Numerical Cell Size and Multidimensional Stability of Planar Detonations

Z. Liang, Y.H. Han, L. Bauwens
University of Calgary, Department of Mechanical & Manufacturing Engineering
2500 University Drive NW, Calgary, Alberta, T2N 1N4 Alberta, Canada

E-MAIL:liangz@ucalgary.ca

We examine the cell size and two-dimensional linear stability of planar detonation waves for one-step Arrhenius rate with arbitrary reaction order. This is motivated by the relationship that may exist between transverse wave length results from linear stability analysis and experimental cell size [1]. A series of two-dimensional stability spectra for different activation energy E, heat release Q and reaction order ν are presented in this paper. Corresponding two-dimensional smoke foils, numerically generated in simulations performed for a range of channel widths from narrow to wide, are also obtained. The predicted cell sizes from numerical simulation and the linear stability results are compared.

A comparison between stability theory and two-dimensional simulations was first presented by Bourlioux and Majda [1]. They found that provided the unperturbed ZND profile exhibits instability at long transverse wavelength with simple stability diagram, the computed regular cell spacing is comparable with the wavelength of the most unstable modes, when the channel width is not too large. However they only examined four sets of parameters and, in most cases, the channel width was limited to 20 half reaction lengths. Nikolic et al. [7] pointed out that from the stand point of analysis and computational studies, the well-posedness of the cell-size concept is not clear. Two-dimensional computations performed in narrow domains result in a cell width that adapts to the domain, with half a cell across as a minimum. Wider computations show that cells which appear regular and periodic in narrow computations become irregular, given a sufficiently wide domain. Additionally, the number of cells obtained in given domain widths, hence their size, retains a strong dependence upon the initial conditions for very long time [3]. Our computations show that the most unstable transverse wavelengths from linear stability analysis are comparable with the minimum channel width in which one full cell is observed in numerical simulations. Wider computations show that cells which appear regular and periodic in narrow channel computations become irregular. The average cell size approaches a consistent limit corresponding to an even larger size.

The numerical solution is constructed using the Weighted Essentially Non-Oscillatory (WENO) finite difference scheme of Shu & Osher [2]. The detonation cellar structure is visualized using numerically generated smoke foils, by transforming the detonation into a frame of reference attached to the unburnt mixture, and plotting the leading shock pressure as a function of time and space [3]. Linear stability of planar detonation waves with the same chemical model is also examined, using the normal mode analysis of Lee & Stewart [4], also used by Short [5, 6], with an iterative shooting method, in both cases for unit reaction order. Spatial integration is performed using a high accuracy adaptive step-size Runge-Kutta method; a standard two-variable Newton-Raphson technique is used to iterate on any of two unknowns.

Figure 1 (a) to (d) shows the change in the linear stability spectrum where the activation energy is reduced from $E = 50$ to $E = 40$, $E = 30$, $E = 10$, with $Q = 50$, $f = 1.2$, $\nu = 0.5$ and $\gamma = 1.2$ fixed. With $E = 50$, the spectrum consists of more than 16 two-dimensionally unstable modes, all of which are also one-dimensionally unstable. Each of these unstable modes exhibits a similar behavior; the growth rate increases monotonically with increasing wave number k, until reaching a maximum. Further increase in k leads to a decay in the growth rate (the real part of the complex eigenvalue α) until a critical wave number is reached when the mode becomes stable [5]. The lowest frequency unstable mode reaches a maximum growth rate $Re(\alpha) = 0.4298$ at $k = 0.815$. The fourth unstable mode with higher frequency exhibits the largest growth rate $Re(\alpha) = 0.7186$ at $k = 4.15$. The wavelength (defined as $W = 2\pi/k$) corresponding to the maximum growth rate is $W = 1.514$. The decrease in activation energy from $E = 50$ to $E = 40$ suppresses most of the higher frequency modes present at $E = 50$, leaving only six one-dimensionally unstable modes. The maximum growth rate appears in the second mode, but drops to $Re(\alpha) = 0.488$ at $k = 1.80$ ($W = 3.489$). A further decrease in activation energy to $E = 30$ leaves only two unstable roots at $k = 0$ and four unstable modes in the spectrum altogether. The maximum growth rate is due to the lowest frequency mode with $Re(\alpha) = 0.2938$ at $k = 0.8$ ($W = 7.85$). At $E = 10$, there is only one unstable mode with maximum growth rate $Re(\alpha) = 0.114$ at $k = 0.74$ ($W = 8.48$).

Figures 2 (a) and (b) shows the change in the linear stability spectrum for $Q = 30$ and $Q = 10$ with $E = 30$, $f = 1.2$, $\nu = 0.5$ and $\gamma = 1.2$ fixed. A decrease in heat release results in a large number of higher frequency modes. At $Q = 30$, nine unstable modes exist starting from $k = 0$. The maximum growth rate $Re(\alpha) = 0.51$ is obtained from the second mode at $k = 1.72$ ($W = 3.65$). At $Q = 10$, a turning point occurs where the growth rates drop abruptly as the heat release is further decreased [8]. The same features appear in the two-dimensional stability spectrum. More than ten roots are unstable for $k = 0$. The unstable roots then start to decrease from the ninth higher frequency mode on. But with increasing k, the maximum growth rate of each mode continues to increase slowly.

