Influence of detailed mechanisms of chemical kinetics on propagation and stability of detonation wave in H\textsubscript{2}/O\textsubscript{2} mixture

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Abstract. In the present paper, detonation in a stoichiometric oxygen-hydrogen mixture is simulated numerically using 4 detailed chemical mechanisms. The effect of chemical kinetics models on the stability of 1D detonation wave and 2D detonation wave propagating in a plane channel is investigated. The number of detonation cells formed in a channel of a given width at different degrees of overdrive is determined. Simulations are performed using a previously developed computational program based on high-order shock-capturing TVD schemes and a finite-rate chemistry solver. The program is implemented in C++ using the CUDA parallel computing platform for running on graphic processor devices (GPU), the open OpenMP standard for multi-threaded applications on multiprocessor systems with shared memory and the MPI protocol for data exchange between processors.

1. Introduction

Numerical simulations of detonation wave (DW) propagation require careful choice of a chemical mechanism as it plays an important role and its parameters can greatly influence the result [1]. Profiles of gas-dynamic quantities, a velocity of DW propagation, a number of detonation cells formed can greatly differ in simulations performed with different chemical models.

There are also widespread reduced chemical mechanisms, in particular a model with a single irreversible reaction and a two-stage model where the induction and heat release periods are separated. For example, the single irreversible reaction model is characterized only by two parameters: the heat release $Q$ and the activation energy $E_a$. By changing these parameters one can investigate their impact on DW stability and study in details the instability development. Some of the results of such research [2] can be seen in figure 1 where, on the left, the DW speed as a function of time is presented. One can notice that the DW speed experiences growing pulsations so that the coefficient of linear growth of DW instability can be measured. On the right, the DW acceleration versus the DW speed is shown. It is clearly seen that later the growth of DW instability is saturated and at a nonlinear stage it finally reaches the limit cycle.
It is clear, however, that the most adequate description of the physicochemical processes occurring during detonation can be achieved on the basis of detailed kinetic mechanisms. As a rule, chemical models for combustion of hydrogen are constructed and verified using available experimental data for slow, diffusive combustion (deflagration). Their applicability when modeling detonation is a delicate subject because of extreme conditions detonation creates and should be studied separately. This is particularly true when investigating detonation instability and formation of cellular structure.

The goal of the present study is to investigate the DW stability with different detailed chemical kinetics models. Detonation in a stoichiometric oxygen-hydrogen mixture is modeled using 4 detailed chemical mechanisms: the ONERA model [3], the Deiterding model [4], which is a hydrogen-oxygen mechanism extracted from the hydrocarbon mechanism of Westbrook [5], the modified Jachimowski model [6] and the Petersen and Hanson model [7]. The previously unexplored effect of chemical kinetics models on the stability of 1D detonation wave and detonation wave propagating in a plane channel is investigated. The linear and nonlinear stages of instability development are studied, the number of cells formed in a 1 cm wide channel in numerical simulation with various chemical mechanisms is determined. The effect of the overdrive factor on DW stability and cellular structure formation is also investigated.

Numerical simulations are performed using a previously developed computational program based on high-order shock-capturing TVD schemes and a finite-rate chemistry solver [8]. The program is implemented in C++ using the CUDA parallel computing platform for running on graphic processor devices (GPU), the open OpenMP standard for multi-threaded applications on multiprocessor systems with shared memory and the MPI protocol for data exchange between processors. The use of these tools allows one to run computational code, both on conventional computing clusters, and on hybrid supercomputers with GPUs.

2. Governing equations

The Euler equations complemented with $N$ equations for chemically reacting species can be written in the conservation law form as follows:

$$\frac{\partial q}{\partial t} + \frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z} = S$$ (1)
\[ Q = \begin{pmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ E \\ \rho Y_1 \\ ... \\ \rho Y_{N-1} \end{pmatrix}, F_x = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ \rho u v \\ \rho u w \\ (E + p)u \end{pmatrix}, F_y = \begin{pmatrix} \rho v \\ \rho v^2 + p \\ \rho v w \\ \rho v Y_1 \\ ... \\ \rho v Y_{N-1} \end{pmatrix}, F_z = \begin{pmatrix} \rho w \\ \rho w^2 + p \\ \rho w v \\ \rho w Y_1 \\ ... \\ \rho w Y_{N-1} \end{pmatrix}, \quad S = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ W_1 \omega \end{pmatrix} \] (2)

Here \( \omega_i \) is the chemical production rate of the \( i \)-th species. Chemical species properties, such as heat capacities \( C_p \) and \( C_v \), specific enthalpy \( H \), and specific entropy \( S \) are determined using polynomial approximations based on Burcat thermodynamic database \([9]\). The code is capable of using any chemical mechanism provided in the CHEMKIN format. In this paper we use 4 different chemical mechanisms \([3-7]\), basic descriptions of which and comparison of profiles of gas-dynamic quantities can be found in \([10]\).

