Numerical Simulation of the Detonation Wave in the Shock-Attached Frame for the Two-Stage Kinetics Model

Yaroslava E. Poroshyna¹, Pavel S. Utkin^{1,2} ¹Moscow Institute of Physics and Technology Dolgoprudny, Moscow region, Russia ²Institute for Computer Aided Design of the Russian Academy of Sciences Moscow, Russia

1 Introduction

Theoretical and numerical studies of the stability of Zeldovich-von Neumann-Doring (ZND) solution describing a stationary detonation wave (DW), as well as pulsating modes of DW propagation, go back to the works of Erpenbeck [1] and Fickett [2]. A large number of subsequent fundamental studies of pulsating DW are associated with the use of a single-stage model of the kinetics of chemical reactions. On the one hand, this is due to the considerable degree of development of this model, the well-established methodology of transition to dimensionless variables using the length of the half-reaction and a large amount of accumulated material. On the other hand, it is known that this model is able to describe the main features of nonlinear dynamics of DW propagation such as one-dimensional pulsations, two-dimensional detonation cells and three-dimensional spin. Among the disadvantages of the model is the impossibility of explicit separation of the induction and reaction zones, which was a background for the creation of two-stage models of kinetics. Apparently, V.P. Korobeinikov, V.A. Levin, V.V. Markov and G.G. Chernyi [3] were pioneers in this area. Important results concerning the stability conditions of DW propagation in the framework of the two-stage kinetic model were obtained in [4]. The non-dimensional parameter defined as the dimensionless activation energy for the induction process multiplied by the ratio of the induction length was introduced.

The aim of this work is the further clarification of the dynamics of pulsating DW in the framework of the two-stage model of kinetics by considering the problem in the shock-attached frame. There are two major numerical approaches for study of detonation in the shock-attached frame, namely [5] and [6], as well as a number of further modifications and developments, such as [7]. We will follow the ideology [5]. This approach is one-dimensional although some attempts to transform it to a two-dimensional one were made in [8] or more recently in [9].

2 Mathematical Model and Statement of the Problem

Correspondence to: pavel_utk@mail.ru

Poroshina, Ya. E.

Mathematical model is based on the reactive Euler equations coupled with the two-stage model of kinetics. The governing system is written in the shock-attached frame (x,t):

$$\frac{\partial \mathbf{u}}{\partial t} + \frac{\partial}{\partial x} (\mathbf{f} - D\mathbf{u}) = \mathbf{s},$$

$$\mathbf{u} = \begin{bmatrix} \rho \\ \rho \\ \rho \\ e \\ \rho \\ \lambda_i \\ \rho \\ \lambda_r \end{bmatrix}, \quad \mathbf{f} = \begin{bmatrix} \rho \\ \nu \\ \lambda_r \end{bmatrix}, \quad \mathbf{s} = \begin{bmatrix} 0 \\ 0 \\ \rho \\ Q \\ \left[1 - H (1 - \lambda_r) \right] K_r (1 - \lambda_r)^k \\ -\rho \\ K_i H (1 - \lambda_r) \cdot \exp(-E_a \rho / p) \\ \rho \\ \left[1 - H (1 - \lambda_r) \right] K_r (1 - \lambda_r)^k \end{bmatrix}, \quad (1)$$

$$e = \rho \varepsilon + \frac{1}{2} \rho v^2, \quad \varepsilon = \frac{p}{\rho(\gamma - 1)}.$$

Here *D* is the leading shock speed, ρ is the density, *p* is the pressure, *v* is the velocity of gas in the laboratory frame, *e* is the total energy density, λ_i is the variable of the induction zone progress which equals 1 in reactants and 0 in the end of the induction zone, λ_r is the variable of the reaction zone progress which equals 0 in the induction zone and reaches 1 in products, *H* is the Heaviside step function, K_i and K_r are the reaction rate constants in the induction and reaction zones respectively, is the activation energy, *Q* is the heat release, *k* is the reaction order in the reaction zone, γ is the heat capacity ratio. It is supposed that the gas obeys the ideal gas state equation.

The system of governing equations (1) is made dimensionless in accordance with [10]. Von Neumann parameters ρ_s and p_s are used as characteristic density and pressure, $v_s = (p_s/\rho_s)^{1/2}$ is used as the velocity scale. The length scale is chosen to be equal to the induction zone length $\Delta_i = (D_{CJ} - v_s)t_i$, where D_{CJ} is the Chapman-Jouguet (CJ) velocity, t_i is the induction time.



