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Brief Communications

Evaluation of non-ideal piston stopping effects on the "adiabatic core" and ignition delay time simulation in rapid compression machines

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ABSTRACT

Piston creep and rebound are two non-ideal piston stopping behaviors in the rapid compression machine. Compared to nominal piston stopping, piston rebound/creep will result in a smaller/bigger 'adiabatic' core zone volume in the reaction chamber and length/shorten the ignition delay time measurements. However, the 'adiabatic core' hypothesis can still be validated under these compressions and ensures the applicability of zero-dimensional method in the model simulation.

1. Introduction

Ignition delay time (IDT) measurements of reactive gas mixtures are an important target parameter for combustion csshemistry mechanism development and validation. Rapid compression machine (RCM) [1,2] can generate a long-lasting environment for fuel auto-ignition, thus it is suitable for relatively longer IDT measurements in the low to intermediate temperature regimes (600–1000 K).

The non-ideal piston stopping (creep/rebound) [2], are very likely to occur in hydraulically damped systems due to the dynamics of oil displacement process, as shown in the supplementary material (SM) Fig. S1. Creep is the slow stopping of the piston in the compressive direction near the end of the compression stroke. Rebound is the piston movement in the expansive direction which then significantly alters the gas temperature in the reaction chamber. Many studies [3–5] have proved the existence of an "adiabatic core" for nominal compressions using creviced pistons, and therefore the heat loss can be reasonably modeled in a zero-dimensional (0-D) reactive gas simulation by adopting non-reactive volume history profiles [6,7]. It is noted that the "adiabatic core" assumption is largely affected by the fluid mechanics effects, and different stopping behaviors might cause change to the flow field in the chamber. However, due to the mechanical nature, ideal piston stopping (infinitely fast piston stopping and locking) can never be achieved. For compressions with non-ideal piston stopping behaviors, their influences on the "adiabatic core" and the 0-D simulation have not been explored. In addition, for the RCM data that has already been published, exploring the non-ideal piston stopping effects will also benefit the interpretation of these data.

22D axisymmetric CFD simulations of the piston compression in the chamber were conducted using ANSYS FLUENT 18.2 [8]. In order to quantify the impact on "adiabatic core", a dimensionless definition of "core zone volume" [5] (V_{core}) was used as a criterion in comparing the cases studied. V_{core} is calculated as per Eq. (1).

$$V_{core} = \frac{\sum \rho_i (T > T_{adiabatic} - 5\ K)}{\sum \rho_i} \tag{1}$$

where i is the cell number, ρ_i is the density within the cell, and $T_{adiabatic}$ is the calculated temperature using adiabatic compression/expansion theory. $\sum \rho_i (T > T_{adiabatic} - 5\ K)$ indicates the summation of the densities in the core zone where the temperature is higher than ($T_{adiabatic}$-5 K).

Two ethanol mixtures were used in the CFD simulations, as shown in Table 1. IDTs of Mix 1 and 2 are respectively around 20 and 85 ms, and thus they can represent conditions with short and long IDTs in the RCM studies.

0-D IDT simulations were performed using the closed homogeneous batch reactors in ANSYS CHEMKIN 18.2 [9]. To assess the effects of non-ideal piston stopping on the simulations, creep, rebound and nominal non-reactive volume-time profiles

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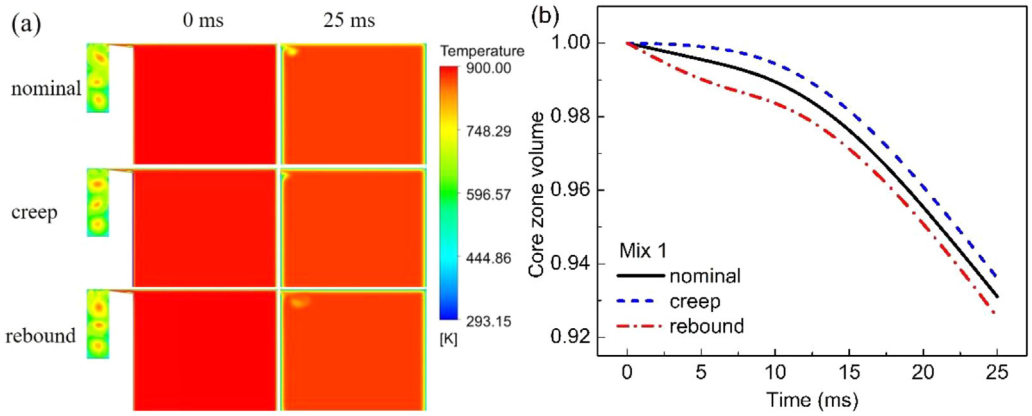

Fig. 1. Temperature distributions (a) and core zone volumes (b) for nominal, creep and rebound stoppings at different times using Mix 1.

