calculations at certain temperature, pressure was embedded with CTC for detailed chemistry calculation. Then this combustion model was integrated with the CFD framework KIVA4 and the chemical library CHEMKIN-II and validated in a RCCI engine. The predicted in-cylinder pressure and heat release rate (HRR)

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show a good consistency with the data from the experiment and better accuracy than that computed from the sole closed reactor model. More importantly, it is observed that this model could save computational time compared with closed reactor model due to less stiff ordinary differential equations (ODEs) computation. A sensitivity analysis of the critical temperature and critical Damköhler number was conducted to demonstrate the effect of these two parameters in the current model.

Keywords: RCCI combustion modeling, CTC model, CHEMKIN, hybrid model

1 Introduction

Internal combustion engines are basically classified into compression ignition (CI) engines and spark ignition (SI) engines, both of which have their pros and cons [1]. CI engines have been widely applied in industry such as in ships and trucks because of its high thermal efficiency. The high thermal efficiency of CI engine is attributed to its instinct features of high compression ratio and combustion organization type. However, because of these features, the high temperature and fuel rich zones lead to higher detrimental emissions such as NO_x and particulate matter (PM). In contrast, SI engines which employ a spark plug to ignite the premixed fuel/air mixture and organize combustion by flame propagation show lower thermal efficiency but better emission performance. Therefore, efforts have been devoted for proposing advanced engine combustion modes for reducing emissions while maintaining high efficiency. Generally, most of these advanced combustion modes are in an effort to aggregate the advantages of CI and SI engines and at the same time, avoid their disadvantages.

HCCI is one of the first proposed types of advanced combustion modes in engines, which has drawn tremendous attention of engine researchers due to its ideal combustion and emission performance. The fundamental idea of HCCI is to combine the advantages of SI and DICI engines while to avoid their disadvantages, as SI engine features low soot emission but low thermal efficiency, DICI engine shows high thermal efficiency but high level NO_x-soot trade-off relation [2]. In HCCI, the combustion occurs at nearly constant volume and homogeneously. As a result, its low combustion temperature and homogeneously lean combustion lead to extremely low emission and a good efficiency. However, because of no direct control strategy of HCCI combustion phasing (the ignition is primarily determined by the fuel/air mixture properties and chemical kinetics), the major challenges in HCCI are the lack of proper combustion phasing control and its undesirably excessive pressure rise rates [2].

To find the best fuels in HCCI engines, Bessonette et al. [3] experimentally investigated the engine performance with different fuel blends for HCCI operations.

They concluded that the best fuel should have the auto-ignition ability between diesel and gasoline. Subsequently, motivated by this result, dual-fuel type advanced combustion mode, PCCI, was proposed. Both modelling and experimental investigation suggest that PCCI presents better combustion controllability than HCCI since a strategy of different blending fuel ratios could be used to control the ignition timing in PCCI [4-6]. To extend the combustion controllability more thus engine operating loads, RCCI was proposed by Kokjohn et al. [7]. The distinct fuel intake manner in RCCI (port fuel injection with low reactivity fuel and direct injection with high reactivity fuel) is able to form fuel stratification in the combustion chamber, suppressing the pressure rise rate (PPR) and broaden the operation loads [6-9]. However, as a variant of HCCI and PCCI concept, RCCI, in nature, still has engine knocking tendency especially at high engine loads. In addition, the fuel diversity in RCCI engine makes fuel design and management a necessity. Due to high cost and time-consuming issues in experiment, calibration and fuel design for RCCI engine in combustion modelling would be an effective and efficient way.

Since RCCI combustion involves low-temperature combustion, auto-ignition and partially premixed combustion, rendering substantial complexity for combustion modelling, different researchers proposed RCCI combustion models and integrated them into CFD framework for RCCI engine simulations.

Kong et al. [10] applied a multi-dimensional CFD software KIVA3-V coupled with CHEMKIN library [11] to solve the chemistry kinetics for HCCI modelling. By taking each cell in the computational domain as a closed reactor, ODEs are solved under a constant volume condition. It was proved that this way showed robust prediction in HCCI modelling researches and widely adopted by the following researchers. Because RCCI is a variant of HCCI, this method has been also applied for RCCI engine simulation and has showed good predictability [7, 12-15]. In fact, considering that in the KIVA framework, the transport and chemical source terms are solved separately [16], this method has also been used for conventional diesel engine simulations in which the combustion is organized by diffusion flame. However, its

computational price is high especially for detailed mechanisms with large size and most of the computational time are consumed by solving the ODEs in CHEMKIN. Moreover, multiple combustion modes including mixing controlled flame and auto-ignition may co-exist in RCCI combustion, an effective method to model the diffusion flame and treat the border between diffusion flame and auto-ignition is important. Thus, efficient and robust methods for integrating the combustion chemistry in RCCI engine simulation are desirable.

