Linear and nonlinear effects in detonation wave structure formation

S P Borisov1,2 and A N Kudryavtsev1,2

1 Khristianovich Institute of Theoretical and Applied Mechanics of SB RAS
630090 Novosibirsk, Russia
2 Novosibirsk State University, 630090 Novosibirsk, Russia
E-mail: borisov@itam.nsc.ru, alex@itam.nsc.ru

Abstract. The role of linear and nonlinear effects in the process of formation of detonation wave structure is investigated using linear stability analysis and direct numerical simulation. A simple model with a one-step irreversible chemical reaction is considered. For linear stability computations, both the local iterative shooting procedure and the global Chebyshev pseudospectral method are employed. Numerical simulations of 1D pulsating instability are performed using a shock fitting approach based on a 5th order upwind-biased compact-difference discretization and a shock acceleration equation deduced from the Rankine–Hugoniot conditions. A shock capturing WENO scheme of the 5th order is used to simulate propagation of detonation wave in a plane channel. It is shown that the linear analysis predicts correctly the mode dominating on early stages of flow evolution and the size of detonation cells which emerge during these stages. Later, however, when a developed self-reproducing cellular structure forms, the cell size is approximately doubled due to nonlinear effects.

1. Introduction

Detonation is one of the most powerful, violent, and intriguing phenomena observed in nature and produced by people. In a good solid explosive, energy is converted at a rate of $10^{10}$ W per square centimeter of the detonation front so that a 20-m square detonation wave (DW) operates at a power equal to all the power the Earth receives from the Sun [1]. Traditionally, detonation studies were focused on producing powerful explosions as well as on their prevention and protection from them. However, the unique feature of detonative processes as very high density energy sources means that suitably controlled detonation fronts represent an attractive and perspective technology for application in many areas. In recent years, there was a significant interest in the use of detonation for development of novel propulsive devices such as standing DW engine [2], pulse detonation engine (PDE) [3], and continuously rotating DW engine [4]. In 2008 the first, 10-s flight of an aircraft powered by an experimental PDE was performed [5]. Moreover, a huge rate of heat release in DWs can also facilitate creation of microengines, entirely new microdevices, in the micrometer to millimeter range, able to produce mechanical work from chemical energy [6].

Nearly all self-sustaining detonations exhibit complicated unsteady 3D patterns known as a cellular or multifront structure [7, 8]. Not long after the discovery that the cellular structure is a widespread and common feature of propagating DWs, it was assumed that its emergence is caused by an instability of a plane detonation front with respect to transverse disturbances.
Existence of such an instability (connected with the strong, exponential dependence of the chemical reaction rate on temperature) was shown, first, for the piecewise-constant basic flow behind the leading shock wave (i.e., in the limit of infinitely fast chemical heat release) [10] and then for the basic flow given by the Zeldovich–Neumann–Doring (ZND) solution of the 1D reactive Euler equations [11]. After a series of papers published by J.J. Erpenbeck in the mid-1960s [12, 13, 14], the linear analysis of DW instability has become a well-established theory. Since the early 1990s, there has been a renewed interest in this theory. The original techniques of Erpenbeck employing the Laplace transform has been replaced by a much simpler approach based on the method of normal modes [15, 16], and the stability of detonation for a simple chemical mechanism with one irreversible reaction has been investigated in a more systematic and nearly exhaustive manner (see the reviews [17, 18, 19] and the book [20]).

Nevertheless, the status of the linear theory of DW instability remains rather uncertain because, in a sharp contrast with the theory of hydrodynamic stability, the former wasn’t ever confirmed directly by experiment. A better understanding of links between the stability theory and mechanisms of formation and self-reproduction of 3D DW structure might help us control detonation behavior in propulsion devices [19]. Relatively recently, a number of investigations were performed aimed at comparison of linear analysis predictions with data of direct numerical simulations in the 1D case [21, 22, 23, 24]. In the present paper, we investigate both the 1D pulsating instability and the 2D instability of a DW propagating in a plane channel trying to elucidate the role of linear and nonlinear effects in formation of the developed DW structure.

