NUMERICAL SIMULATION OF DETONATION WAVE PROPAGATION IN THE NONUNIFORM MEDIUM IN THE SHOCK-ATTACHED FRAME

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Three different numerical algorithms are proposed for the simulation of one-dimensional (1D) pulsating detonation wave (DW) propagation in the periodic nonuniform medium using the shock-attached frame (SAF) of reference. These algorithms ("explicit," "semi-implicit," and "implicit") differ in the way of leading shock speed calculation. The algorithms are analyzed in the problem of shock wave (SW) interaction with the sine waves in density. We show that the "semi-implicit" and "implicit" algorithms for the leading shock speed calculation provide the most robust simulation but nevertheless fail at a certain time at the beginning of the process because of the internal shocklets interaction with the leading shock.

Introduction

The study of the dynamics of DW propagation in a medium characterized by nonuniform distribution of parameters is an actual problem in the context of detonation engine development. Due to the unsteadiness of the processes, the separate supply of fuel and oxidizer, the conditions in the combustion chamber are far from uniform. The arrangements with DW propagation in a channel with transverse (see, for example, [1] and references therein) or longitudinal (see [2] and

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references therein) concentration gradients can be considered as ideal limiting cases for the real life problems. The first one also includes the problem of DW propagation along the inert gas layer(s) [3] and the second one — DW propagation through the inert gas gap(s) [4].

In our previous works, we studied the dynamics of 1D pulsating DW in the SAF. The studies were performed with a one-step [5] and a two-step [6] chemical kinetics models. In all considered problems, a DW propagated in the uniform mixture. So, we decided to improve our algorithm for simulating DW propagation in the nonuniform mixture.

Mathematical Model and Numerical Algorithm

Let us consider reactive Euler equations coupled with a two-step model of kinetics [7]. The governing system of equations is written in the SAF (x, t):

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

Here,

$$\mathbf{u} = \begin{bmatrix} \rho \\ \rho v \\ e \\ \rho\lambda_i \\ \rho\lambda_r \end{bmatrix};\ \mathbf{f} = \begin{bmatrix} \rho v \\ \rho v^2 + p \\ (p+e)v \\ \rho v\lambda_i \\ \rho v\lambda_r \end{bmatrix};\ \mathbf{s} = \begin{bmatrix} 0 \\ 0 \\ \rho Q[1 - H(1-\lambda_r)]K_r(1-\lambda_r)^k \\ -\rho K_i H(1-\lambda_i)\exp\left(-\dfrac{E_a\rho}{p}\right) \\ \rho[1 - H(1-\lambda_r)K_r(1-\lambda_r)^k \end{bmatrix}$$

where

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

All notations are standard: D is the leading SW (LSW) speed; λ_i is the variable of the induction zone progress which equals to 1 in reactants and 0 at the end of the induction zone; λ_r is the variable of the reaction zone progress which equals to 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; E_a is the activation energy; Q is the heat release; and k is the reaction order in the reaction zone.

The interval $[-L; 0]$ is considered as the computational domain. On the rear left end of the computation domain $x = -L$, different boundary conditions are imposed including Chapman–Jouguet (CJ) conditions, extrapolation of zero order, and nonreflecting boundary conditions. On the right end of domain, the boundary conditions correspond to Rankine–Hugoniot conditions for the shock propagating in the uniform (constant preshock parameters) or nonuniform (nonconstant preshock parameters as known functions of time or space coordinate) medium. The total number of computational cells is denoted as N. The computational mesh is uniform. The Zel'dovich – von Neumann – Doering (ZND) solution is used as an initial condition.

The computational algorithm is based on the principle of splitting by physical processes. Firstly, the gasdynamic equations are integrated on the time step with no chemical reactions included ($\mathbf{s} = 0$). The spatial discretization of the governing system is performed using the finite volume method. At this hyperbolic step, the Courant–Isaacson–Rees numerical scheme in conservative formulation of the second approximation order is applied. At the second step, the chemical reactions are considered without convection terms. Such a system is solved with the use of the explicit Euler method. The numerical algorithm in general follows [5].