This study proposed a CTC model based on the original CTC model for DICI combustion [17] and coupled it with a closed reactor model for RCCI combustion simulation. It is able to solve the detailed chemical kinetics in RCCI combustion and show favorable computational price and accuracy than the commonly used sole closed reactor model with CHEMKIN. This hybrid model was integrated into the KIVA4 codes and validated by comparing with the experimental data from a RCCI engine fueled with gasoline/diesel. It is observed that this model can give reasonable combustion characteristic compared with the measured data. A better accuracy than the sole closed reactor model with CHEMKIN can be found as well. More importantly, an evident computational overhead reduction of the current model can be observed than the closed reactor model with CHEMKIN.

2 Methodology

In conventional simulations of diesel diffusion flame, for the cells lower than a critical temperature T_c , all the chemistry and internal energy change in these cells will be treated by auto-ignition models (SHELL in the classical SHELL-CTC model with generic chemistry; closed reactor model in CHEMKIN with detailed chemistry). In the existing RCCI engine combustion models, all the auto-ignition and diffusion flame are handled by the closed reactor model with the CHEMKIN library without considering the sub-grid turbulence-chemistry interaction. To illustrate the current model in a direct way, a schematic figure is shown as Fig. 1. Compared with the figure of quasi-steady diesel combustion plume as presented from Sandia National Laboratories [18], it is observed that due to the low temperature, the spray vapor

transport to the end of the combustion chamber with slight first-stage low temperature combustion. At the end of the spray tip, the mixing between the vapor and the air is still controlling the combustion. This study proposed a hybrid model with computing the auto-ignition cells by closed reactor model with CHEMKIN and calculating the mixing controlled combustion by CTC, as shown in Fig. 1.

Nevertheless, the classical CTC model was formulated with a generic chemical model and is not capable of dealing with detailed chemistry. In the following sections, the formulation of CTC with detailed chemistry is presented; a brief introduction of the closed reactor model treated by CHEMKIN library is then described; the solution algorithm and the couple of these two models are finally introduced.

2.1 Formulation of CTC model

The characteristic time combustion (CTC) model is a classical model to be used in conventional diesel combustion [17, 19]. The assumption in this model is that in the high temperature conditions, the chemistry in the system tends to be in equilibrium after a certain period of time. Thus in this model, the conversion rate of the partial density for specie n is given by

$$\frac{dY_n}{dt} = -\frac{Y_n - Y_n^*}{\tau_c} \quad (1)$$

where Y_n is the mass fraction of specie n , Y_n^* is the instantaneous equilibrium value of the mass fraction, τ_c is the characteristics time-scale to achieve such an equilibrium state. It is noted that the most critical parameter in Eq. (1) to be modelled is the characteristic time-scale τ_c and the instantaneous equilibrium value Y_n^* .

Typically, the characteristic time is approximately formulated by the sum of the laminar timescale and the turbulent timescale [17], i.e.

$$\tau_c = \tau_l + f \cdot \tau_t \quad (2)$$

where τ_l is the laminar timescale; τ_t is the turbulent timescale; f is a delay coefficient that determines the controlling role of turbulent effects.

Since the current CFD framework KIVA4 adopts RNG $\kappa-\varepsilon$ turbulence model [20], the turbulent characteristic timescale was estimated by

$$\tau_t = C_2 \cdot k / \varepsilon \quad (3)$$

where k and ε are calculated in the turbulence model. C_2 is a model constant with a value of 0.1 in the original RNG $\kappa-\varepsilon$ model, which is considered as a tunable parameter in the current study. The sensitivity analysis of C_2 will be shown in the following section.

The laminar timescale could be calculated by an eigen-analysis of the Jacobian matrix of the chemistry ODEs by

$$\tau_l = 1 / |\lambda_g(J)| \quad (4)$$

where J is the Jacobian matrix of the chemistry ODEs; λ_g is the eigenvalue of J .