### 2. Governing equations and numerical techniques

A chemically reacting flow governed by the Euler equations for a perfect gas which undergoes a one-step irreversible reaction is considered:

\[
\begin{align*}
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) &= 0, \\
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) + \nabla p &= 0, \\
\frac{\partial E}{\partial t} + \nabla \cdot ((E + p) \mathbf{u}) &= 0, \\
E &= \frac{1}{2} \rho \mathbf{u}^2 + \frac{1}{\gamma - 1} \frac{p}{\rho} - \lambda Q, \\
\frac{\partial \rho \lambda}{\partial t} + \nabla \cdot (\rho \lambda \mathbf{u}) &= \rho \dot{\omega}, \\
\dot{\omega} &= K (1 - \lambda) \exp \left(-\frac{\rho E_a}{p}\right).
\end{align*}
\]

Here, the dependent variables are density \( \rho \), velocity \( \mathbf{u} \), pressure \( p \), specific total energy \( E \) and reaction progress \( \lambda \); \( t \) is time, \( \gamma = 1.2 \) is the ratio of specific heats, \( K \) is the predexponential factor, \( E_a \) is the activation energy, and \( Q \) is the specific heat release.

The 1D ZND solution of (1) consists of a leading plane nonreactive shock front followed by a chemical reaction zone [1, 20]. This structure is stationary in the frame of reference moving with the shock front speed \( D \). The value of \( K \) can be specified in such a way that the reaction half-length, i.e., the distance between the shock front and the location where the reaction progress variable \( \lambda = 1/2 \), will be equal to unity for the ZND solution. Thereafter, all lengths are assumed to be normalized with the reaction half-length.

The ZND solution exists provided that \( M = D/c_0 \geq M_{CJ} \) where \( c_0 \) is the sound speed ahead of the front and \( M_{CJ} \) is the Chapman–Jouguet (CJ) Mach number

\[
M_{CJ} = \sqrt{\frac{(\gamma^2 - 1)Q}{2c_0^2}} + \sqrt{\frac{(\gamma^2 - 1)Q}{2c_0^2}} + 1.
\]

The CJ detonation is a self-sustaining, freely propagating DW while overdriven detonations with \( M > M_{CJ} \) can be considered as DWs driven by a piston moving with a constant velocity far behind the shock front. The overdrive parameter is defined as \( f = (M/M_{CJ})^2 \).
To investigate stability of a plane DW, small disturbances are added to the ZND solution, and the shape of shock front is also assumed to be distorted:

$$q(x, y, z) = \tilde{q}(x) + \tilde{q}(x) e^{\alpha t} e^{i(k_y y + k_z z)}, \quad \psi(y, z, t) = 0 + \tilde{\psi} e^{\alpha t} e^{i(k_y y + k_z z)}. \quad (3)$$

Here, $q$ denotes any of flow variables, and the disturbed shape of shock front is given by the equation $x = \psi(y, z, t)$ where $x$ is the coordinate normal to the undisturbed shock front, and $y, z$ are two other Cartesian coordinates. The frame of reference is attached to the undisturbed shock front (located at $x=0$), $\tilde{q}(x)$ is the ZND solution, $k_y$ and $k_z$ transverse components of the disturbance wave number, $\alpha = \alpha_r + i\alpha_i$ is a complex number whose real part is the growth rate, the flow is unstable at $\alpha_r > 0$. It is worth noting that the axes $y, z$ can be always orientated in such a way that one of the components $k_y, k_z$ will vanish, so we will assume that $k_z = 0$.

The linearized reactive Euler equations along with the linearized Rankine–Hugoniot jump conditions at $x = 0$ and the radiation condition far from the shock front, at $x \rightarrow \infty$ results in an eigenvalue problem with respect to $\alpha$. It is solved with either an iterative shooting procedure [15] or a pseudospectral Chebyshev method [25]. The latter provides an eigenvalue map and enables us to avoid time-consuming “carpet search” of initial guesses. Since the radiation condition for multidimensional disturbances leads to a nonlinear eigenvalue problem, non-reflective boundary conditions proposed in [26] are employed instead when solving the spectral problem.

