Numerical simulation of nonlinear dynamics of 1D pulsating detonations

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Abstract. The development of 1D instability of a detonation wave is numerically simulated for a two-stage chemical model. The shock-fitting approach is employed to track the leading detonation front. In order to determine its motion, the equation for the acceleration of the shock wave derived from the Rankine-Hugoniot conditions and the characteristic relations is integrated along with the reactive Euler equations. The fifth-order WENO scheme is used, time stepping is performed with the four-stage Runge-Kutta-Gill method. It is shown that in a certain range of parameters of the problem (the degree of overdrive \( f \), the dissociation energy \( E_d \) and the activation energy \( E_a \)), the Zeldovich-Neumann-Döring stationary solution is unstable with respect to 1D disturbances. The evolution of disturbances at later nonlinear stages is studied. Nonlinear saturation of the growth of disturbances leads to the formation of a stable limit cycle. When changing the parameters of the problem, the period doubling bifurcation can occur leading to the appearance of pulsations with two different maxima of the amplitude.

1. Introduction
Linear stability of detonation waves (DWs) was studied almost exclusively using the simplest one-step chemical mechanism with one irreversible Arrhenius-type reaction [1]. Nonlinear dynamics of 1D unstable detonations in the framework of this model was also studied in detail [2, 3, 4, 5]. It was shown that, for weakly unstable detonations, the growth of disturbances leads to a periodic self-oscillating regime corresponding to a stable limit cycle in the phase plane. With increasing the activation energy, several successive period doubling bifurcations occur followed by transition to a chaotic regime.

The simplest one-step model correctly describes many features of the detonation phenomenon. However, it does not correspond to any specific combustible mixture and cannot claim quantitative agreement with experimental data. When solving practical problems connected with the propagation of detonations in gaseous mixtures, two-stage models, first proposed in [6], are most often used. In this paper we consider the nonlinear dynamics of 1D disturbances in a two-stage chemical model developed in [7, 8] for describing the detonation combustion of hydrogen and widely used later in numerical simulation of detonations.

2. Governing equations and numerical techniques
2.1. Two-stage chemical model
Instead of considering detailed kinetic schemes, which can include, depending on the composition of the combustible mixture, tens, hundreds, and even thousands of chemical reactions, in the
two-stage model the chemical transformations that occur when a fuel burns are described by two variables, the fraction of the induction period \( Y \), \( 0 \leq Y \leq 1 \), and the current molar mass of the mixture \( \mu \). The flow is governed by the Euler equations (in our case, 1D ones) complemented with two additional equations:

\[
\frac{\partial \mathbf{Q}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S}, \quad \mathbf{Q} = [\rho, \rho u, \rho E, \rho Y, \rho \mu]^T, \quad \mathbf{F} = [\rho u, \rho u^2 + p, u(\rho E + p), \rho uY, \rho u\mu]^T, \quad \mathbf{S} = (0, 0, 0, \rho W_Y, \rho W_\mu)^T.
\]

The pressure and the total energy are

\[
p = \frac{\rho RT}{\mu}, \quad E = e(T, \mu) + \frac{1}{2} u^2,
\]

where is the internal energy is given by

\[
e(T, \mu) = E_d \left( \frac{1}{\mu} - \frac{1}{\mu_{\text{min}}} \right) + \left[ \frac{\mu}{\mu_{\text{min}}} + \frac{1 - \delta}{2} + \left( \frac{\mu}{\mu_{\text{min}}} + \delta - 1 \right) \frac{\theta/T}{e^{\theta/T} - 1} \right] \frac{RT}{\mu} \quad (3)
\]

Here, for the stoichiometric hydrogen–oxygen mixture, \( E_d = 4.6024 \cdot 10^8 \) J/kmol is the mean dissociation energy of reaction products, \( \mu_{\text{min}} = 6 \) kg/kmol and \( \mu_{\text{max}} = 18 \) kg/kmol are the molar masses in completely dissociated and completely recombined states, respectively, \( \delta = \frac{\mu - \mu_{\text{min}}}{\mu_{\text{max}} - \mu_{\text{min}}} \), \( \theta = 3500 \) K is the effective temperature of excitation of vibrational degrees of freedom, and \( R \) is the universal gas constant.