However, the Jacobian matrix either evaluated numerically or analytically and its decomposition could cause undesirable computation overhead. Hence, a semi-empirical one-step reaction rate from a single droplet auto-ignition experiment for n-heptane and iso-octane [21] are used to predict the laminar timescale:

$$\tau_{gasoline} = A_1^{-1} \cdot [C_8H_{18}]^{0.25} \cdot [O_2]^{1.25} \cdot \exp(-E_1 / RT) \quad (5a)$$

$$\tau_{diesel} = A_2^{-1} \cdot [C_7H_{16}]^{0.25} \cdot [O_2]^{1.25} \cdot \exp(-E_2 / RT) \quad (5b)$$

$$\tau_l = x(C_7H_{16}) \cdot \tau_{diesel} + x(C_8H_{18}) \cdot \tau_{gasoline} \quad (5c)$$

in which, the bracket here implies the mole concentration; $A_1 = 5.1e+11$; $E_1 = 125.52$ kJ/mol; $A_2 = 4.6e+11$; $E_2 = 167.36$ kJ/mol; R is the universal gas constant; T is the temperature; x means the mole fraction of one single fuel in the binary fuels.

The delay coefficient f in Eq. 2 is calculated by:

$$f = \frac{1 - e^{-r}}{1 - e} \quad (6)$$

where r is a parameter to indicate the completeness of combustion and could be approximated by:

$$r = \frac{Y(CO_2) + Y(H_2O)}{1 - Y(N_2)} \quad (7)$$

where Y means the mass fraction of a certain species.

Another important parameter in CTC model is the equilibrium partial density. Unlike the classical CTC model [17] which only 7 species were considered and the equilibrium partial density could be evaluated by assuming an incomplete combustion with products of CO, H₂O and CO₂ or a complete combustion with products of CO and H₂O and solving a serial of linear equations, the current model was proposed to account for detailed chemistry. Thus, in order to evaluate the equilibrium partial density Y^* , a chemical equilibrium solver CEQ [22] was coupled into the current CFD code KIVA4. CEQ adopted Gibbs function continuation algorithm to achieve better computational stability and solved the local species mass fraction as a function of local enthalpy and pressure:

$$Y^* = Y_i^{EQ}(H, P) \quad (8)$$

In addition, the classic CTC is supposed to be proposed for diffusion flame computation in conventional diesel engine combustion which is known as the type of mixing-controlled combustion. Hence, if applied in RCCI combustion, besides the temperature, another border in the CTC model should be designed to identify the diffusion flame regime. In this study, the Damköhler number indicating the chemical reaction timescale (reaction rate) to the transport phenomena rate occurring in the system is adopted:

$$Da = \tau_t / \tau_l \quad (9)$$

where Da is the Damköhler number. Hence, if the Damköhler number in a certain cell is larger than a critical Damköhler number Da_c , the transport phenomena in that cell dominates the rate thus this cell will be computed by the CTC model. In sum, the precondition that the cell should be taken as in the diffusion flame regime is that its temperature is larger than T_c as well as its Damköhler number is larger than Da_c .

2.2 Closed reactor model with CHEMKIN

In the current study, except for the cells whose temperatures are greater than T_c and thus considered to be tended into equilibrium, the chemistry in other cells are

deemed to be trapped in closed reactors, in which the species conversion and the enthalpy change are solved by a chemistry solver – CHEMKIN. A skeletal primary reference fuel (PRF) chemical mechanism consisting of 48 species and 153 reactions was adopted for the combustion chemistry of gasoline and diesel [23] in this study. The convection and diffusion transport between cells are modelled by the RNG $\kappa-\varepsilon$ turbulence model [20]. Once considering the chemical process in a cell, this cell was considered as a closed system, in which the sub-grid scale turbulence chemistry interaction is not considered. Using CHEMKIN to model the combustion in the two limits from chemistry-controlled combustion to mixing-controlled combustion has been proved working well [16]. The basic principle in CHEMKIN is that the change of each species in one closed computational cell was given by