Methods of the Leading Shock Wave Calculation

The SAF formulation demands additional equations for the calculation of D. The governing system of equations in the characteristic form along C_+-characteristics is used [8]:

$$\left.\begin{aligned} \frac{D_+ p}{Dt} + c\rho\frac{D_+ v}{Dt} - (\gamma-1)\rho\left[1 - H(1-\lambda_r)\right]K_r(1-\lambda_r)^\nu = 0\,; \\ \frac{D_+ x}{Dt} = v + c - D\,; \end{aligned}\right\} \quad (1)$$

$$\frac{D_+}{Dt} = \frac{\partial}{\partial t} + (v+c)\frac{\partial}{\partial x}\,.$$

Just behind the LSW, $\lambda_r = 0$. So, Eqs. (1) can be rewritten as

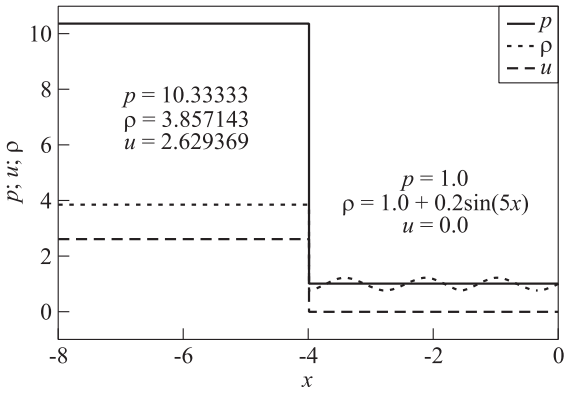

Figure 1 Schematic of the Shu test [9]

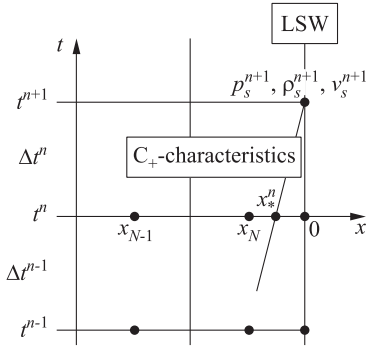

Figure 2 The sketch to the algorithm of the LSW speed equation integration

$$\left.\begin{aligned} &\frac{D_+ p}{Dt} + c\rho \frac{D_+ v}{Dt} = 0\,; \\ &\frac{D_+ x}{Dt} = v + c - D\,. \end{aligned}\right\} \qquad (2)$$

Different numerical methods can be used to find D from Eqs. (2). We considered three approaches, calling them "explicit," "semiexplicit," and "implicit."

Let us illustrate the approaches on the well-known Shu test [9] considering SW interaction with the sine waves in density (Fig. 1). The Shu test is an inert analog to the problem of DW propagation in the periodic nonuniform reactive medium [10–13]. The "explicit" method implies (Fig. 2):

$$\left.\begin{aligned} &p_s^{n+1} - p_*^n + \frac{1}{2}\left((\rho c)_*^n + (\rho c)_s^{n+1}\right)\left(v_s^{n+1} - v_*^n\right) = 0\,; \\ &\rho_0^{n+1} = \rho_{\text{init}} + \varepsilon \sin\left(a x_0 + a\sqrt{\frac{\gamma p_0^{n+1}}{\rho_0^{n+1}}}\,\mathrm{M}^{n+1} t^{n+1}\right)\,; \\ &-x_*^n = \left(c_*^n + v_*^n - D^n\right)\Delta t^n\,. \end{aligned}\right\} \qquad (3)$$

