

A Parametric Validation of Autoignition Numerical Studies on Compact Rapid Compression Machine

Pravendra Kumar, Shinji Nakaya, Mitsuhiro Tsue
Department of Aeronautics and Astronautics, The University of Tokyo
Tokyo, Japan

1. Introduction

In diesel and homogeneous charge compression ignition (HCCI) engines, chemical reactions through ignition govern the combustion dynamics. The enhancing use of computation is required accurate modeling of chemical kinetics to explore the insight of combustion dynamics inside practical engines. Ignition delay measurement of hydrocarbon fuels is an important parameter to validate chemical kinetics. Therefore, a hydraulically operated Compact Rapid Compression Machine (CRCM) is designed and developed to measure the ignition delay. The present CRCM facility can produce high pressure and high temperature environment in the combustion chamber using free piston driven by pressurized hydraulic oil. Rapid Compression Machines (RCMs) and shock tubes have been used to obtain ignition delay at high pressure, however, CRCM has its unique characteristics to obtain high pressure at very fast compression [14] [12]. Preliminary results indicate that the CRCM has shorter compression period than those of conventional RCMs by a factor of 3-10 which is fast enough to avoid the heat loss during the compression process. It guarantees nearly adiabatic process even with very compact chamber dimensions are considered in this study, since the compression process does not influence much by diffusion process for at least 10 milliseconds after the end of compression [4]. Direct measurement of temperature at the end of compression is still difficult, although several research have been conducted [4][10]. It is confirmed by many research groups that heat loss has significant effects on uniformity of temperature, one of the essential conditions to model the chemical kinetics [2][3]. Therefore, to hold the uniformity of temperature or adiabatic core [13], heat loss must be negligible or minimum, since the vortex created by the piston motion causes the nonuniformity. The non-uniformity can be solved by adopting crevice method [15]. Due to the fast compression, consequently negligible heat loss may eliminate the necessity of crevice method in the present CRCM, since the fundamental principle of an ideal RCM is the rapid adiabatic heating of gas to a high pressure and temperature [15].

In this study, an analytical model is developed based on CRCM thermodynamics incorporated essential physics assuming no chemical heat release to investigate the heat loss. Moreover, a 2D axisymmetric model is developed to model the autoignition process using reduced mechanism for n-butane combustible mixtures. Analytical and axisymmetric models are validated against the experimental pressure time history obtained from the CRCM. Furthermore, Ignition delay obtained using 2D axisymmetric model is validated

against the zero-dimensional study using detailed reaction mechanism. The fuel considered in this study shows the negative temperature coefficient (NTC) in which ignition delay increases with increasing temperature [13]. Moreover, near to the turnover states[7], it is difficult to predict two-stage ignition from pressure trace. Therefore, two-stage ignition is investigated based on OH formation near to the turnover states in the numerical simulation.

2. Experimental Methods

The schematic of CRCM facility is shown in Fig.1.0. Using this CRCM, within a few milliseconds the order of 70 MPa hydraulic pressure could be achievable that enables the piston to move at high speed and facilitate process towards adiabatic compression which is essential to study the chemical kinetics [13]. The hydraulic pressure and combustion chamber pressure were measured using pressure transducers (Kyowa PG-2TH and PCB 102B). The compression ratio was controlled by changing the stroke and the cavity size of the free piston. The cavity provided in the piston forms the final combustion chamber after the end of the compression (TDC). In the present combustion chamber assembly, both the free piston and piston cylinder as shown in Fig.1.0 (b) and (c) are made of polycarbonate. The free piston stops at TDC and was remained there due to the hydraulic pressure which is higher than that the pressure in the combustion chamber.