$$\frac{dY_n}{dt} = v \cdot \dot{\omega}_n \cdot MW_n \quad (10)$$

where v is the specific volume, Y_n is the mass fraction of species n , MW_n is the molecular weight. Within a certain time step, $\dot{\omega}_n$ is the production rate at a given temperature and molar concentrations. Hence, if nsp is the number of species in chemical mechanism, a set of ordinary differential equations (ODEs) with nsp equations will be built and then solved by DVODE [24]. In this way, the energy governing equation can be obtained under constant pressure conditions as

$$dQ - v \sum_{n=1}^{nsp} e_n \dot{\omega}_n MW_n = 0 \quad (11)$$

Where dQ is the change of the internal energy, e_n is the internal energy of Species n . Together with the enthalpy change caused by other physical phenomena (e.g., fuel evaporation et al.), the temperature change is estimated in KIVA4 by locating the specific enthalpy in a pre-stored temperature vs. enthalpy database, in which interpolation might be used if needed.

2.3 Solution algorithm

The solution algorithm in this hybrid model is intuitive:

1. Critical temperatures T_{cut} for initiating the closed reactor model (700 K is recommended and was used in the current study) and T_c for initiating the CTC model (1200 K is recommended and was used in the current study) and a critical Damköhler number Da_c (1000 is recommended and was used in the current study) are pre-set as inputs into the program.

2. With the compression of the piston during the engine simulation, the temperature increases to a critical point T_{cut} where the closed reactor model starts to compute the low-intermediate temperature auto-ignition in the computational domain.

3. The CTC model will be initiated for diffusion flame if the temperature of any cells is higher than T_c and the Damköhler number is larger than Da_c . Simultaneously, the closed reactor keeps dealing with the other cells.

The temperature and Damköhler number of each cell will be compared with the critical temperatures at each time step to categorize the cells into the proper model.

3 Results and discussions

3.1 Validation

To validate the current model, the calculated combustion characteristics including pressure and heat release rate are compared with the experimental data. The current hybrid model was compared with the closed reactor model with CHEMKIN in terms of accuracy and computational cost.

The experiments were conducted in a single cylinder dual fuel GW4D20 engine fueled with gasoline and diesel. The operating conditions and engine specifications are listed in Table 1. More than 6 different starts of injections (SOI) were tested experimentally, in which three of them were chosen for this validation. Two of them are single injections with SOI of -35, -30 degree after the top dead center (ATDC) while the other one is a double injection with the first SOI -60 degree ATDC and second one -35 degree ATDC. For more details of this experiment, please refer to our previous study [12]. Because of 8 evenly distributed injector holes in the injector in this testing engine, a 45 degree computational grid with 8060 cells was created as shown in Fig. 2. By setting the same initial thermodynamic conditions in KIVA4-

CHEMKIN-CTC and KIVA4-CHEMKIN, the simulations were conducted on the clusters in National University of Singapore (NUS) High Performance Computing (HPC) center.

The comparison among the current hybrid model, sole closed reactor model with CHEMKIN and the experimental data is presented in Fig. 3, 4 and 5. It is noted that all the data calculated from the current hybrid model were obtained by setting $C_2 = 0.1$ and $Da_c = 1000$ for all cases. It is observed that for all different SOI and different injection strategies, the current hybrid model predicted the pressure traces better than the pure closed reactor model. With respect to the heat release rate, it is more obvious to note that in Fig. 3 and Fig. 4, the sole closed reactor model with CHEMKIN underestimate the HRR peak while the current hybrid model captured the HRR peak more accurately. This might be attributed to the fact that the pure closed reactor resolves the diffusion flame by assuming a perfectly stirred reactor without considering the turbulence under the grid scale. Moreover, it is interesting to be noted that the difference between the pressure and HRR trace of the SOI -60 deg. ATDC case is not substantial, indicating that with a separate advanced injection, the flame is more of a premixed combustion type and in the hybrid model more cells are computed by the closed reactor model with CHEMKIN.

In addition, in Fig. 6 for the SOI=-30 case, it is shown that in the temperature spatial contours the combustion occurs at the end of the spray tip where the Damköhler number is larger than the critical Damköhler number (as indicated by the $Da=1000$ contour line), implying that at the beginning of the combustion, the combustion is of mixing controlled type. It is also noted that after the combustion occurrence, the temperature and Damköhler number in more and more cells are becoming larger than the critical Damköhler number and temperature, thus the percentage of cell numbers computed in CTC dramatically increases.