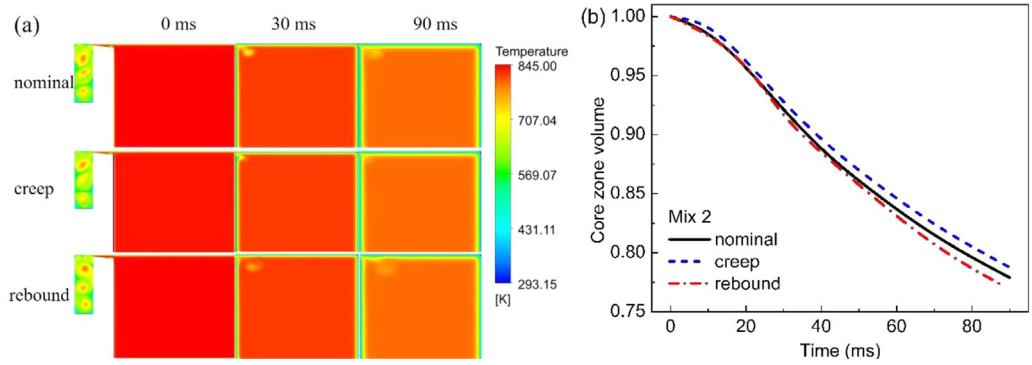

Fig. 2. Temperature distributions (a) and core zone volumes (b) for nominal, creep and rebound stoppings at different times using Mix 2.

Table 1
Components of the ethanol mixtures (mole fraction).

Mixture	Ethanol	O_2	N_2	Ar
Mix 1	3.72%	11.17%	0.00%	85.11%
Mix 2	3.72%	11.17%	12.16%	72.95%

were adopted. The detailed ethanol mechanism from Mittal et al. [10] was used in the simulations.

The temperature distributions and core zone volume profiles for different compressions using Mix 1 are compared in Fig. 1(a) and (b). The piston moving profiles used in the simulations are provided in the SM, Fig S 2. Time zero (0 ms) is defined as the time instant at which the pressure reaches its maximum value for the non-reactive cases. At 0 ms, temperature distributions for all the compressions are very homogenous and the core zone volumes are all around 100%. At the latter stage, it is seen that the creep and rebound piston stopping respectively increases and reduces the adiabatic core zone volume compared with the nominal case. After 0 ms, cold gas disturbance caused by the vortex tends to grow as time proceeds from a small region in the piston head to a relatively larger region in the chamber. As a result, core zone volumes begin to decrease due to both the growth of roll-up vortex and the boundary layer. At 30 ms, most of the hot gas remains unaffected and the core zone volumes for all these compressions are above 90%. However, a larger cold gas disturbance is observed before the entrance of the piston crevice in the rebound case followed by the nominal and creep cases. This is mainly because when piston rebound occurs near EOC, the backward movement of the piston causes more cold gas to escape from the crevice. Then, as the piston moves forward again, the cold gas disturbance in front of the piston is forced to transport further. The temperature distribution histories for the piston rebound process are provided in Fig. S4 of the SM. For creep piston stopping, on the other hand, the slow movement (velocity and deceleration) of the piston during its seating process provides a lower driving force for cold gas transport and thus the roll-up vortex is less pronounced. For a longer IDT test condition using Mix 2, similar trend is observed in the temperature distributions and core zone volume profiles for different compressions are shown in Fig. 2. As time proceeds, cold gas disturbance evolves, and the core zone volume decreases to around 75%~80% at 90 ms.