In a two-stage model it is assumed that the entire process of chemical transformations can be divided into two stages, the induction stage and the heat release stage. During the induction stage, the molar mass of the gas does not change, there is no heat release, and the variable \( Y \), initially equal to 1, changes according to the equation

\[
\frac{dY}{dt} = W_Y = -\frac{1}{\tau_{\text{ind}}}, \quad \tau_{\text{ind}} = \frac{K_a \mu_{O_2}}{\rho z} \exp \left( \frac{E_a}{RT} \right),
\]

where \( E_a = 7.17556 \cdot 10^7 \) J/kmol is the activation energy, \( K_a = 5.38 \cdot 10^{-11} \) kmol/s/m³ is the pre-exponential factor, \( \mu_{O_2} = 32 \) kg/kmol is the molar mass of oxygen, and \( z = 8/9 \) is the mass fraction of oxygen.

When \( Y \) reaches zero the molar mass starts to change, that is accompanied by heat release. The molar mass changes according to the equation

\[
\frac{d\mu}{dt} = W_\mu = W_1(\mu) \rho^2 - W_2(T, \mu) \rho, \quad W_1(\mu) = \frac{4K_+}{\mu} \left( 1 - \frac{\mu}{\mu_{\text{max}}} \right)^2 \quad (5),
\]

\[
W_2(T, \mu) = 4K_+ K_- \left( \frac{\mu}{\mu_{\text{min}}} - 1 \right) \left( \frac{T}{T_0} \right) ^{\beta/2} \left[ 1 - \exp \left( \frac{-\theta}{T} \right) \right] ^{\beta} \exp \left( - \frac{E_d}{RT} \right).
\]

Here \( K_+ = 6 \cdot 10^8 \) m⁶/(kmol²s) is recombination rate constant, \( K_- = 1.769 \cdot 10^3 \) kmol/m³ is the equilibrium constant, \( T_0 \) is the initial temperature of the mixture, and \( \beta = \frac{\mu_{\text{max}} - \mu_{\text{min}}}{\mu_{\text{max}} - \mu_{\text{min}}} \).

The profile of the stationary solution (Zeldovich–von Neumann–Döring, ZND, solution) obtained with the two-stage model has a kink at the point where the induction period expires. This nonphysical singularity can lead to problems, in particular to the loss of accuracy in
numerical simulations, and significantly affect the stability characteristics since the equations of
the linear stability theory include derivatives of the basic flow quantities. To avoid the potential
problems, we modified the two-stage model having replaced $W_\mu, W_Y$ by

$$
\tilde{W}_\mu = W_\mu \exp(-\eta Y), \quad \tilde{W}_Y = W_Y \left[1 - \exp(-\eta Y)\right],
$$

(6)

Where $\eta$ is a smoothing parameter. Thus, the two stages cease to be sharply separated. Figure 1
shows the temperature profiles of the stationary solution of the equations (1) for various values
of the parameter $\eta$. Hereafter dimensionless variables are plotted with the induction length $\ell_{ind}$
as the reference length, the pre-shock speed of sound as the reference velocity and other flow
properties measured in their pre-shock values.

In the subsequent calculations, $\eta = 10$ is taken. As can be seen from the figure, at this value
the profile is very close to that obtained from the original model, with a well-defined induction
zone in which heat release can be considered negligible.