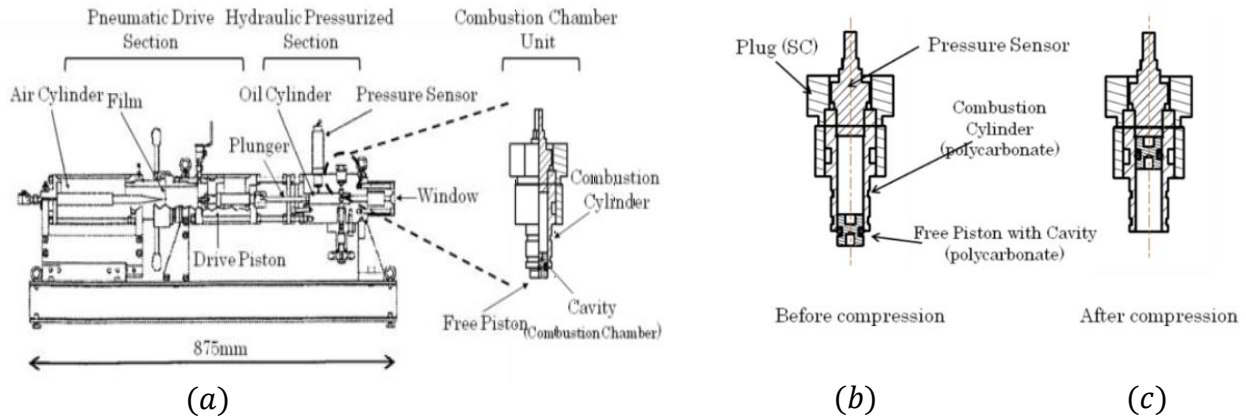


Figure 1.0 Schematic of experimental setup (a) CRCM, (b) combustion chamber before compression, (c) combustion chamber after compression

3. Analytical Model

The analytical expressions for domains shown in Fig.2.0 (a) & (b) were deduced and resulting algebraic equations 1 to 7 along with the isentropic relations were solved. In this model, the closed system with air as working fluid of mass m was considered with specific heat ratio (γ) of 1.4 and gas constant $R = 287$ which obeys the ideal gas law. Heat loss (q) was modeled using heat conduction from domain to wall which depends on gas temperature (T_t) inside chamber and actual surface area (A_{ct}). The heat transfer coefficient h was approximated using thermal conductivity (k) of fluid and δ (as shown in Fig.3.0 (b)) which are obtained from the present CFD model based on maximum heat loss by considering the smallest δ near to the wall. The thermodynamic quantities ρ , p , T , C_v are the density, pressure, temperature and specific heat at constant volume respectively. The geometrical parameters V , S , A_p , r_p , r_{cav} , l and u_p are the volume, stroke length, cross sectional area of cylinder, radius of cross section of cylinder, radius of cavity of free piston, length of cavity and piston velocity respectively. The subscripts o, cav and t belong to the initial condition, cavity and time dependent parameters respectively. All parameters are in SI units.

In the earlier studies, D. Lee et al. [8] analytically modeled one-dimensional chemical kinetic incorporated with heat transfer along the walls, though their study was to design the effective crevice volume to suppress the vortex. A. Ahmed et al.[2], recently carried out the investigation to identify the effect of heat

loss and γ on ignition delay during post compression. In the present study, heat loss is modeled in both pre-compression and post-compression process. Since the heat loss during the pre-compression causes the lower pressure than the one obtained adiabatically, that affects the gas temperature and thus variation in the ignition delay for the identical initial conditions. The time dependent h calculated from CFD model is shown in Fig.2.0(c) along with heat loss which was approximated from analytical model. It is noted that the maximum heat loss occurs during the compression which might be due to piston work, however, the magnitude is much lower in post compression which reveals that the thermal boundary layer does not degrade due to slower diffusion than the compression process.