The forward (f) and reverse (r) reaction rates are determined using the Arrhenius formula:

\[ k_{f,r} = A_{f,r} T^{\beta_{f,r}} e^{-\frac{E_a}{T}}, \] (3)

where \( T \) is the temperature and the constants \( A, \beta, E_a \) are parameters of a chemical model.

2.1. Numerical methods

The Euler equations are solved using shock-capturing MUSCL (monotonic upwind schemes for conservation laws) TVD schemes. The flow variables are reconstructed on the cell boundaries from cell-centered values with a 2nd or 3rd order of accuracy and then are limited using minmod slope limiter. Numerical fluxes are calculated with the HLLE (Harten-Lax-van Leer-Einfeldt) approximate Riemann solver. Time advancement is carried out using either explicit Runge-Kutta TVD schemes of 2nd or 3rd order, or semi-implicit ASIRK2C scheme of 2nd order \([11]\), which is more efficient in terms of the computational time, because it allows one to integrate stiff chemical source terms using considerably larger time steps.

In order to investigate linear and nonlinear stages of DW propagation and cellular structure formation modifications to the existing code are made. This allows saving the DW position history and the DW front shape. In 1D numerical simulation a point where Mach number equals 1 for the first time is taken as a DW position. In 2D case such points traced across a channel form the DW curved front form and their average X coordinate is taken as a DW position.

3. Numerical simulations

The problem of DW propagation in a channel filled with the stoichiometric mixture of \( \text{H}_2 \) and \( \text{O}_2 \) is investigated. The initial pressure is set to 10132.5 Pa. On the right boundary the supersonic inflow conditions with the Mach number depending on the overdrive factor are imposed. The Zeldovich-von Neumann-Doering (ZND) solution profile is used as an initial flowfield, and the values of parameters corresponding to the end state of the ZND profile are fixed at the left boundary of the computational domain. As the DW propagation velocity changes periodically due to the ZND solution instability a buffer zone with inflow parameters is placed between the DW wave and the right boundary in order to maintain the DW within the computational domain.

At first we determine the Chapman-Jouguet (CJ) Mach number for all 4 detailed chemical kinetic mechanisms. For this purpose we use a modified Fortran program for the ZND solution calculation. It determines the CJ Mach number in a series of ZND solution computations by changing the inflow Mach number until the outflow Mach number is equal to 1. The resulting CJ Mach number is close to 5.025 for all 4 studied chemical models. The 1D simulations are performed on an Intel Xeon E5-2695 v4 processor with up to 10 CPU cores per one simulation, while the 2D simulations are performed using 8 Nvidia GeForce 1080Ti GPUs of a computational cluster.
3.1. 1D numerical simulations
In this section we compare 1D numerical simulations of DW with different detailed chemical models and investigate the influence of a model on DW instability. The influence of the overdrive factor is also considered.

The computational domain length $L$ and the grid resolution are determined so that in all cases there are 40 grid cells with the half-reaction zone. The latter is determined by $H_2$ concentration – its value reduces by half at the zone end. This gives the largest domain length equal to 2 cm and up to 2500 grid cells overall.

The results are presented in figure 2. Here the DW position is shown as a function of time for different chemical models and overdrive factors. From figure 2 it can be clearly seen that the DW stability is strongly affected by the overdrive factor: the DW is more stable for higher values of $f$, the instability is totally suppressed for $f > f_{cr}$. This result is valid for all chemical models considered though there is a significant difference in values of $f_{cr}$: it is close to 1.1 for ONERA and Petersen and Hanson models, 1.3 for the Deiterding model and 1.4 for modified Jachimowski model. Such noticeable difference in $f_{cr}$ makes the choice of chemical model particularly important in simulations aimed at comparison with real-life experiments.

![Figure 2. DW position as a function of time for different models and overdrive factors.](image)
3.2. 2D numerical simulations

It is well known that the ZND solution is unstable to transverse disturbances. 2D numerical simulations allow us to investigate the effect of the instability on cellular structure formation for different chemical models. In 2D case we use same chemical models as in 1D case and for each model we perform simulations at three values of the overdrive factor: 1.0, 1.2, 1.4. The DW propagates in a channel with width \( H = 1 \text{ cm} \). The channel length \( L \) depends on the overdrive factor. Typical values are \( L = 6 \text{ cm} \) for \( f = 1 \), \( L = 3 \text{ cm} \) for \( f = 1.2 \) and \( L = 1.5 \text{ cm} \) for \( f = 1.4 \). Grid resolution is 400 points per 1 cm, so the maximum grid size is 400×2400 points. The results of 2D numerical simulations for the ONERA model are presented in figure 3.

![Figure 3. 2D numerical simulations with ONERA chemical model for different overdrive factors.](image)

The upper part of figure 3 illustrates the initial, linear stage of cellular structure formation. It is noticeable that at this stage the higher values of \( f \) result in smaller cells. The lower part of figure 3 shows the cellular structure during the later, nonlinear stage. It is evident that the cell size has changed drastically: nonlinear effects have led to merging of small detonations cells into larger ones.

