

# Simplified Chemical Reaction Model and Its Application in Flame Acceleration and Detonation

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## 1 Introduction

The studies of flame acceleration mechanism, deflagration to detonation transition(DDT) mechanism are of great significance for the prevention and prevention of industrial explosion disasters and the design of detonation propulsion. While, in many studies on the numerical simulation of combustible gas flame acceleration and DDT, the one-step model or the detailed chemical reaction model was used. These models are not able to meet the accuracy of the simulation and cost-effective applications, so the development of a more efficient simplified model is necessary.

This paper established and verified the accuracy of the REDIM(Reaction-Diffusion-Manifold) model based on the experiment of the explosion characteristics of methane and oxygen premixed gas in small-scale pipelines conducted by my lab. As a comparison, one-step reaction model:  $\text{CH}_4+2\text{O}_2\rightarrow\text{CO}_2+2\text{H}_2\text{O}$  was selected. Also, the elementary reaction model (14 components and 19 reaction steps) was selected, in which the components involved in the reaction are  $\text{H}_2$ ,  $\text{O}_2$ ,  $\text{H}$ ,  $\text{O}$ ,  $\text{OH}$ ,  $\text{H}_2\text{O}$ ,  $\text{CH}_3$ ,  $\text{CH}_4$ ,  $\text{CO}$ ,  $\text{CO}_2$ ,  $\text{HCO}$ ,  $\text{CH}_2\text{O}$ ,  $\text{CH}_3\text{O}$  and  $\text{C}_2\text{H}_6$ . And , this 14 components and 19 reaction steps model had been proved [1] to be suitable not only for diffusion flames, but also for premixed flames, its result of combustion speed and flame characteristics, such as temperature etc. was in good agreement with the experimental results.

Large eddy numerical simulations were carried out by using three reaction models (one-step reaction model, 14-component 19-step model and REDIM model) for experiments conducted by my lab. By comparing with other two model's numerical results and the experimental results, the accuracy and high-efficiency (low computational cost) of the REDIM model were verified.

## 2 The experiment on explosion characteristics of methane oxygen premixed gas

The experiment (Fig.1 and Fig. 2) of the small-scale pipeline(20 mm\*20 mm square section and length of 1.5 m) methane oxygen premixed gas explosion characteristics is conducted by the State Key Laboratory of Explosion Science and Safety Protection, Beijing Institute of Technology. The experimental system including small scale pipeline, high speed photography system, ignition system, external trigger system and pressure data acquisition system, etc.