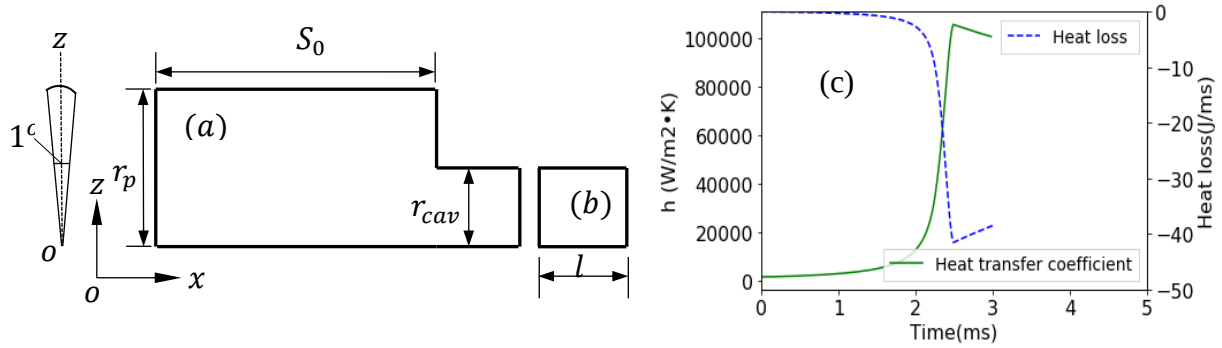


Figure 2.0 (a) Analytical domain before compression, (b) after compression (c) Time dependent heat transfer coefficient (CFD model) and heat loss (analytical model)

$$\rho_t = \frac{m}{V_t} \quad (1)$$

$$V_t = S_0 A_p + V_c - \left[\int_0^t u_p(t) dt \right] A_p \quad (2)$$

$$p_t = \rho_t R T_t \quad (3)$$

$$m C_v \frac{dT_t}{dt} = -h(T_t - T_0) A_{ct} + p_t u_p(t) A_p \quad (4)$$

$$A_{ct} = 2\pi [r_p^2 + r_{cav} l + r_p (S_0 - S_t)] \quad (5)$$

$$q = -h [T_t - T_0] A_{ct} \quad (6)$$

$$h = \left(\frac{\rho}{\rho_0} \right)^{\frac{k}{\delta}} \quad (7)$$

4. CFD Model

2D axisymmetric numerical simulations were carried out to investigate the autoignition phenomena within the combustion chamber of the CRCM proposed in this study. In order to incorporate compression and to have autoignition, a modified solver was developed from the standard OpenFoam libraries with dynamical mesh utility and layer removal-addition technique [6]. The laminar compressible flow is considered aside with the ODE combustion solver to handle detailed and reduced reactions mechanism. PIMPLE algorithm was used to solve the algebraic finite volume equations for transient model [1]. The diameter of the combustion chamber was considered 4 mm, with 2.5 mm of depth. The stroke length was kept at 16.5625 mm to keep the compression ratio (CR) of 27.5, which is identical to the experiment and analytical model. The computational domain by considering 1° wedge was used as shown in Fig.3.0 (a). The wall boundary conditions are adopted based on the heat loss model deduced analytically, keeping the fixed wall temperature at 301 K. with no-slip conditions. Beside this, piston motion is based on the velocity profile considered in the work of D. Lee et al. [4] without solving the equation of motion, since the piston speed is too fast that enables the compression of gases nearly at adiabatic in the CRCM chamber. Nevertheless, the diffusion process affect the compression at least 10 ms after the end of compression [4], the velocity profile may not be the prime factor to affect the compression process.

An attempt has been carried out to validate the pressure obtained from the deduced analytical model and numerical simulation against the experimental data of CRCM as shown in Fig. 3.0 (c). The pressure profile from analytical model is found to be well matched with one obtained from numerical simulation for identical parameters.

