

A numerical high-speed reacting flow model based on the AMReX frame

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1 Abstracts

A numerical high-speed reacting flow model based on the AMReX [1] frame is developed. The multi-species Euler equation is considered as the governing equation of the high-speed reacting flow, since the diffusion effect is negligible. The thermal properties of the multi-species are assumed to be the function of temperature, and the nasa-7 model is employed to calculate these properties. Point-implicit method is used to solve the reaction source term to avoid the stiff problem. The 1D, 2D and 3D $H_2/O_2/Ar$ detonation is simulated based on the model, and the results demonstrate the efficacy of the model. The leading shock wave and the transverse wave of the 2D and 3D detonation are highly resolved in the results, suggesting the model is suitable for the simulation of detonation.

2 Numerical Model

The Euler equation is employed to depict the high-speed reacting flow, since the diffusion effect, including viscous diffusion, thermal diffusion as well as species diffusion, is insignificant in such problem. The governing equation is as follows,

$$\begin{aligned}\frac{\partial(\rho_k)}{\partial t} + \frac{\partial(\rho_k u_j)}{\partial x_j} &= \dot{S}_k \\ \frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j + p \delta_{ij})}{\partial x_j} &= 0 \\ \frac{\partial \rho E}{\partial t} + \frac{\partial[\rho(E + p)u_j]}{\partial x_j} &= 0\end{aligned}\quad (1)$$

where ρ_k denotes the density of the k th species; \dot{S}_k denotes the source term caused by the chemical reaction; $E = e + u_i u_i / 2$ is the total energy of the gas, where e is the internal energy. The thermal properties of the gas species is calculated using the NASA-7 model,

$$\begin{aligned}\frac{C_{p,k}}{R_u/M_k} &= a_{0,k} + a_{1,k}T + a_{2,k}T^2 + a_{3,k}T^3 + a_{4,k}T^4 \\ \frac{h_k}{R_u/M_k} &= a_{0,k}T + \frac{a_{1,k}}{2}T^2 + \frac{a_{2,k}}{3}T^3 + \frac{a_{3,k}}{4}T^4 + \frac{a_{4,k}}{5}T^5 + a_{5,k} \\ \frac{s_k}{R_u/M_k} &= a_{0,k} \ln T + a_{1,k}T + \frac{a_{2,k}}{2}T^2 + \frac{a_{3,k}}{3}T^3 + \frac{a_{4,k}}{4}T^4 + a_{6,k}\end{aligned}\quad (2)$$

where T is the temperature; $a_{0,k} \sim a_{6,k}$ are the NASA-7 coefficients for the k th species; R_u represents the universal gas constant; M_k denotes the molecular weight for the k th species; $C_{p,k}$, h_k , s_k denote the constant pressure specific heat, enthalpy and entropy for the k th species, respectively.

The Euler equation is numerically discretized using finite-volume approach. The convection flux is reconstructed using modified second order MUSCL scheme with the mini-mod limiter [2]. And then the HLL solver [3] is employed for the estimation of the face flux. The three-order Runge-Kutta method is adopted for the temporal integration. As for the source term of the component equation, Arrhenius law is employed to calculate the reaction rate of each component. And to avoid the stiffness problem caused by the short time scale of the chemical reaction, the point-implicit method is adopted for calculation of chemical source term.

The 1D, 2D and 3D $H_2/O_2/Ar$ detonation is investigated in our study. A detailed reaction mechanism with 7 species and 8 element reactions [4] is employed in the simulation, which has been used for the simulation of the detonation. For all the simulations, the gas mixture is composed of the stoichiometric hydrogen and oxygen diluted by 70% argon. And the initial state for the gas mixture is 293 K, 100 kPa. The initial condition for the 1D simulation is shown as Figure 1 (a), while the initial condition for the 2D simulation is shown as Figure 1 (b). For the 1D and 2D simulation, the mesh size for the base grid is 25 μm , with a maximum refine level of 3, meaning the finest mesh size is 3.125 μm . For the 3D simulation base mesh size is 50 μm , with a finest mesh size is 6.25 μm . The domain size for the 1D, 2D, 3D simulation is 204.8 mm, 51.2 mm \times 12.8 mm, 51.2 mm \times 6.4 mm \times 6.4 mm, respectively. The timestep is controlled by the CFL number with the value of 0.2, and in all steps, the timestep is smaller than 10^{-9} s.