Furthermore, because of fewer cells computed by the closed reactor model with CHEMKIN in the hybrid model, less stiff chemistry ODEs system were solved by DVODE. Hence, it is expected that there would be a reduction of computation time of

the hybrid model because in the CTC model, solving the chemistry in these cells only needed to solve very simple equations through Eq. (1-7) and undergo the equilibrium solver calculation. Indeed, as shown in Figure 7, the hybrid model can save maximally more than 40% computational time than the sole closed reactor model. As discussed above, the SOI -60 deg. ATDC case computed with the CTC model within a short duration, which could explain the fact that in Fig. 7, the computational time difference between the current hybrid model and the closed reactor model in this case is trivial.

3.2 Sensitivity analysis of tunable model parameters

One of the advantages of this current hybrid than the sole closed reactor model with CHEMKIN is that it avoids its dependence of the combustion solely on fuel chemistry mechanism. A tunable parameter C_2 could be easily adjusted for different engines to properly simulate the experimental conditions. It has to be mentioned that when simulating the same engine for different operating conditions, C_2 should not be changed. In this section, a sensitivity analysis of the tunable constant C_2 in Eq. (3) was conducted. As shown in Eq. (3), an increase of the value of C_2 could increase the turbulence timescale. A longer turbulence timescale indicates a longer characteristic time to reach the equilibrium thus a slower species conversion rate. Hence, a slower pressure rise rate would be expected with a larger C_2 value. As presented in Fig. 8, by varying the value of C_2 among 0.05, 0.1 and 0.15 while keeping all of the other parameters constant as in the SOI -30 degree ATDC case, an obvious different computed pressure rise rate can be observed. Specifically, a larger C_2 value can lead to slower combustion and slow different pressure rise due to the larger estimated turbulence time scale and slower species conversion rate in the mixing controlled combustion. It is pointed out that the change of C_2 could significantly lead to an obvious pressure rise rate change. Hence, users of this model should be tuning this constant cautiously to get an accurate prediction when this model is used for a new engine.

Another model parameter that might affect the model performance is the critical Damköhler number Da_c . The chosen value $Da_c=1000$ in the present validation is based on the observation of a previous mixed-mode large eddy engine simulation [25]. As shown in Eq. (9), it is speculated that a too small Da_c value might lead to a possible scenario that some high-temperature premixed combustion cells are mistakenly computed as diffusion flame cells in CTC and consequently the species conversion rate could be overestimated. Varying Da_c from 10 to 1000 while keeping all of the other parameters constant as in the SOI -30 degree ATDC case, the calculated pressure traces were compared and shown in Fig. 9. It is observed that during the combustion process (rapid pressure rise), the difference among these three cases is not obvious, indicating that after the fuel spray at -30 degree ATDC, the Da number of most of the high-temperature cells are larger than 1000 and the flame is of mixing-dominant type. The enlarged figure shows that the pressure of the $Da_c = 1000$ case slightly deviate downwards from the other two cases, implying that the Damköhler number of some cells fell into the range between 100 and 1000. After the pressure peak where most of the fuel atomization and evaporation have been ended but most of the cell temperatures are still larger than T_c , using CTC to compute the combustion could overestimate the species conversion rate. Hence, from Fig. 9, it is observed that during the expansion stroke, the $Da_c = 10$ case shows overestimated pressure than other cases because most of the high temperature cells are still computed by CTC in this case.

4 Conclusion

Under some certain scenarios when mixing controlled combustion is substantial in RCCI combustion, it is more accurate to model the diffusion flame with turbulence-chemistry interaction considered. A hybrid model with the classical CTC model and closed reactor model was proposed for RCCI combustion modeling, as a substitute of the conventional sole closed reactor model. A semi-empirical one-step reaction rate from a single droplet auto-ignition experiment was adopted for the laminar timescale evaluation while the turbulence timescale was estimated by the RNG $\kappa-\varepsilon$ model. To

account for detailed chemistry in this hybrid model, a CEQ equilibrium solver was employed to solve the species concentrations under equilibrium state. This detailed chemistry CTC model was then coupled with the closed reactor model with CHEMKIN library, forming a hybrid model which is able to compute the auto-ignition and mixing controlled diffusion flame under RCCI conditions.