Figure 1. The leading shock wave (LSW) propagation in a low-frequency regime with different resolutions of induction zone: green line – 32 cells, blue line – 64 cells, violet line – 128 cells, red lines – 256 cells.

The interval [-L;0] is considered as the computational area. On the rear left end of the computation domain x = -L different boundary conditions are imposed including CJ conditions, extrapolation of zero

27th ICDERS – July 28th - August 2nd, 2019 – Beijing, China

order and non-reflecting boundary condition [5]. On the right end of domain the boundary conditions respond to Rankine-Hugoniot conditions on the shock, see the next Section. The grid is uniform with the resolution 128 cells per induction zone. This resolution was chosen after the grid convergence study (see Fig. 1) with the use of the maximum values of activation energy and heat release used in this research which respond to the low frequency regime, see section 4. The total number of computational cells is denoted as N. ZND-solution is used as an initial condition.

3 The Algorithm for the Shock Speed Calculation

The computational algorithm is based on the principal of splitting by physical processes. Firstly, the gas dynamics equations are integrated on the time step with no chemical reactions taken into account (s = 0). The spatial discretization of the governing system is performed using finite volume method. On this hyperbolic step Courant-Isaacson-Rees numerical scheme in conservative formulation of the second approximation order is applied. On the second step the chemical reactions are considered without convection terms. Such system is solved with the use of explicit Euler method. The numerical algorithm in general follows [7].

The shock-attached frame formulation of the governing equations leads to the modification of the numerical flux which includes now the unknown LSW speed D^{n+1} from the next time layer. The additional equations on the C₊-characteristics to calculate D^{n+1} are derived from the characteristic form of the governing system:

$$\begin{cases} \frac{dx}{dt} = v + c - D, \\ \frac{dp}{dt} + \rho c \frac{dv}{dt} = 0. \end{cases}$$
(2)

This system is discretized according to [5] under the assumption of local linear approximation of the characteristic curve C_+ (see Fig. 2):

$$\begin{cases} -x_*^n = (c_*^n + v_*^n - D^n) \Delta t^n, \\ p_0^{n+1} - p_*^n + \frac{1}{2} ((\rho c)_*^n + (\rho c)_0^{n+1}) (v_0^{n+1} - v_*^n) = 0. \end{cases}$$
(3)

The unknown x_*^n is found from the first equation of (3). Gas velocity v_*^n and sound velocity c_*^n at the point (x_*^n, t^n) are expressed with the use of linear interpolation between points $(0, t^n)$ and (x_N^n, t^n) . The new LSW speed D^{n+1} is determined from the second equation of (3). All unknown values on the (n+1)-th time layer are expressed using the LSW Mach number M^{n+1} with the use of Rankine-Hugoniot conditions:

$$\frac{p_0^{n+1}}{P_0} = \frac{2\gamma}{\gamma+1} \left(M^{n+1} \right)^2 - \frac{\gamma-1}{\gamma+1}, \quad \frac{\rho_0^{n+1}}{R_0} = \frac{(\gamma+1) \left(M^{n+1} \right)^2}{2 + (\gamma-1) \left(M^{n+1} \right)^2}, \quad \frac{v_0^{n+1}}{C_0} = \frac{2}{\gamma+1} \frac{\left(M^{n+1} \right)^2 - 1}{M^{n+1}}, \quad \lambda_{i0}^{n+1} = 1, \quad \lambda_{r0}^{n+1} = 0,$$

where P_0 , R_0 and C_0 are pressure, density and sound velocity before the DW. The gas is considered to be quiescent before the DW. Thus, the second equation in the discretized system is solved relative to M^{n+1} using Newton iterations. Obtained shock speed D^{n+1} is used then for the numerical flux calculation.

27th ICDERS – July 28th - August 2nd, 2019 – Beijing, China



Figure 2. The sketch to the algorithm of the LSW speed equation integration

4 Pulsating Detonation Wave Simulation

We now consider four sets of parameters from [10] that correspond to the very high frequency regime (VHF), high frequency regime (HF), low frequency (LF) and transient (T) regimes of oscillations (see Tab. 1). It can be noted that the choice of the activation energies and rate constants of the reaction zone for each regime is based on the fact that such regimes are close to the neutral stability boundary.