Pressure traces from the CFD and 0-D simulations of Mix 1 and 2 are compared in Fig. 3. It can be observed that the non-reactive and reactive pressure traces from the CFD simulations coincide with each other before the heat release stage caused by the evolving chemistry. The volume profiles derived from the non-reactive CFD pressure traces are then adopted in the CHEMKIN 0-D simulation. Compared with the nominal compression, the pressure for the creep piston stopping case keeps nearly constant for 5 ms and then drops, instead of immediate dropping down after EOC. In addition, T_C in creep case is lower than that in the nominal or rebound cases because the compression is not fully completed at time zero, and thus the compression ratio at 0 ms is smaller than that in nominal or rebound cases. For the rebound piston stopping case, the pressure after 0 ms drops at a much faster rate and then rises again. Generally, the IDTs calculated using 0-D reactors are slightly shorter than those from the CFD calculations, which is mainly because of the heat transfer and species diffusion between the hot core zone and cold boundary layer gas/roll-up vortex considered in CFD calculations. As shown in Fig. 4, the core zone temperature calculated by CFD is slightly lower than that by 0-D method, and the moments of the fastest consumption of the fuel and pro-

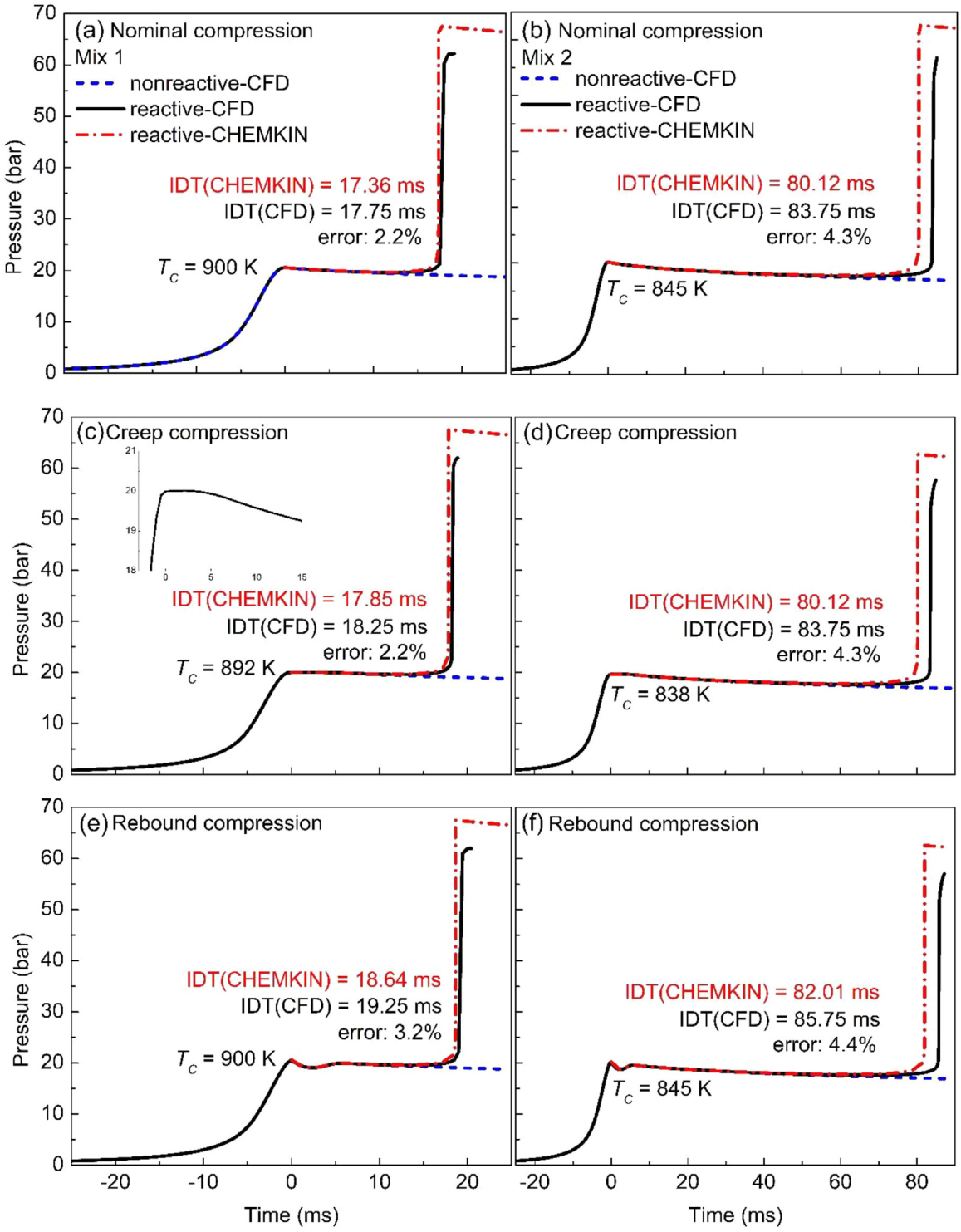

