

The Effect of Low Temperature Chemistry on Detonation Propagation in Dimethyl Ether Mixture

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1 Introduction

Cool flame, whose generation mainly relies on low temperature chemistry, has recently regained attention in research due to its critical role in engine knock, emission reduction, fuel efficiency, flame stabilization, and low carbon fuel development [1]. Among above, engine knock is a current concern topic. It is generally accepted that engine knock is the result of auto-ignition and detonation [2]. Early studies reported the phenomenon of reduced run-up distance to detonation of pentane/oxygen mixture in 'cool flame region' [3]. The role of low temperature chemistry in detonation has been gained a deeper understanding in recent work by investigating the ZND structure [4]. However, there is still a lack of understanding of the effect of low temperature chemistry on detonation during the auto-ignition process of fuel. Therefore, this work mainly focuses on the ZND structure and cellular structure of dimethyl ether's (DME) detonation waves during auto-ignition processes by one-dimensional/two-dimensional simulation.

2 Numerical set up and results

This work studied the effect of low temperature chemistry on detonation by numerical simulation. The results proved that the partially oxidization of low temperature chemistry has a certain impact on the features of detonation. As a typical fuel with low temperature chemistry, dimethyl ether (DME) with an equivalence ratio of 1 is used as the fuel, diluted by argon. The mole fraction of the mixture is DME: O₂: AR=1:3:11.28. The simulation covers different dimensional results, including homogeneous ignition, ZND structure and two-dimensional detonation. Among above, the gas state at different time in homogeneous ignition results are assigned as the initial states to the latter two. ZND structure is simulated by SDToolbox. The method of integration is LSODA, and the max time step is 1e-12 s. In the study of ZND structure, the decrease in induction length (L) and CJ speed (D_{CJ}) was observed as the initial conditions move from the first stage ignition zone to the second stage ignition zone, namely, L and D_{CJ} goes down with the increase of reaction progress c . Two sets of one-dimensional simulation were conducted to confirm that this decrease is caused by partially sensitization. For the partially sensitized mixture, CJ speed decline more sharply than the fresh mixture with the same initial temperature and pressure. On the other hand, the induction length descent of partially sensitized mixture is less than fresh mixture.

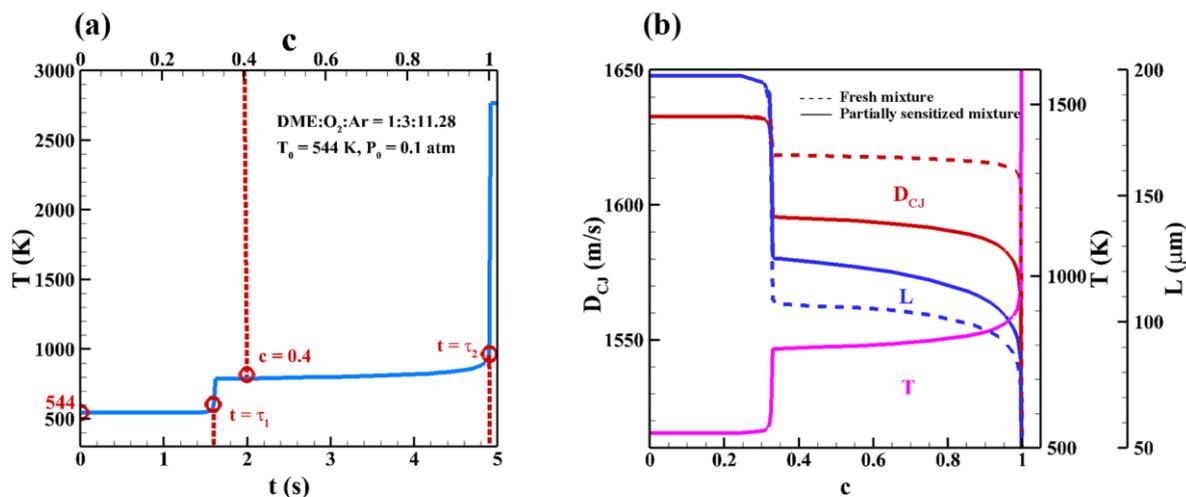


Figure 1: (a) Homogeneous ignition over time and the reaction progress c . (b) Change of the initial temperature, CJ speed and induction length with c .