By comparing its prediction performance with both the experimental data and the predicted data from the sole closed reactor model with CHEMKIN library, it is proved that this hybrid model is robust to model RCCI combustion and gave reliable prediction for the combustion characteristics. More importantly, it is capable of reducing the computational time maximally more than 40% compared with the sole closed reactor solver, due to fewer stiff ODEs solved in the CHEMKIN solver.

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6 References

- [1] Heywood JB. Internal combustion engine fundamentals: Mcgraw-hill New York; 1988.
- [2] Lu X, Han D, Huang Z. Fuel design and management for the control of advanced compression-ignition combustion modes. *Prog Energ Combust* 2011;37:741-83.
- [3] Bessonette PW, Schleyer CH, Duffy KP, Hardy WL, Liechty MP. Effects of fuel property changes on heavy-duty HCCI combustion. SAE 2007-01-0191.
- [4] Kokjohn S, Reitz R. Characterization of Dual-Fuel PCCI Combustion in a Light-Duty Engine. Proceedings of the International Multi-Dimensional Engine Modeling User's Group Meeting. 2010.
- [5] Kokjohn SL, Hanson RM, Splitter DA, Reitz RD. Experiments and modeling of dual-fuel HCCI and PCCI combustion using in-cylinder fuel blending. SAE 2009-01-2647.
- [6] Splitter D, Kokjohn S, Rein K, Hanson R, Sanders S, Reitz RD. An optical investigation of ignition processes in fuel reactivity controlled PCCI combustion. SAE 2010-01-0345.
- [7] Kokjohn S, Hanson R, Splitter D, Kaddatz J, Reitz R. Fuel reactivity controlled compression ignition (RCCI) combustion in light-and heavy-duty engines. SAE 2011-01-0357.
- [8] Splitter D, Hanson R, Kokjohn S, Reitz RD. Reactivity controlled compression ignition (RCCI) heavy-duty engine operation at mid-and high-loads with conventional and alternative fuels. SAE 2011-01-0363.
- [9] Splitter D, Wissink M, Kokjohn S, Reitz RD. Effect of compression ratio and piston geometry on RCCI load limits and efficiency. SAE 2012-01-0383.
- [10] Kong S-C, Reitz RD. Application of detailed chemistry and CFD for predicting direct injection HCCI engine combustion and emissions. *Proc Combust Inst* 2002;29:663-9.
- [11] Kee RJ, Rupley FM, Miller JA. Chemkin-II: A Fortran chemical kinetics package for the analysis of gas-phase chemical kinetics. 1989.

- [12] Li J, Yang W, An H, Zhou D, Yu W, Wang J, et al. Numerical investigation on the effect of reactivity gradient in an RCCI engine fueled with gasoline and diesel. *Energ Convers Manage* 2015;92:342-52.
- [13] Li YP, Jia M, Chang YC, Liu YD, Xie MZ, Wang TY, et al. Parametric study and optimization of a RCCI (reactivity controlled compression ignition) engine fueled with methanol and diesel. *Energy* 2014;65:319-32.
- [14] Zhou D, Yang W, An H, Li J, Shu C. A numerical study on RCCI engine fueled by biodiesel/methanol. *Energ Convers Manage* 2015;89:798-807.
- [15] Zhou DZ, Yang WM, An H, Li J. Application of CFD-chemical kinetics approach in detecting RCCI engine knocking fuelled with biodiesel/methanol. *Appl Energ* 2015;145:255-64.
- [16] Kokjohn SL, Reitz RD. Investigation of the roles of flame propagation, turbulent mixing, and volumetric heat release in conventional and low temperature diesel combustion. *J Eng Gas Turbines Power* 2011;133:102805.
- [17] Kong S-C, Han Z, Reitz RD. The development and application of a diesel ignition and combustion model for multidimensional engine simulation. SAE 950278.
- [18] Dec J. A Conceptual Model of DI Diesel Combustion Based on Laser-Sheet Imaging. SAE 970873.
- [19] Abraham J, Bracco F, Reitz R. Comparisons of computed and measured premixed charge engine combustion. *Combust Flame* 1985;60:309-22.
- [20] Han Z, Reitz RD. Turbulence modeling of internal combustion engines using RNG κ - ϵ models. *Combust Sci Technol* 1995;106:267-95.
- [21] Westbrook CK, Dryer FL. Simplified reaction mechanisms for the oxidation of hydrocarbon fuels in flames. *Combust Sci Technol* 1981;27:31-43.
- [22] Pope SB. The computation of constrained and unconstrained equilibrium compositions of ideal gas mixtures using Gibbs function continuation. Cornell University, Ithaca, NY, Report No FDA 2003:03-2.
- [23] Zhou D, Yang W, Li J, Tay KL. Simplified fuel cracking process in reduced mechanism development: PRF-PAH kinetic models for combustion and soot prediction. *Fuel* 2016;182:831-41.
- [24] Brown P, Hindmarch A, Byrne G. DVODE: Computer Subroutine Package for Solving Ordinary Differential Equations. 1992.
- [25] Hu B, Rutland CJ, Shethaji TA. A Mixed-Mode Combustion Model for Large-Eddy Simulation of Diesel Engines. *Combust Sci Technol* 2010;182:1279-320.