Fig. 3. Comparison of the pressure traces from CFD and 0-D simulations of Mix 1 (a, c and e) and 2 (b, d, and f). Solid lines and dash lines are respectively the reactive and nonreactive pressure traces from CFD results; dash dot lines are the 0-D simulation results using CHEMKIN.

duction of the intermediate species (C_2H_4) are arrived earlier in 0-D method. Besides, the maximum concentration of C_2H_4 is also lower in the result of CFD simulation, demonstrating the species diffusion between hot core gas and cold boundary layer gas. The IDT errors of 0-D simulations under different compressions are within 5%, because most of the gas in the reaction chamber remains unaffected as discussed above. However, the rebound case shows a slightly larger error, compared with the nominal and creep cases. As for longer IDT studies, errors in the 0-D simulations become larger which is mainly because of the growth of boundary layer and vortex, and the core zone gas expansion caused by piston crevice in the slow heat release process before thermal runaway. This comparison then indicates that the deviation between 0-D and multi-dimensional simulation is going to be more pronounced as time proceeds which is inevitable in practical RCM experiments.

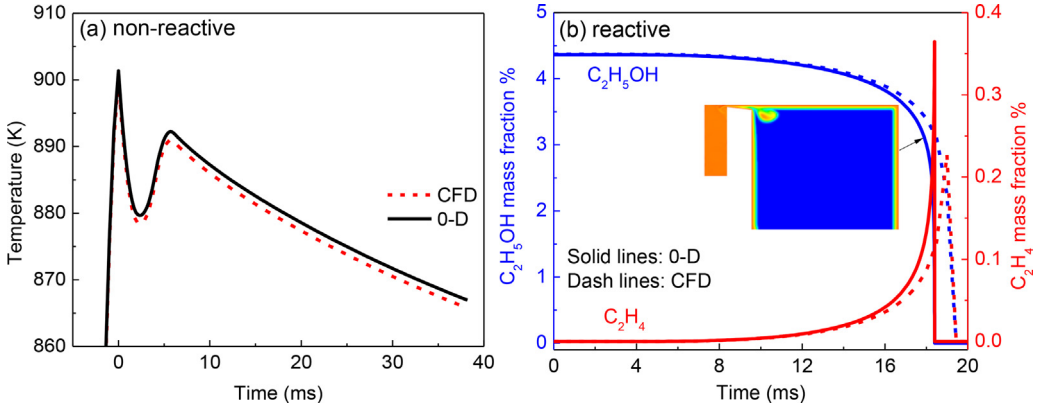

Fig. 4. Temperature and species profiles comparison between CFD and CHEMKIN (0-D) simulations.