The specific values of the parameters of the problem are: $\rho_{\text{init}} = 1.0$; $\varepsilon = 0.2$; $x_0 = -4.0$; $a = 5.0$; and $p_0 = 1.0$. The parameters with the subscript 's' are the unknown parameters just behind the LSW at the next time step. They can be expressed through the LSW Mach number M^{n+1} using the Rankine–Hugoniot relations. The parameters with the subscript '0' correspond to the immediate conditions ahead of the LSW. The density ahead of the LSW is also unknown because the instantaneous LSW speed is unknown. The parameters with the subscript '$*$' are calculated using linear interpolation between the points x_N and $x = 0$ at the corresponding time layer. The coordinate x_*^n is found from the last equation of Eqs. (3) explicitly and then the system of the first two equations for M^{n+1} and ρ_0^{n+1} is solved using Newton iterations.

In the "semi-implicit" modification, the first equation in Eqs. (3) changes:

$$p_s^{n+1} - p_*^n + (\rho c)_s^{n+1} \left(v_s^{n+1} - v_*^n\right) = 0\,.$$

The remaining parts of the method are the same.

The "implicit" method of the LSW speed calculation reads:

$$p_s^{n+1} - p_*^n + (\rho c)_s^{n+1} \left(v_s^{n+1} - v_*^n\right) = 0\,;$$

$$\rho_0^{n+1} = \rho_{\text{init}} + \varepsilon \sin\left(a x_0 + a \sqrt{\frac{\gamma p_0^{n+1}}{\rho_0^{n+1}}}\, \mathrm{M}^{n+1} t^{n+1}\right)\,;$$

$$-x_*^n = \left(c_s^{n+1} + v_s^{n+1} - D^{n+1}\right) \Delta t^n\,.$$

All the equations are solved for M^{n+1}, ρ_0^{n+1}, and x_*^n with Newton iterations simultaneously.

Simulation Results and Discussion

All three methods were compared for Shu test simulation. The length of the computational domain was equal to $L = 10$, the number of cells was equal to $N = 4000$. The "explicit" algorithm failed at the time of 1.311. The "semi-implicit" and "implicit" algorithms demonstrated similar results that cannot be distinguished by eyes (see a solid line in Fig. 3*a*). However, they both failed at the times greater than 2.043. The main reason is the formation of the internal shocklets with very

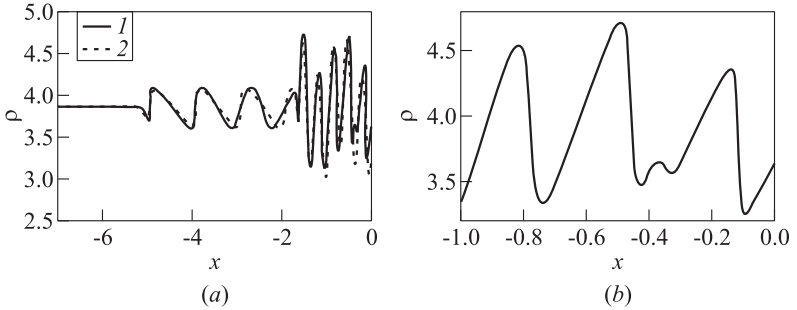

Figure 3 Density distribution in Shu test [9]: (*a*) comparison of the SAF simulation (*1*) with the simulation from [9] (*2*) at the time of 1.8; and (*b*) shocklets in the SAF simulation

sharp front (see Fig. 3*b*) in the considered problem. After several interactions of these shocklets with the LSW, all methods failed. This situation is somehow similar to that reported in [14]. In [14], the SAF fifth accuracy order algorithm was proposed for simulating 1D detonation wave propagation. However, the algorithm was applicable only to the stable and weakly unstable detonation without internal shock and DWs. The algorithm was improved recently in [15] to deal with more unstable regimes but with a loss of accuracy. So, it is possible that the considered test is too challenging even for the implicit SAF algorithms and they nevertheless can be used for the simulations of not strongly unstable detonation propagation in nonuniform media. Another opportunity is more careful adjustment of the Newton iterations in the implicit algorithm.

Acknowledgments

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