In order to investigate this process in more detail, the position of DW front at different values of the \( y \) coordinate is recorded. The time histories of DW positions on the channel bottom wall and averaged over the channel width in simulations with the ONERA chemical model are displayed in figure 4. The positions are taken in the frame of references moving with the velocities equal to the corresponding DW ZND speeds.

It is seen that up to some moment the DW speed in this frame of references is close to zero. The flow is essentially 1D. At \( f = 1 \) small longitudinal oscillations of the DW position are present during this stage while at \( f = 1.2 \) the longitudinal oscillations gradually decay. At \( f = 1.4 \) no such oscillations are visible. However, approximately at \( T \approx 4 \times 10^{-5} - 5 \times 10^{-5} \text{ s} \) 2D flow disturbances start to develop, transverse waves emerge on the DW front and cellular detonation structure form. The amplitude of 2D pulsations depends on the overdrive value, with the strongest pulsations observed for the CJ detonation. The development of 2D instability causes an increase in the DW propagation speed. At \( f = 1.4 \) the DW speed increases by some constant value; at \( f = 1.2 \) the increase is more significant and the DW speed oscillates slightly.
around its increased value. At $f = 1$ it experiences strong pulsations though an increase in the averaged speed which is also distinctively visible. This behavior is common for all 4 chemical models but times needed for the emergence of 2D disturbances are different.

To characterize the process of formation and development of the cellular structure quantitatively the number of cells as function of time is determined using the Fourier transform of the DW front shape. The results for the ONERA model and three different overdrive factors are presented in figure 5. Earlier in numerical simulations [12] for a simple model with one irreversible reaction it was observed that the number of detonation cells halved during the nonlinear stage. It is not the case in the present simulations with the detailed chemistry mechanisms. Although there is a clear tendency to merging of detonation cells after the onset of the nonlinear stage, the final number of cells depends substantially on the overdrive – see figure 5. However, more detailed studies are necessary to determine mechanisms responsible for the final selection of the cell size during nonlinear stages of flow evolution.

**Figure 4.** Time history of averaged DW position (left) and time history of its position on the channel bottom wall (right).

**Figure 5.** Number of detonation cells as a function of time.
For better understanding of general picture, in table 1 we provide an overview of the obtained results for different chemical models and overdrive factors. It is noticeable that there is a scattering in the number of cells obtained at the linear stage with different models. At nonlinear stage results are closer to each other with the ONERA and Petersen and Hanson models giving, for high overdrive factor $f$, a slightly higher number of cells than Deiterding and modified Jachimowski models.

Table 1. Number of cells for different chemical models and overdrive factors.

| Chemical model       | $f = 1$ linear | non-linear | $f = 1.2$ linear | non-linear | $f = 1.4$ linear | non-linear |
|----------------------|---------------|------------|-----------------|------------|-----------------|------------|
| ONERA model          | 7             | 1          | 4-6             | 2          | 11              | 5-8        |
| Deiterding model     | 7             | 1-2        | 9               | 2          | 9-12            | 4-6        |
| Mod. Jachimowski model | 5-6          | 1-2        | 5-6             | 2          | 8-10            | 4-5        |
| Petersen and Hanson model | 6-7          | 1          | 12              | 2-3        | 12-13           | 5          |

Conclusions

Four detailed chemical kinetics models have been investigated using numerical simulation. 1D and 2D DWs with different overdrive factors $f$ have been simulated with focus on the disturbance development and cellular structure formation.

1D numerical simulations show that the overdrive factor $f$ at which the flow becomes stable can vary significantly depending on the chemical model used. Unlike a simplified chemistry model with one irreversible reaction, the detailed chemical models demonstrate more rapid growth of 1D instability, it is particularly true for the ONERA and Petersen and Hanson models. This circumstance makes it difficult to investigate the linear growth of instability and to determine the growth rate.

2D numerical simulations of a DW propagating in a plane channel show that emergence of transverse waves on the DW front affects the DW speed and leads to cellular structure formation. A comparison of 4 detailed chemical kinetics models shows quantitative differences. The number of detonation cells differs, especially on later stages of DW propagation or with higher overdrive factor $f$.

Considering the above, it is planned to perform numerical simulations of linear development and cellular structure formation in a wider channel. Also, it is planned to conduct numerical simulation for gas mixtures diluted with an inert gas to obtain enlarged and more regular pattern of detonation cells. Also 3D numerical simulations have to be done in order to compare with real-life experiments and investigate the effect of shock waves propagating in both transverse directions and their influence on cellular structure characteristics.

Acknowledgments

This work was supported by the Russian Foundation for Basic Research (Grants № 18-33-00740, 18-08-01442, 16-57-48007). Numerical code development was partly carried out within the framework of the Program of Fundamental Scientific Research of the state academies of sciences in 2013-2020 (project No. AAAA-A17-117030610138-7).
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