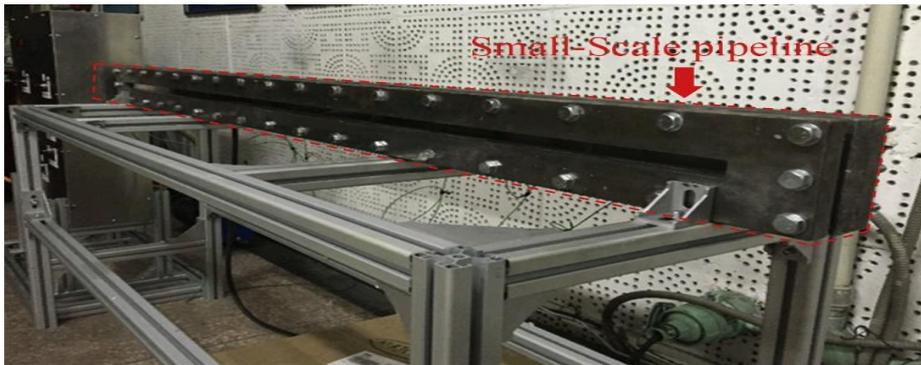


Figure 1 Picture of small-scale pipeline experiment system device

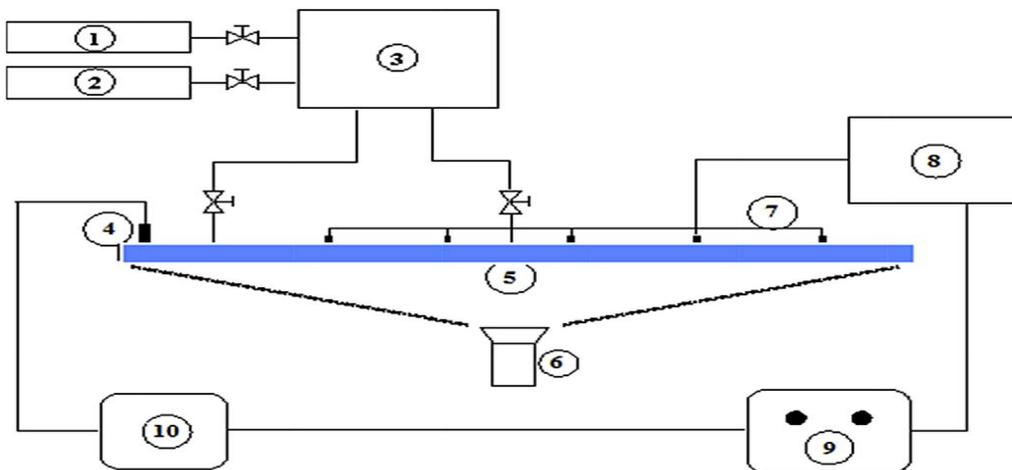


Figure 2 Diagram of the experimental system

(1) - pure methane, (2) - pure oxygen, (3) - gas mixing device, (4) - ignition electrode, (5) - horizontal channel, (6) - high-speed video camera, (7) - pressure and temperature recorder, (8) - data recorder, (9) - synchronization controller, (10) - spark igniter.

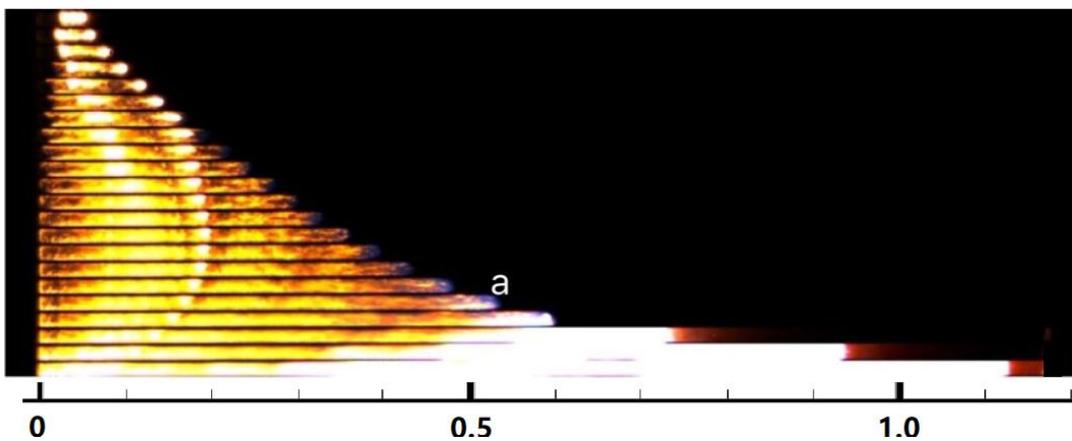


Figure 3 High-speed camera image of premixed gas explosion flame propagation

Fig.3 is a high-speed image of the combustion of a methane oxygen premixed gas in a small-sized pipe and DDT at initial pressure of 40 kPa and equivalent ratio of 1.0. In Fig.3, a white light appears on the flame surface at position (0.52 m). Here, a partial explosion occurred. The local explosion caused the flame propagation speed to increase, and the pipeline pressure increase, which triggered the deflagration to detonation transition.

### 3 Establishment of REDIM (reaction-diffusion manifold)

REDIM[2~4] had followed the main concept of decomposition of time scales (time scales analyzed by eigenvalues of the Jacobian matrix). It was based on the assumption of existence of invariant slow manifolds in the thermo-chemical composition space (states space) of a reacting flow. REDIM technology took into account the coupling process between chemical reactions and molecular transport when using mathematical methods to automatically generate low-dimensional manifolds. It can solve both the fast-reacting combustion and the slow-burning that controls the chemical reaction rate during the diffusion. It had achieved a unified description of the fast and slow reaction zones.

Based on the above experiment, the simplified chemical model REDIM was established. In the generated REDIM manifold, the CO<sub>2</sub> mass fraction was selected as the reference variable. By inputting experimental parameters and boundary conditions into the REDIM program, and setting the gradient value of the parameter (CO<sub>2</sub> mass fraction), the REDIM table required in this paper was automatically obtained by the REDIM program. This table was a chemical reaction lookup table. Given the reference coordinate value, i.e. the parameter (CO<sub>2</sub> mass fraction), the parameters such as CH<sub>4</sub>, O<sub>2</sub>, CO and OH, and the CO<sub>2</sub> generation rate can be obtained from the REDIM table to support subsequent calculations.