![Figure 1. ZND temperature profiles at different values of the smoothing parameter.](image)

2.2. Shock-fitting approach
Numerical simulations are performed using the shock-fitting approach. The leading detonation
front is one of the boundaries of the computational domain. To determine its position and
velocity, the equations of motion of the front are integrated along with the reactive Euler
equations (1). By differentiating the Rankine-Hugoniot conditions with respect to time, the
acceleration of the shock wave can be expressed through the time derivative of any of the flow
quantities just behind the shock. The latter, in turn, can be replaced by spatial derivatives using
the Euler equations. Since the spatial derivatives at the boundary have to be approximated by
one-sided finite differences, it is most correct, from numerical point of view, to express the
acceleration of DW in terms of $\mathcal{L}$, a linear combination of the derivatives of the flow quantities.
entering into the relation on the characteristic arriving at the shock wave [9]. For the two-stage model it is given by the following formula:

\[
\mathcal{L} = \left( \frac{1}{\rho} \frac{\partial \rho}{\partial t} + \frac{\gamma}{c} \frac{\partial u}{\partial t} + \frac{1}{T} \frac{\partial T}{\partial t} - \frac{1}{\mu} \frac{\partial \mu}{\partial t} \right) = -(u + c) \left( \frac{1}{\rho} \frac{\partial \rho}{\partial x} + \frac{\gamma}{c} \frac{\partial u}{\partial x} + \frac{1}{T} \frac{\partial T}{\partial x} - \frac{1}{\mu} \frac{\partial \mu}{\partial x} \right) - (7)
\]

\[
\frac{1}{T} e_{\mu} + \frac{1}{\mu} W_{\mu}, \quad \gamma = 1 + \frac{R}{\mu e_{T}}, \quad c^2 = \frac{\gamma RT}{\mu}.
\]

Here \(e_{T}\) and \(e_{\mu}\) are the partial derivatives of the internal energy with respect to relevant variables and \(c\) is the speed of sound.

The fifth-order WENO scheme [10] is used to evaluate the spatial derivatives. The length of the computational domain is 50 \(\ell_{\text{ind}}\), the number of grid points is 5,000. Time integration is performed with the four-stage Runge–Kutta–Gill scheme [11]. Since the dependence of the internal energy on the temperature (3) is nonlinear, at each stage of the Runge–Kutta–Gill integration the temperature is determined with Newton iterations. The same iterative method is used in calculating the flow quantities just behind the shock wave from the Rankin-Hugoniot relations.

3. Results

The stationary ZND solution is used as initial data in numerical simulations. The influence of the degree of overdrive \(f = (M/M_{CJ})^2\), the activation energy \(E_a\), and the dissociation energy \(E_d\) was studied. Here \(M\) is the DW Mach number and \(M_{CJ}\) is the Chapman–Jouguet Mach number.

![Figure 2](image1.png)

**Figure 2.** Evolution of DW velocity at \(f = 1\), \(E_a = 7.17556 \cdot 10^7\) J/kmol, and \(E_d = 4.6024 \cdot 7.17556 \cdot 10^7\) J/kmol. \(E_a = 4.6024 \cdot 10^8\) J/kmol.

![Figure 3](image2.png)

**Figure 3.** Phase portrait at \(f = 1\), \(E_a = 7.17556 \cdot 10^7\) J/kmol, and \(E_d = 4.6024 \cdot 10^8\) J/kmol.

3.1. Influence of the degree of overdrive \(f\)

The numerical simulation of the propagation of the self-sustaining DW has shown that at \(f = 1\), \(E_a = 7.17556 \cdot 10^7\) J/kmol, and \(E_d = 4.6 \cdot 10^8\) J/kmol the DW is unstable to 1D disturbances. The instability leads to the formation of a pulsating detonation regime. Figure 2 shows the
evolution of the DW velocity. The initial stage of the instability development is singled out in blue. The oscillations are periodic and their amplitude is constant starting at about $t = 200$.