A high-order shock-fitting approach is used to perform direct numerical simulation of evolution of 1D disturbances. The 1D reactive Euler equations are solved along with an equation for shock wave acceleration. The shock wave acceleration $dD/dt$ can be expressed from the Rankine–Hugoniot conditions in terms of time derivatives of flow variables just behind the shock front, which, in turn, can be replaced using the Euler equations by their spatial derivatives. Since the spatial derivatives just behind, the shock front must be calculated using one-sided differences, it is preferable to use the Riemann invariant $L$ corresponding to the characteristic running towards the shock front, which leads to the equation

$$\frac{dD}{dt} = \frac{(\gamma + 1) L/2}{2\rho_0 D - \rho_s c_s \left[1 + (c_0/D)^2\right]}, \quad (4)$$

$\mathcal{L} = \frac{\partial p_s}{\partial t} - \rho_s c_s \frac{\partial u_s}{\partial t} = -(u_s - D - c_s) \left(\frac{\partial p_s}{\partial x} - \rho_s c_s \frac{\partial u_s}{\partial x}\right) + (\gamma - 1) \rho Q \dot{\psi}$.

Here, the subscripts 0 and $s$ denote quantities ahead of and just behind the shock front, respectively. The spatial derivatives are approximated by the 5th-order upwind-biased compact differences [27], and the reactive Euler equations (1) along with (4) are integrated in time with the 5th-order, 6-stage SSP (Strong Stability-Preserving) Runge–Kutta scheme [28].

In the 2D case, numerical simulations are performed using the high-order shock-capturing finite-difference WENO (Weighted Essentially Non-Oscillatory) scheme [29].

3. Linear analysis for DW in a plane channel

In general, plane DWs are unstable over a wide range of the parameters $Q$, $E_a$ and $f$. Figure 1 shows the eigenvalue maps at $Q = 50$, $E_a = 50$, $f = 1$ and different values of the transverse wave number $k_y$. There are 10 unstable eigenmodes at $k_y = 0$, however their number decreases as $k_y$ grows so that the flow becomes stable if $k_y$ exceeds a neutral wave number $k_y^N \approx 28$.

The growth rates of all these modes are shown in figure 2. For each value of $k_y$, there exists a maximally unstable mode. The dependence of the maximum growth rate on $k_y$ is given by the envelope (shown as a bold solid line). For a DW traveling in a plane channel, boundary conditions for the transverse velocity $v$ require $k_y = \pi n/H$, $n = 1, 2, 3...$, where $H$ is the channel height.
If $H < \pi/k_y^N$ then the channel is too narrow for existence of unstable transverse disturbances, and formation of cellular DW structure can hardly be expected.

**Figure 1.** Eigenvalues at $k_y = 0, 15, 28$.

**Figure 2.** Growth rates as functions of $k_y$.

For wider channels, the growth rate is maximum for some value of $n = N$. It is natural to suppose [30] that the corresponding mode will dominate at early (at least) stages of DW structure evolution so that formation of the cellular structure containing $N$ detonation half-cells (or $N/2$ entire cells) can be expected.

As an example, the number of detonation half-cells $N$ and the cell size $a = 2H/N$ predicted by the linear theory at $Q = 50$, $E_a = 12.5$, $f = 1$ are shown in Figures 3 and 4, respectively.

**Figure 3.** Predicted number of half-cells for DW in plane channel.

**Figure 4.** Predicted cell size for DW in plane channel.

It is seen that as $H$ increases, the cell size also increases to fit boundary conditions and the number of cells does not change until a sudden transition to the next value of $n$ happens. For very large channel heights the cell size approaches the limiting value $2\pi/k_y^M$ where $k_y^M$ is the
wave number corresponding to the maximum growth rate over all wave numbers (see Figure 2). Such behavior is in close agreement with that was observed in experiments.

4. Numerical simulations of pulsating 1D instability
Numerical simulations of the 1D instability cannot elucidate mechanisms governing formation of the cellular detonation structure, however they allow us to test predictions of the linear theory concerning growth rates of unstable disturbances, study mode competition phenomena and investigate the instability saturation and formation of nonlinear quasi-equilibrium states. In the present computations, the ZND solution with no imposed disturbances is taken as the initial condition. Nevertheless, as a result of accumulation of rounding errors, disturbances can emerge and, in unstable cases, grow.

The computations performed for $Q = 50$, $f = 1$ and varying values of $E_a$ show that the behavior of disturbances agrees with the linear analysis. The disturbances grow at $E_a > E_a^N = 25.26$ and their numerical growth rate during the linear stage is very close to predicted one. After saturation, a stable limiting cycle is observed in the phase space $(D, dD/dt)$ if the activation energy slightly exceeds $E_a^N$. At larger values of $E_a$, the single limiting cycle gives way to a doubly periodic solution and, as the activation energy further increases, the system becomes more and more chaotic. These results agree very well with those in [24].