The relationship between the CO<sub>2</sub> production rate and the mass fraction in the REDIM model was compared with those of the one-step model and 14-species, 19 step model. Then, the accuracy of the established REDIM manifold was verified.

### 4 Governing equations and numerical methods

Based on the three reaction model (one-step model ; 14-species, 19 step model ; REDIM model), LES governing equation with chemical reaction was established. It included the mass conservation equation, the momentum conservation equation, the energy conservation equation, and the species mass fraction transport equation.

The FSD (flame surface density) model was used in the single-step reaction model and the 14-species, 19 step model, where the one-step model case needed to calculate one transport equation, 14-species, 19 step model needed to calculate the transport equation for each species. In the REDIM model, the flame surface density model was combined with the REDIM method to generate a manifold to form a new combustion model.

In the simulation, the 5th-order WENO finite difference scheme was used for the spatial discretization, the 6th-order central difference scheme was adopted for the viscous term, and the 3rd-order TVD-Runge-Kutta method was adopted for the time-discrete direction. The validity of the numerical algorithm was verified by using the WENO algorithm to solve the two-dimensional Riemann problem.

The calculation area was a small pipe closed at both ends of 20 mm × 1500 mm (see Figure 4), and premixed gas having a stoichiometric ratio was set. The boundary of the was a non-slip reflection solid wall. The ignition area was consistent with the experimental situation. it was placed at the left

end of the pipe, that was, a high temperature zone was added. The temperature in the high temperature zone was 2625K, the pressure was 40 kPa, and the velocity was 0 m/s. The initial velocity, temperature and pressure in the calculation area were 0 m/s, 298 K and 40 kPa respectively, and the grid size was 1 mm.

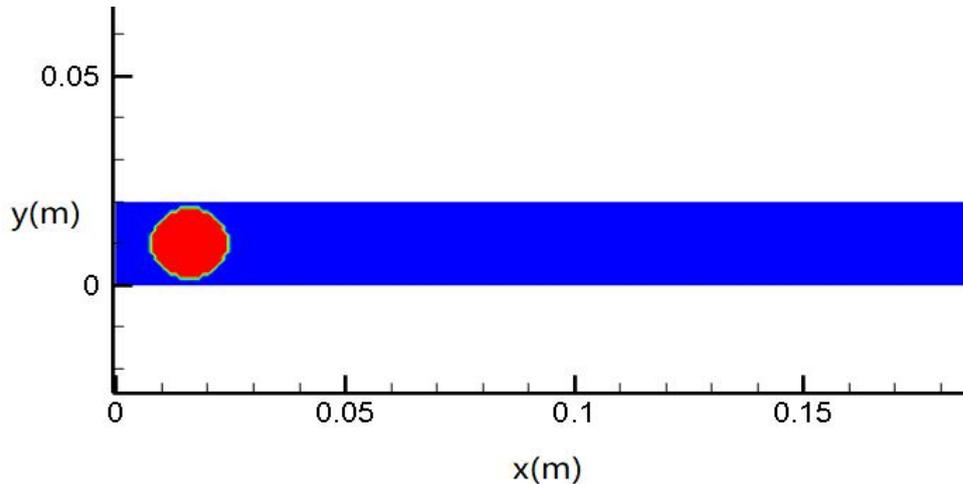
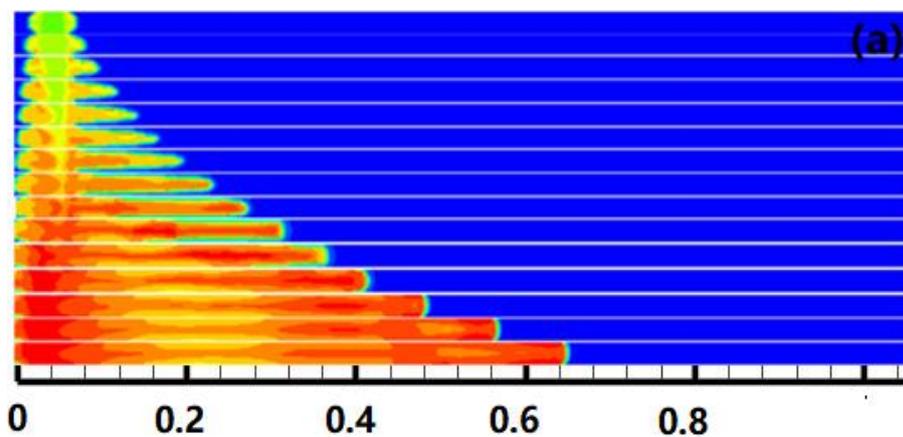