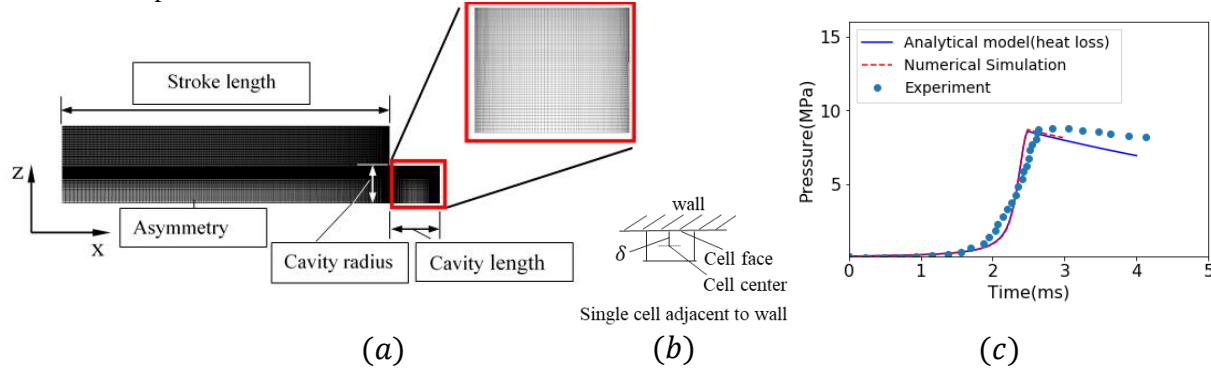


Figure 3.0 (a) Computational domain (b) Comparison of analytical, numerical and experimental pressure time history at identical conditions

On the other hand, the experimental data fits marginally with analytical solution and numerical one, though the pressure drop is found to be approximately similar. It is noted that the experimental pressure trace has little deviation from the analytical model and numerical. This might be due to the assumption not to consider the friction caused by piston O-ring in experiments as well as not solving the piston motion equation while modeling the analytical and numerical cases. From the numerical simulation, mass averaged value of $\gamma = 1.38$ is calculated.

5. Results and Discussion

Numerical investigations of autoignition phenomena have been studied as well as corresponding zero-dimensional analysis with detailed kinetic mechanism of NUI, Galway [5]. Table 1.0 shows the initial conditions used in the cases and it also shows the results obtained from numerical simulations as well as zero-dimensional studies. τ_{NS} and τ_0 belong to the ignition delay obtained from numerical simulations and zero-dimensional studies. P_c , T_c and τ_c are the pressure, temperature at TDC and compression time respectively. The numerical simulations are based on reduced chemical kinetics with 57 species and 230 reactions for n-butane combustible mixtures [11]. Table 2.0 shows the mixture composition which were at equivalence ratio 1.0 for n-butane combustible mixtures.

For the case A, the pressure and OH mass fraction histories are shown in Fig.4 (a). After TDC, the total ignition delay 1.3 ms is obtained as given in Table 2.0. Case A shows the two-stage ignition though it is not observed from the pressure time history, OH mass fraction profile showed the two-stage ignition clearly as OH formation starts after a delay from TDC which is called ignition delay for first stage ignition. After this period, OH formation increases for a short period and become constant for a period that belongs to the second stage ignition delay and leads to the final ignition, consequently, sudden pressure rises. Therefore, OH formation is more sensitive than pressure profile to predict the two-stage ignition in numerical simulations.

For the case B, diluents of nitrogen (diatomic) and argon (monoatomic) were considered 50-50% by mole fraction. Involving AR with large γ than nitrogen results higher pressure and temperature. Wurmel et al. 2007 [14], observed higher pressure and temperature in case of AR. Therefore, they recommend to use monoatomic diluent gases for RCMs studies in order to achieve higher temperature except helium which is not suitable for RCMs studies due to its low heat capacity and low molecular weight as well as high thermal conductivity and thermal diffusivity [15]. However, the two-stage ignition is not observed for the case B (which can be seen from OH formation) as shown in Fig.4(b). Beside this, heat loss was modeled at walls

boundaries based on analytical model present in this study above. In comparison to the Case A, higher temperature and higher pressure were obtained in Case B. This is might be due to large γ in case of AR as stated above.