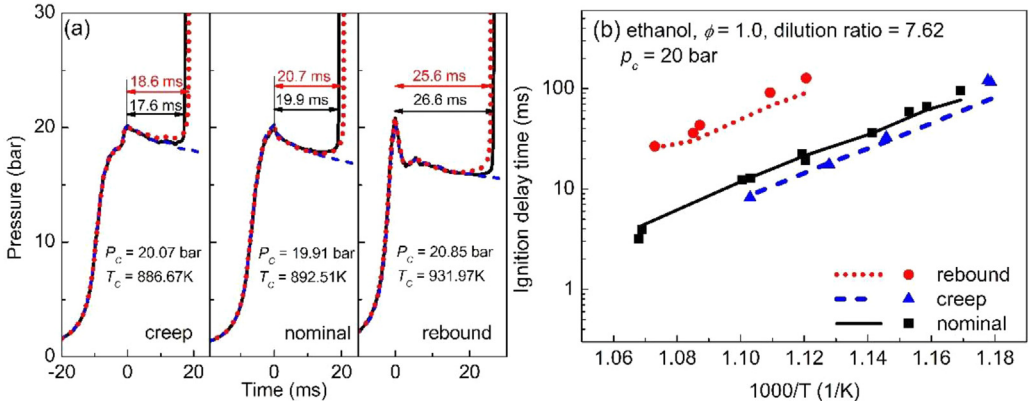

Fig. 5. (a) Typical pressure traces of the stoichiometric ethanol/Ar/O_2 mixture in nominal, creep, and rebound compressions. Solid and dash lines are respectively the measured reactive and non-reactive pressure traces, and dot lines are the pressure traces of the model prediction; (b) IDT measurements and model predictions of the stoichiometric ethanol/Ar/O_2 mixture. Scatters are the experimental data; lines are the model predictions.

Experiments were conducted in a RCM at Xi'an Jiaotong University. Details of this RCM are provided in Ref [5, 11] including the creviced piston design and the IDT measuring validations. In this RCM, the groove and ring hydraulic mechanism [12] is used in the piston stopping design. We intentionally adjust the driving pressure and the oil venting channel in the hydraulic piston to realize the creep or rebound compressions in the experiments.

IDTs of the ethanol mixtures were further experimentally measured under nominal, creep and rebound compressions and then used in a mechanism validation. As shown in Fig. 5(a), pressure traces with nominal, creep and rebound compressions are all well predicted by the 0-D simulations. Fig. 5(b) presents the measured IDT data as a function of the inverse temperature, together with the 0-D simulations. It is seen that the measured IDTs for different piston stoppings show observable discrepancies. Compared with the nominal compression, rebound prolongs the measured IDTs by an average of 80% while creep leads to shorter measurements by an average of 30%. The rebound experiments show a much larger difference compared with the CFD results, indicating more pressure drop and heat loss in the reaction chamber. The pressure (and temperature) decreases dramatically after the EOC due to volume expansion leading to a reduced global reaction rate of the mixture and consequently longer IDTs. For creep piston stopping, there will be a short period of high temperature before the EOC due to the slow piston movement. Consequently, more pre-EOC chemistry occurs and leads to shortened IDTs. By adopting the corresponding volume history profiles in the 0-D simulation, the mechanism captures the discrepancies caused by the creep and rebound piston stoppings. 0-D simulations using AramcoMech 3.0 [13] were also conducted, and the results show a very similar trend for different compressions even though the IDT predictions are slightly different. The model predictions using AramcoMech 3.0 [13] are provided in Fig. S5 of the SM.

Uncertainties in the kinetic mechanism will also make a difference when comparing the 0-D simulations with the experimental data. As a simulation begins, errors are accumulated with the changing thermal conditions. The rebound compression, for example, experiences lower temperature conditions compared with the nominal compression. Thus, if the kinetic mechanism has more uncertainty in the low-temperature region, more errors will be accumulated in predicting IDTs for piston rebound compressions. A slightly larger discrepancy is observed between the simulations and experimental results for rebound conditions, as shown by Fig. 5(b), which is possibly due to the relatively lager uncertainties of the kinetic mechanism at low temperatures.

Piston rebound will result in a larger cold gas disturbance in the reaction chamber, while piston creep tends to inhibit the disturbance transport compared to nominal piston stopping. In this work, these disturbances will not invalidate the "adiabatic core" and most of the gas in the reaction chamber remains unaffected. Consequently, creep and rebound stopping behaviours only have a minor impact on the accuracy of 0-D simulations compared to the error induced by the 0-D method itself (around 5%). However, the flow condition of the rebound case could exceed the scope of the laminar model, and future simulations using Large Eddy Simulation (LES) or Direct Numerical Simulation (DNS) should be conducted to further explore the piston rebound effect. Data in more severe rebound compressions could cause the failure of 0-D simu-

lation method because of the fast decaying trend of the 'adiabatic core' shown in the present study especially for long IDT measurements.

Comparisons on the IDTs of ethanol mixtures with experimentally designed nominal, creep and rebound piston stoppings indicates that non-ideal piston stoppings will notably alter IDT measurements. Yet, by adopting the corresponding volume history profiles of creep and rebound, 0-D simulations can capture the discrepancies of the experimental data under these conditions.

Declaration of Competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.combustflame.2020.04.007.

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