Figure 4 Calculation model of flame explosion characteristics

## 5 Results of numerical simulations and analysis

Large eddy numerical simulations were carried out using three reaction models (one-step reaction model, 14-component 19-step model and REDIM model) for experiments of DDT in small-scale pipeline. By comparing with the experimental results and the other two reaction model's results, the accuracy and high-efficiency (low computational cost) of the REDIM model were verified.

Figure 5(a)(b)(c) are temperature cloud diagram of the numerical simulation by the one-step reaction model, the 14-component 19-step reaction model, and the REDIM model respectively during flame acceleration and deflagration to detonation transition.



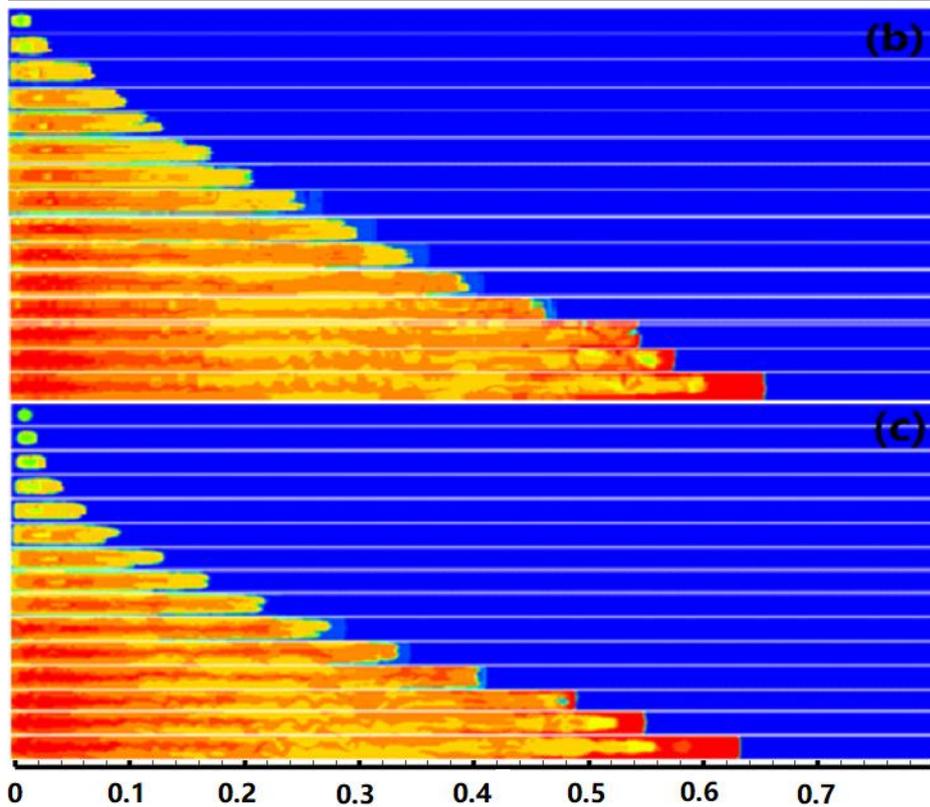


Figure 5 Simulation of the temperature cloud during flame propagation and DDT

(a) one-step reaction; (b) 14-species, 19 step; (c) REDIM

From Fig3 and Fig.5, The position of detonation (0.38 m) for the one-step reaction model was very different from the experimental results(0.52 m, see Fig.3), while the simulation results of the 14-species, 19 step model (0.5 m) and REDIM result (0.49 m) was very close to the experiment result (see Fig.3).

The whole process of flame propagation was divided into 4 phases or stages:(1) laminar flame acceleration (2) pressure wave formation phase in front of the flame, (3) reaction gradient formation phase (4) DDT phase.

Some further comparative numerical simulations and analysis were conducted for 4 phases in this paper. For example, in the reaction gradient mechanism formation stage, the Figure 6(a)(b)(c) were the temperature evolution diagram on the axis for the one-step model, the 14-component 19-step model, and the REDIM model respectively.