Table 1.0 Summary of autoignition study

Initial Conditions					Results			
	P_0 (MPa)	T_0 (K)	τ_c (ms)	CR	P_c (MPa)	T_c (K)	τ_{NS} (ms)	τ_0 (ms)
Case A	0.1	301	2.5	27.5	8.10	882	1.3	0.79
Case B	0.1	301	2.5	27.5	8.80	936	0.79	0.69

Table 2.0 Mixture compositions

Component		n-C4H10	O2	N2	AR
Fraction [mol.%]	Case A	3.00	19.4	76.7	0
	Case B	3.00	19.4	38.8	38.8

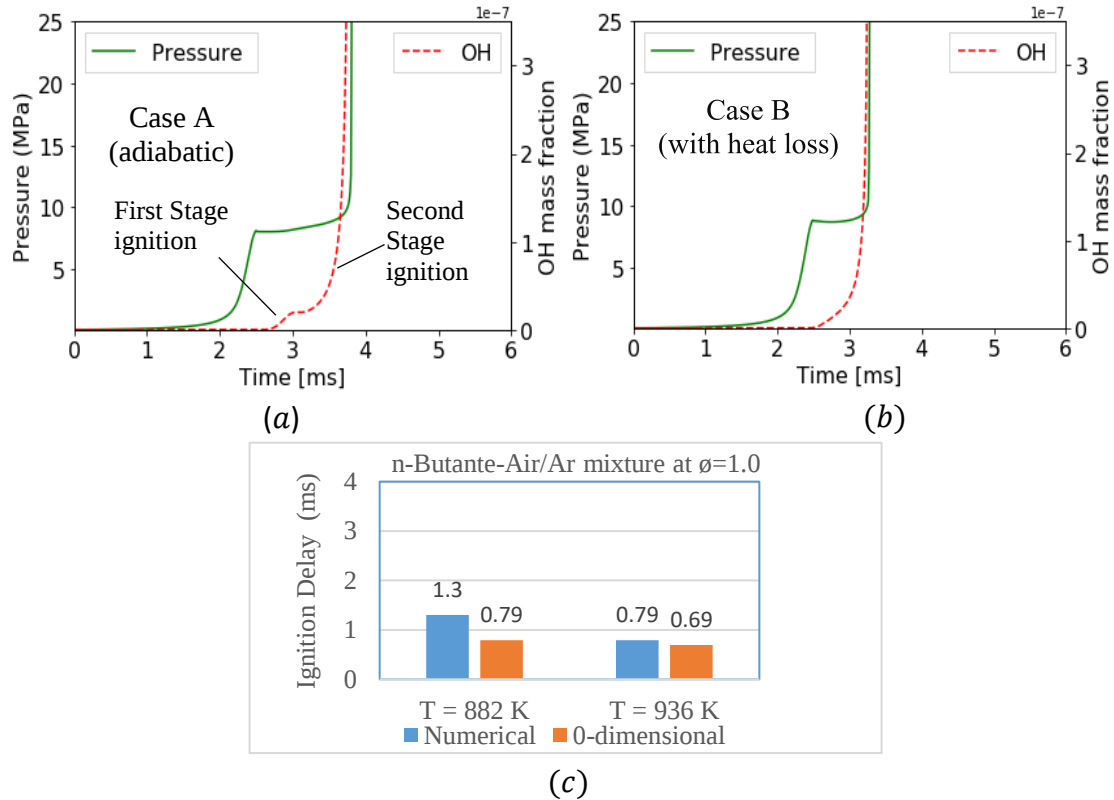


Fig.4 (a) Pressure-time and OH formation-time histories (Case A), (b) Pressure-time and OH formation-time histories (Case B), and (c) Comparison of ignition delay from numerical and zero-dimensional.

Fig.4(c) shows the comparison of ignition delay from numerical and zero-dimensional (adiabatic conditions) studies. It is noted that longer ignition delay is observed in case of numerical simulations. This is due to the facts that unavoidable non-uniformity due to cooler boundary layer of temperature causes non-uniform heat release and chemical kinetics considered in CFD calculations [9], and choosing numerical schemes to solve the governing equations. In addition, the ignition delay gets decreased with increase in the

temperature. More interestingly, the difference of ignition delay between numerical and zero-dimensional gets decreased with increase in the temperature at TDC.