Regime	E_a	Q	K _r	ν	γ
VHF	1.0	10.3875	2.1	0.5	1.2
HF	5.0	2.789	3.2	0.5	1.2
LF	10.0	10.3875	0.15	0.5	1.2
Т	5.0	10.3875	0.37	0.5	1.2

Table 1: Test cases parameters



Figure 3. LSW pressure dynamics for (a) VHF and (b) HF regimes of pulsating DW propagation with zero-order extrapolation used as rear boundary conditions. Red curves – authors' simulations, black ones – simulations from [10]. N = 2560, L = 20.

27th ICDERS – July 28th - August 2nd, 2019 – Beijing, China



Poroshina, Ya. E.

Figure 4. LSW pressure dynamics for (a) T and (b) LF regimes of pulsating DW propagation with zero-order extrapolation used as rear boundary conditions. Red curves – authors' simulations, black ones – simulations from [10]. N = 12800, L = 100.



Figure 5. LSW pressure dynamics for (a) LF (N = 12800, L = 100) and (b) HF (N = 2560, L = 20) regimes of pulsating DW propagation with different rear boundary conditions. Red curves correspond to zero-order extrapolation, green ones – to CJ conditions.

Fig. 3 illustrates these regimes of oscillations calculated using our technique in comparison with the data from [10]. It can be observed that VHF (period of pulsations is less than induction time) and HF (period of pulsations is greater than induction time but comparable to it) regimes on Fig. 3a and Fig. 3b are in good accordance with [10]. The periods of oscillations are equal and the amplitude of pulsations is slightly higher than in [10] due to the absence of LSW numerical smearing in the shock-attached frame simulations. For LF and T regimes some differences are visible. First of all, although the amplitude of pulsations in our simulations tends to be almost twice as great as in [10], see Fig. 4a. Secondly, there is a considerable difference in the amplitude of pulsations of the LF regime while the period of oscillations is almost the same as in [10], see Fig. 4b. Such differences may be caused by the differences in the method of simulation, the length of the computational domain and the choice of the rear boundary conditions.

27th ICDERS - July 28th - August 2nd, 2019 - Beijing, China

Poroshina, Ya. E.

Elongation of the computational domain length up to 750 units confirms the obtained result. Fig. 5 shows that rear boundary condition does not play significant role in the resulting mode of detonation propagation within this problem.

5 Conclusions

The computational algorithm was proposed for the simulation of detonation wave propagation using twostage kinetics model in the shock attached frame. The algorithm was applied for the simulation of four regimes of detonation propagation, namely very high frequency, high frequency, low frequency and transient regimes. Very high frequency and high frequency regimes correlate well with the data from [10]. There are discrepancies in amplitude and period of pulsations in low frequency and transient regimes in comparison with [10]. The obtained results were confirmed in simulations with variation of computational domain length and rear boundary conditions.

References

[1] Erpenbeck JJ. (1962). Stability of steady-state equilibrium detonations. Phys. Fluids. 5: 604.

[2] Fickett W, Wood WW. (1966). Flow calculations for pulsating one dimensional detonations. Phys. Fluids. 9: 903.

[3] Korobeinikov VP, Levin VA, Markov VV, Chernyi GG. (1972). Propagation of blast waves in combustible gas. Acta Astronaut. 17: 529.

[4] Ng HD, Radulescu MI, Higgins AJ, Nikiforakis N, Lee JHS. (2005). Numerical investigation of the instability for one-dimensional Chapman-Jouguet detonations with chain-branching kinetics. CTM. 9: 385.

[5] Kasimov AR, Stewart DS. (2004). On the dynamics of self-sustained one-dimensional detonations: A numerical study in the shock-attached frame. Physics of Fluids. 16: 3566.

[6] Henrick AK, Aslam TD, Powers JM. (2006). Simulations of pulsating one-dimensional detonations with true fifth order accuracy. JCP. 213: 311.

[7] Lopato AI, Utkin PS. (2016). Toward second-order algorithm for the pulsating detonation wave modeling in the shock-attached frame. CST. 188: 1844.

[8] Taylor BD, Kasimov AR, Stewart DS. (2009). Mode selection in weakly unstable two-dimensional detonations. CTM. 13:6.

[9] Romick TC, Aslam TD. (2016). Two-Dimensional Detonation Propagation using Shock-Fitting. LA-UR-16-24776. 15th International Detonation Symposium, 2014-07-13 (San Francisco, New Mexico, United States)

[10] Leung C, Radulescu MI, Sharpe GJ. (2010). Characteristics analysis of the one-dimensional pulsating dynamics of chain-branching detonations. Phys. Fluids. 22: 126101.