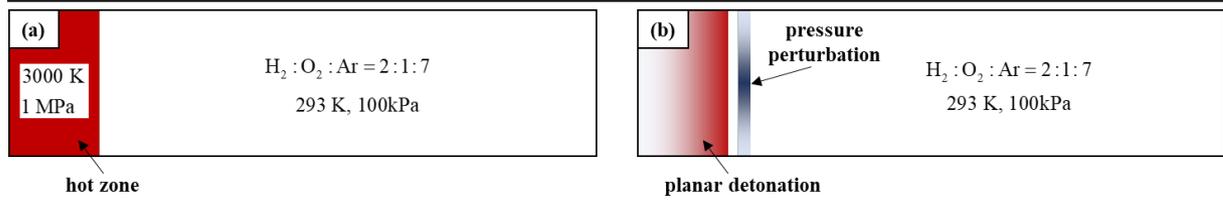


Figure 1 Schematics of the initial condition for 1D simulation (a), and the initial condition for the 2D simulation (b).

3 Result and Discussion

The 1D simulation result is presented in Figure 2. The post-shock pressure of the 1D numerical result is 2.92 MPa, which is the same as the theoretical value (2.92 Mpa) of the CJ detonation calculated by the Shock and Detonation Toolbox [5]. Such consistency demonstrates that the numerical model is appropriate for the simulation of detonation wave.

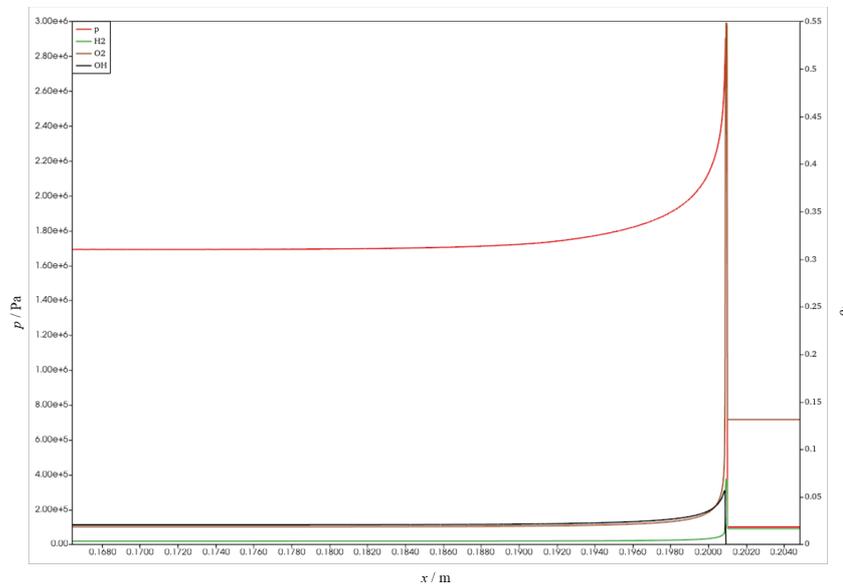


Figure 2 The pressure and the mass fraction of H₂, O₂, OH along the x direction of the 1D detonation.

Figure 3 exhibits the results the simulation results for the 2D cellular detonation. Comparing Figure 3 (a) with Figure 3 (b), we find that the region containing the leading shock front is well refined. The leading shock wave as well as the transverse wave can be easily identified in Figure 3 (b). And combined with Figure 3 (c), the incident shock and the Mach stem can be classified. The leading shock with a high OH density behind it is just the Mach stem. And the pressure behind the Mach stem is higher than the pressure behind the incident shock, but it's not evident in Figure 3 (b). The Figure 3 (d) record the trajectory of the triple point and can be served as the numerical soot figure for the detonation. And the cell size measured from Figure 3 (d) is about 2.2 mm. And in the experiments, the cell size of the detonation in the same condition is at the order of 1 mm. Therefore, the 2D numerical result matches well with the experiment result.