Figure Captions

Figure 1. Figure 1. Schematic figure of RCCI combustion. Different colors mean different combustion zones. The mixing controlled diffusion flame are calculated by the CTC model while auto-ignition are computed by the closed reactor model in the current hybrid model.

Figure 2. Computational grid of the testing engine at 0 deg. ATDC.

Figure 3. Comparisons of pressure traces and HRRs as a function of crank angle with SOI=-30 degree ATDC. The solid lines indicate the computed results. The dash line indicates the experimental results.

Figure 4. Comparisons of Pressure traces and HRRs as a function of crank angle with SOI=-35 degree ATDC. The solid lines indicate the computed results. The dash line indicates the experimental results.

Figure 5. Comparisons of Pressure traces and HRRs as a function of crank angle with SOI=-60 degree ATDC with double injections. The solid lines indicate the computed results. The dash line indicates the experimental results.

Figure 6. Percentage of cell numbers computed in each solver as a function of crank angle with SOI=-30 degree ATDC in the current hybrid model. The temperature spatial contours are shown at the beginning of mixing controlled combustion occurrence (-5 deg. ATDC) and at -3 deg. ATDC. The red dash line in the spatial contours indicates the $Da=1000$ contour line.

Figure 7. Normalized computational time and injection profile with different start of injections. The solid lines indicate the injection profiles. The open symbols indicate the computational time of the hybrid model. The closed symbols indicate the computational time of the closed reactor model with CHEMKIN.

Figure 8. Comparison of pressure traces as a function of crank angle under various C_2 (0.05, 0.1, 0.15), computed with the SOI=-30 case. The enlarged graph shows the rapid pressure rise part of the pressure traces.

Figure 9. Comparison of pressure traces as a function of crank angle under various Da_c (10, 100, 1000), computed with the SOI=-30 case. The enlarged graph shows the rapid pressure rise part of the pressure traces.

Table Captions

Table 1. Engine specifications and operating conditions.

Figure 1. Schematic figure of RCCI combustion. Different colors mean different combustion zones. The mixing controlled diffusion flame are calculated by the CTC model while auto-ignition are computed by the closed reactor model in the current hybrid model.

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Figure 6. Percentage of cell numbers computed in each solver as a function of crank angle with SOI=-30 degree ATDC in the current hybrid model. The temperature spatial contours are shown at the beginning of mixing controlled combustion occurrence (-5 deg. ATDC) and at -3 deg. ATDC. The red dash line in the spatial contours indicates the Da=1000 contour line.

Figure 7. Normalized computational time and injection profile with different start of injections. The solid lines indicate the injection profiles. The open symbols indicate the computational time of the hybrid model. The closed symbols indicate the computational time of the closed reactor model with CHEMKIN.

Figure 8. Comparison of pressure traces as a function of crank angle under various C_2 (0.05, 0.1, 0.15), computed with the SOI=-30 case. The enlarged graph shows the rapid pressure rise part of the pressure traces.

Figure 9. Comparison of pressure traces as a function of crank angle under various Da_c (10, 100, 1000), computed with the SOI=-30 case. The enlarged graph shows the rapid pressure rise part of the pressure traces.

Table 1. Engine specifications and operating conditions.

Engine	GW4D20 diesel engine
Fuel	Gasoline/diesel
Bore×stroke (mm)	93.1×92
Compression ratio	16.7:1
Engine speed (rpm)	1600
Injection manner	Port + direct injection
SOI (ATDC)	-60, -35, -30
Intake tem. (K)	368
IMEP(bar)	5.06