In Figures 5 and 6 the results of simulations performed at $Q = 50$, $E_a = 50$, $f = 1.4$ are compared with the linear analysis predictions. At these conditions, there are two unstable modes. As is seen, in numerical simulations the disturbances grow with the rate which is very close to the amplification coefficient predicted by the linear theory for the faster growing mode (Figure 5). This mode dominates for the entire stage of linear evolution. The spatial distribution of velocity disturbance during this stage nearly perfectly matches the linear eigenfunction of the more unstable mode (Figure 6).

The period of DW oscillations during the stage of linear evolution is also very close to the period $2\pi/\alpha_i$ of the dominating mode. At a later moment it increases abruptly up to a value which is slightly larger than the period of the second, slower growing, mode and continues to increase permanently while the computation proceeds.
5. Numerical simulation of formation of cellular detonation structure

To investigate the process of formation of the cellular structure, DW propagation in a plane channel of height $H = 100$ is simulated. The length of computational domain $L_x$ is 80. A special techniques of periodic translations of the computational domain is used to keep the propagating DW inside the domain. The grid resolution is varied, the finest grid comprises of $2720 \times 3400$ cells; up to 80 cores of a multiprocessor cluster are used for the computations. A plane wave ZND solution with a superimposed long-wave (half-sine) disturbance of the transverse velocity is taken as the initial condition. The computations are performed at different values of the parameters $Q$, $E_a$, and $f$.

A numerically generated smoke foil resulted from a typical computation at $Q = 50$, $E_a = 12.5$, and $f = 1$ is shown in Figure 7 along with enlarged views of its leftmost and rightmost parts. At these parameters, the linear analysis predicts the existence of a single unstable mode. Its growth rate is maximum at the transverse wavenumber $k_y^{\text{M}} = 1.095$ which corresponds to the number of half-cells across the channel $N$ between 34 and 35. As can be seen, detonation cells become visible approximately at $x = 180$. In spite of long-wave excitation, at first they are small. Later, however, their size increases and becomes roughly constant at $x \geq 350$. The cellular structure is far from completely regular so that both smaller and larger cells can be observed at any distance from the initial detonation front position.

![Figure 7. Numerical smoke foils for DW propagation in 2D channel, $H = 100$.](image)

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 transverse velocity flowfield:

$$\hat{\nu}_k(x, t) = \frac{2}{H} \int_0^H v(x, y, t) \sin \left( \frac{k \pi y}{H} \right) \, dy.$$  \hspace{1cm} (5)

The number of half-cells deduced from the wavenumber of Fourier harmonics with the maximum amplitude is shown in Figure 8. The line marked “max” is obtained by taking also the maximum of $|\hat{\nu}_k(x, t)|$ over the longitudinal coordinate $x$, whereas the second line (“ave”) is built from the data averaged over some interval of $x$.

As is it seen just after formation of detonation cells their number is in good agreement with the one predicted by the linear theory. However, in a well-developed cellular structure the number of cell is approximately halved. This pairing process is obviously caused by nonlinear effects. Thus, it seems that the linear analysis predictions are valid only for early stages of formation of the cellular structure. It is worth noting that this conclusion disagrees with the results obtained
in [31] where in numerical simulations of a weakly unstable detonation at $Q = 0.4$, $E_a = 50$, $f = 1$ the most unstable linear mode remains dominant even in the developed cellular regime.

![Figure 8. Time variation of number of half-cells for DW in plane channel.](image)

![Figure 9. Time evolution of velocity of DW propagating in plane channel.](image)

Another interesting feature of cellular DW propagation is the time evolution of the velocity of leading shock front shown in Figure 9. The theoretical CJ velocity is indicated by a white horizontal line. It can be seen that the averaged velocity obtained from the numerical simulation is slighter larger than its theoretical value predicted by the ZND model.

6. Conclusions
Numerical simulations confirm that the linear analysis predicts correctly the characteristics of disturbances which develop and dominate on early stages of flow evolution as well as the size of detonation cells emerging during these stages. It has been observed, however, that later, when a developed self-reproducing cellular structure forms, the cell size is approximately doubled — obviously due to nonlinear effects. A further exploration of non-linear mechanisms responsible for this “pairing” phenomenon can be considered as an interesting challenge for future research.

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