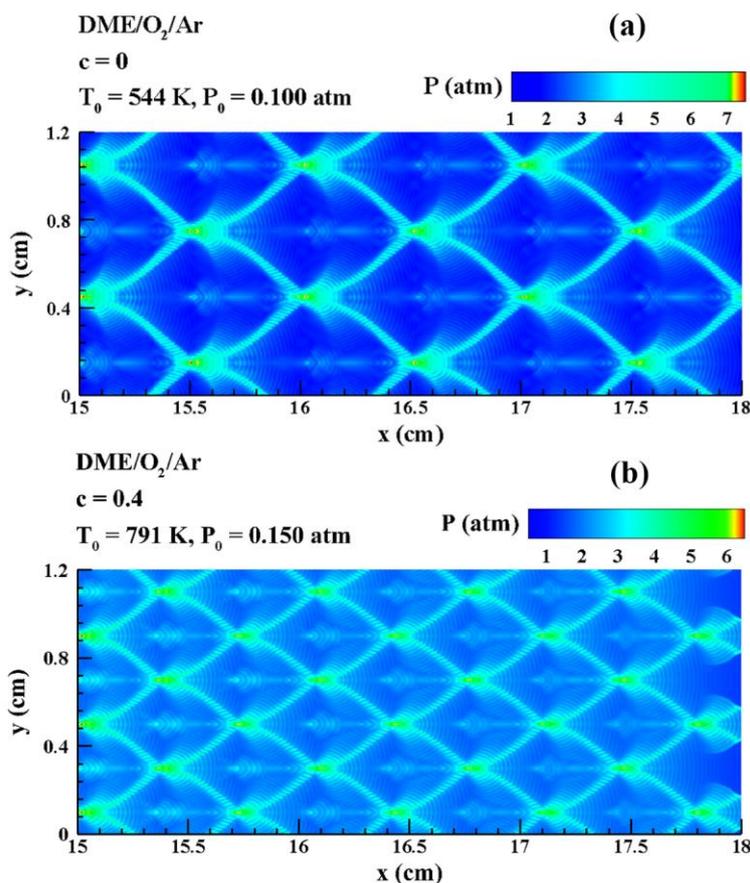


Figure 2: Detonation cell structure for (a) $c=0$ and (b) $c=0.4$.

In two-dimensional simulation, the computational domain is a $20\text{cm} \times 1.2\text{cm}$ rectangle with periodical boundary conditions at upper and lower edges, and wall boundary conditions at left and right edges. A high temperature and pressure zone is set at the left end to initiate the detonation. In order to apply disturbance, the hot spot zone and the unburned zone are separated by sinusoidal boundary. In unburned

area, the initial temperature and pressure were set to be 544 K and 0.1 atm. As a comparison, another simulation uses the gas state of reaction progress $c = 0.4$ as the initial condition for the unburned zone.

The calculation uses PeleC [5], which solves the reacting compressible Navier-Stokes on a structured grid with adaptive mesh refinement. For time stepping, an iterative scheme on a spectral deferred correction (SDC) approach is chosen. A piecewise linear interpolation to reconstruct values at face is used in hyperbolic system.

In two-dimensional simulation, grid independence verification was performed. The results of the minimum grid from 15 microns to 500 microns are consistent. The cell size is about 0.6 cm for reaction progress $c = 0$, and the cell size is about 0.4 cm for $c = 0.4$. The proportion of decrease in cell size is approximately the same as that of decrease in the induction length. Validation under different hot spot conditions was also conducted. If the period of the sinusoidal boundary is very small, the number of transverse waves in the computational domain will decrease from a relatively large number at the beginning to a steady-state number which matches the cell size. If a small rectangular perturbation is set in hot spot zone instead of a sinusoidal boundary, the number of transverse waves will gradually increase to the steady-state number.

3 Discussion and conclusion

From the one-dimensional and two-dimensional results, several important properties of detonation have undergone significant changes before and after the low temperature reactions, including CJ speed, induction length and cell size. These changes happen during the transition between the first stage and the second stage of auto-ignition. From one dimensional results, it is caused by temperature, pressure, and mole fraction jointly. If cell size represents the sensitivity of detonation [6], two-dimensional results shows that low temperature chemistry partially oxidization can sensitize the unburned mixture.

4 Future plan

Low temperature chemistry has a comprehensive impact on detonation, so this work requires full-scale research on it. The study will continue to advance, with a focus on analyzing the sensitization phenomenon in greater detail, which means the detonation energy density, DDT process and the speed of reaching the steady state. As expected, they will be affected to some extent by the low temperature chemistry.

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