6. Conclusion

Based on the analytical model, walls boundary condition in the CFD model with heat loss implemented which could be useful to study the effect of heat loss on ignition delay. Furthermore, autoignition study of numerical simulations are validated using zero-dimensional model. The time dependent γ is calculated and the mass weighted average value, 1.38 of it is considered for the approximation of combustion chamber temperature at TDC in the experiments. This parameter is important to estimate the accurate temperature at TDC, since, a little deviation in temperature leads to inaccurate prediction of ignition delay and thus propagation of error while validating the chemical kinetic. It is found that the OH formation is more sensitive than pressure profile to predict fuel's two-stage ignition near to the turnover states numerically.

7. References

- [1] H.J. Aguerre, S.M. Damián, J.M. Gimenez, N.M. Nigro, Modeling of Compressible Fluid Problems With Openfoam Using Dynamic Mesh Technology, *Tornello. XXXII* (2013) 995–1011.
- [2] A. Ahmed, M. Hantouche, M. Khurshid, S.Y. Mohamed, E.F. Nasir, A. Farooq, W.L. Roberts, O.M. Knio, S.M. Sarathy, Impact of thermodynamic properties and heat loss on ignition of transportation fuels in rapid compression machines, *Fuel*. 218 (2018) 203–212.
- [3] S.S. Goldsborough, C. Banyon, G. Mittal, A computationally efficient, physics-based model for simulating heat loss during compression and the delay period in RCM experiments, *Combust. Flame*. 159 (2012) 3476–3492.
- [4] J.F. Griffiths, J.P. Macnamara, C. Mohamed, B.J. Whitaker, C.G.W. Sheppard, Temperature fields during the development of autoignition in a rapid compression machine, *Faraday discussions* 119 (2002): 287–303.
- [5] D. Healy, N.S. Donato, C.J. Aul, E.L. Petersen, C.M. Zinner, G. Bourque, H.J. Curran, n-Butane: Ignition delay measurements at high pressure and detailed chemical kinetic simulations, *Combust. Flame*. (2010).
- [6] H. Jasak, Dynamic Mesh Handling in OpenFOAM, 47th AIAA Aerosp. Sci. Meet. Incl. New Horizons Forum Aerosp. Expo. (2009).
- [7] W. Ji, P. Zhao, T. He, X. He, A. Farooq, C.K. Law, On the controlling mechanism of the upper turnover states in the NTC regime, *Combust. Flame*. (2016).
- [8] D. Lee, S. Hochgreb, Rapid compression machines: Heat transfer and suppression of corner vortex, *Combust. Flame*. 114 (1998) 531–545.
- [9] G. Mittal, S. Gupta, Computational assessment of an approach for implementing crevice containment in rapid compression machines, *Fuel*. 102 (2012) 536–544.
- [10] G. Mittal, C.J. Sung, Aerodynamics inside a rapid compression machine, *Combust. Flame*. 145 (2006) 160–180.
- [11] J.C. Prince, C. Treviño, F.A. Williams, A reduced reaction mechanism for the combustion of n-butane, *Combust. Flame*. (2017).
- [12] A. Ramalingam, K. Zhang, A. Dhongde, L. Virnich, H. Sankhla, H. Curran, A. Heufer, An RCM experimental and modeling study on CH₄ and CH₄/C₂H₆ oxidation at pressures up to 160 bar, *Fuel*. 206 (2017) 325–333.
- [13] C.-J. Sung, H.J. Curran, Using rapid compression machines for chemical kinetics studies, *Prog. Energy Combust. Sci.* 44 (2014) 1–18.
- [14] J. Würmel, E.J. Silke, H.J. Curran, M.S. Ó Conaire, J.M. Simmie, The effect of diluent gases on ignition delay times in the shock tube and in the rapid compression machine, *Combust. Flame*. 151 (2007) 289–302.
- [15] J. Würmel, J.M. Simmie, CFD studies of a twin-piston rapid compression machine, *Combust. Flame*. 141 (2005) 417–430.