It can be seen from Fig 6(b) and Fig 6 (c) that due to the onset of hot spots in the preheating zone, temperature pulse appear in front of the flame surface after the hot spot was ignited. While the temperature pulse was not obvious in one-step model result in Fig 6(a)

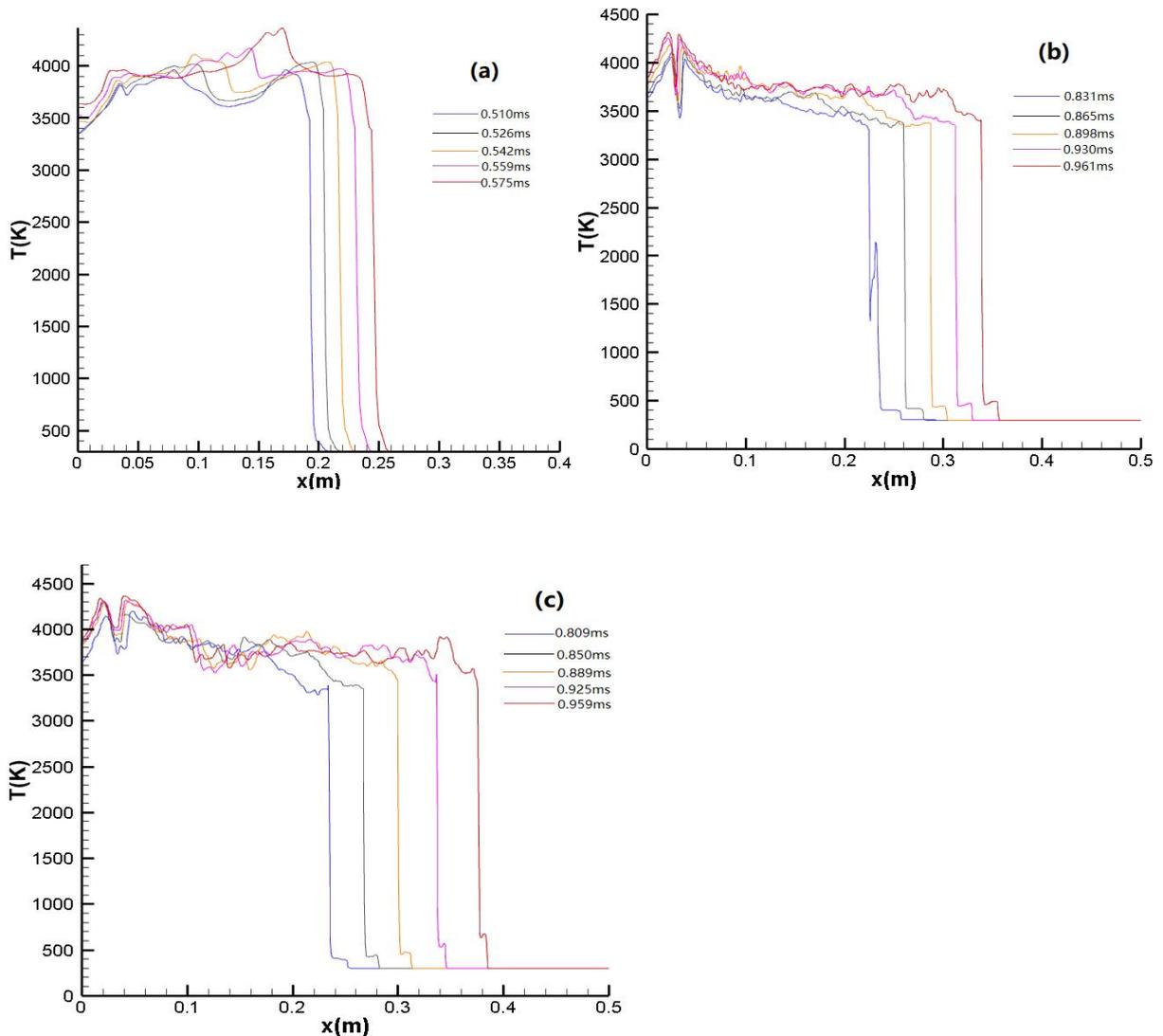


Figure 6 Temperature evolution diagram on the axis,  
 (a) one-step reaction; (b) 14-species, 19 step; (c) REDIM

## References

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