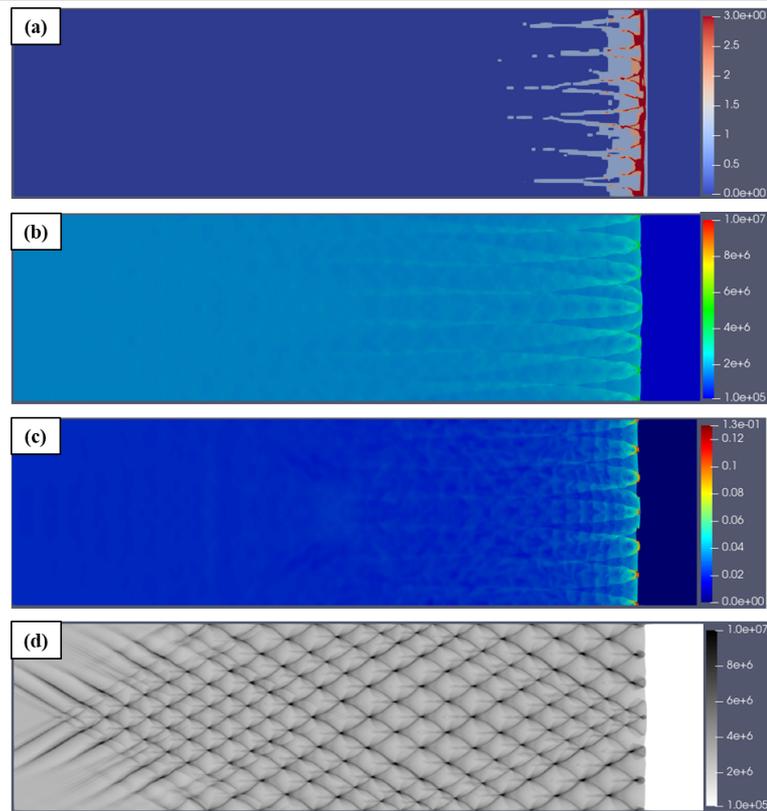


Figure 3 The contours of the mesh refinement level (a), the pressure (b), the OH density (c) and the maximum pressure (d) for the 2D detonation.

The 3D simulation result is presented in Figure 4. Here, the maximum pressure contour at different section is plotted. It can be seen in the figures that the cell pattern is more chaotic, and the cell size is smaller compared with the 2D simulation. The reason may be that the difference in the 3D confinement and the 2D confinement. And for the 3D condition, the cell size is about 0.8 mm, and the result is still close to the experiment result.

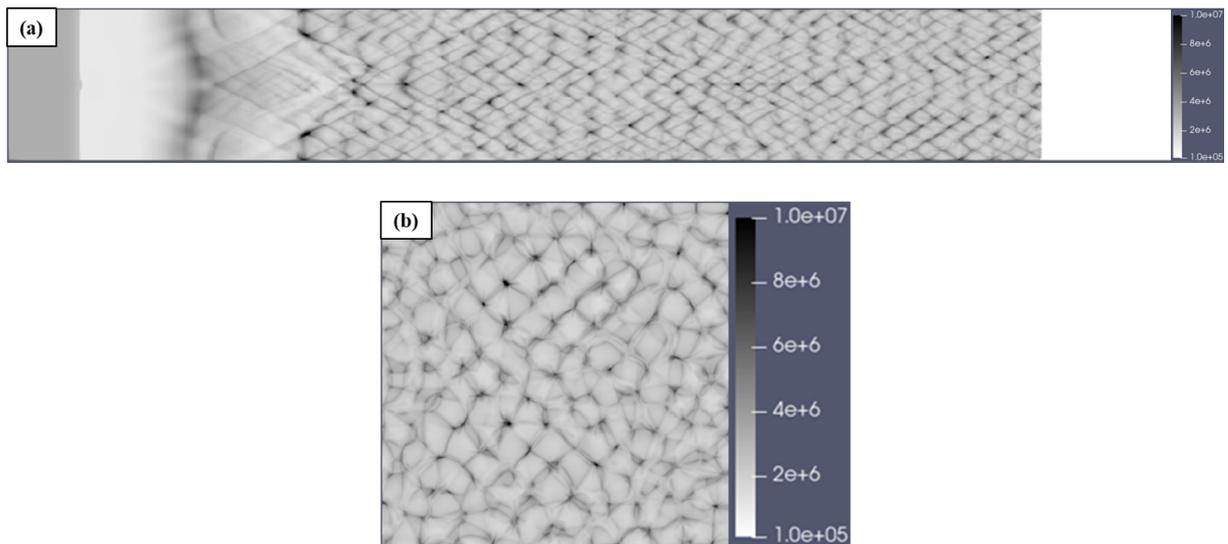


Figure 4 The contours of the maximum pressure at x - y plane with $z = 3.2$ mm (a), the maximum pressure at y - z plane with $x = 43.5$ mm (b).

4 Conclusion

A numerical high-speed reacting flow model based on the AMReX frame is proposed. And the simulation results for the 1D, 2D, 3D detonation are presented. For the 1D detonation simulation, the post-shock pressure exhibits good agreement with the CJ theory. And for the 2D and 3D simulation, the cell size measured in the numerical soot figure also align well with the experimental results. And these consistencies demonstrate that the numerical model is suitable for the simulation of detonation wave. And here only a shallow analysis has been conducted, so, more information is supposed to be explore from the numerical results.

References

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