Figure 3 shows the phase plane $(D, dD/dt)$. Only the initial (blue) and final (red) parts of the phase trajectory are depicted. It is obvious that the initial point representing the ZND solution is an unstable focus under these parameters. Moving away from this point, the trajectory after $t \approx 200$ winds onto a stable limit cycle corresponding to periodic self-oscillations.

An increase in $f$ to 1.05 does not lead to a qualitative change in the picture, although the instability develops more slowly. However, at $f = 1.1$ the flow becomes stable. The initial oscillations caused by perturbations originated from the limited accuracy of the calculation of the ZND solution dampen over time and, after that, the DW propagates at a constant speed.

3.2. Influence of the activation energy $E_a$

Increasing the activation energy leads to a more unstable state. Thus, at $f = 1$, $E_a = 7.42556 \cdot 10^7$ J/kmol, $E_d = 4.6024 \cdot 10^8$ J/kmol, the instability develops significantly faster and the amplitude of the DW velocity oscillations increases. Figure 4 shows that the character of the oscillations has changed significantly so that two maxima of different magnitude are observed during the period. The corresponding limit cycle, which the trajectory reaches at $t \approx 120$, has a self-intersection point, see figure 5. Thus, as a result of the cycle doubling bifurcation, the system enters a two-period regime.

A further increase in $E_a$ leads to an even stronger instability. In fact, even at $E_a = 7.67556 \cdot 10^7$ J/kmol, it is difficult to identify a stable cycle on the phase plane and the flow becomes chaotic.

A decrease in activation energy, on the contrary, has a stabilizing effect. At $E_a = 6.92556 \cdot 10^7$ J/kmol the system is still unstable and the self-oscillation regime occurs at $t \approx 700$. The decrease in the activation energy to $E_a = 6.67556 \cdot 10^7$ J/kmol leads to suppression of the instability.
3.3. Influence of the dissociation energy $E_d$
As can be expected, a decrease in $E_d$ leads to an increase in instability, while an increase in $E_d$ cause its weakening. Thus, as the dissociation energy is reduced to $E_d = 4.4024 \cdot 10^8$ J/kmol (as earlier, $f = 1$, $E_a = 7.17556 \cdot 10^7$ J/kmol), the picture is qualitatively similar to that shown in figures 4 and 5.

With the increase in $E_d$ up to $4.8024 \cdot 10^8$ J/kmol the pulsations of the DW velocity are first visible only by the time moment $t \approx 150$, see figure 2. The corresponding picture in the phase plane, figure 7, shows very distinctively the instability development at the initial stage, a transient process, during which gradually damped oscillations around the limit cycle occur, and the final transition to the periodic regime.

![Figure 6. Evolution of DW velocity at $f = 1$, $E_a = 7.17556 \cdot 10^7$ J/kmol, and $E_d = 4.8024 \cdot 10^8$ J/kmol.](image)

![Figure 7. Phase portrait at $f = 1$, $E_a = 7.17556 \cdot 10^7$ J/kmol, and $E_d = 4.8024 \cdot 10^8$ J/kmol.](image)

4. Conclusions
It is shown that a plane self-sustaining DW, which is a stationary solution of the Euler equations with a two-stage chemical model, is unstable with respect to 1D disturbances. The development of instability leads to the formation of a pulsating detonation regime with a periodic variation in the velocity of the leading DW front. Overdriven detonations are more stable; an increasing in the degree of overdrive $f$ up to 1.1 completely suppresses the instability.

The effect of the activation energy $E_a$ and the dissociation energy $E_d$ on the 1D instability is studied. Detonations become more unstable with increasing $E_a$ and, as a result of the cycle doubling bifurcation, two-period oscillations appear with two different maxima of the DW velocity during the period. A further increase in the activation energy leads to a highly unstable state with chaotic dynamics. On the contrary, a decrease in $E_a$ can completely suppress the instability.

Variation of the dissociation energy $E_d$ has the opposite effect; the DW becomes more stable as the $E_d$ increases and more unstable as it decreases.

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