In order to better understand the relationship between stability analysis and cell spacing, a typical case is selected, which is one-dimensionally ($k = 0$) stable and has simple instability characteristics. Figure 3 shows a series of corresponding numerical smoke foils when the channel width is varied from 9 to 50 times $L_{1/2}$, for the same parameters sets as Figure 1 (d).

The detonation runs from left to right on the figures below. The initial data consist of the ZND profile to which a half sine disturbance is added in the transverse velocity at the shock. The initial perturbation develops into the characteristic fish scale pattern. The computation is pursued until the cells reach a more or less periodic regime. The results shown correspond to that regime. It is shown that half a cell occurs for widths less than $10L_{1/2}$ and the transition from half a cell to one full cell occurs between 9 and 10 $L_{1/2}$. For width up to $14L_{1/2}$, one and a half cells appear and the transition from one and a half cells to two cells is observed between 24 to $25L_{1/2}$. Transition from two and a half to three cells occurs between 40 to $41L_{1/2}$. Four cells occur for $50L_{1/2}$. In narrow channels, the minimum cell width of approximately $10L_{1/2}$ is larger than the predicted cell size at $8.5L_{1/2}$ based upon the most unstable wave length, but in wider channels, the cells adopt a larger size, of approximately $14L_{1/2}$. Detailed comparison will be provided in the final paper.

References

[1] Bourlioux, A. & Majda, A.J. (1992) *Combustion And Flame* **90**: 211–229.
[2] Shu, C. W. & Osher, S. (1988) *Journal of Computational Physics* **77**: 439–471.
[3] Williams, D.N. (2002) Ph.D thesis, University of Calgary.
[4] Lee & Stewart, D. S. (1990) *J. Fluid Mech.* **216**: 103-132.
[5] Short, M., (1997) *SIAM J. Appl. Math.* 57:307-326.
[6] Short, M. & Stewart, D.S., (1998) *J. Fluid Mech.* 368:229-262.
[7] Nikolic, M., Williams, D.N. & Bauwens, L. (1999)Gaseous and Heterogeneous Detonations. 153–162.
[8] Liang, Z. & Bauwens, L. 2003 The 24^{th} International Symposium On Shock Waves. Submitted.

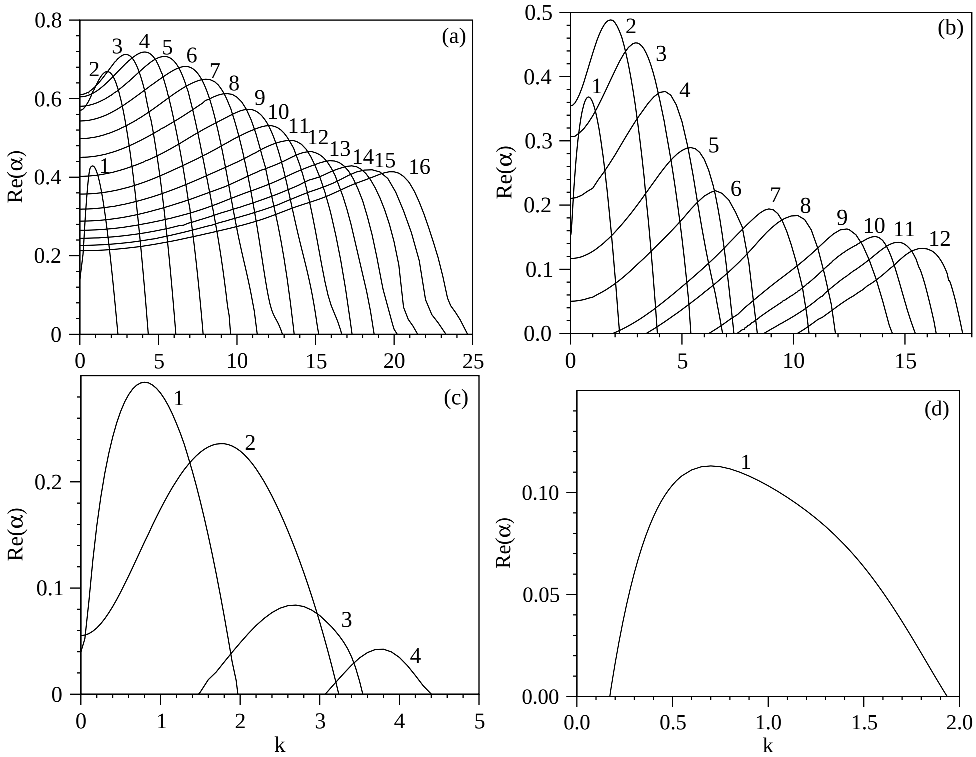

Figure 1. Stability spectrum showing $Re(\alpha)$ vs. k for (a) $E = 50$, the first fifteen unstable modes; (b) $E = 40$, the fist twelve unstable modes; (c) the four unstable modes for $E = 30$; (d) the single unstable mode for $E = 10$ (with $\nu = 0.5$, $Q = 50$, $f = 1.2$ and $\gamma = 1.2$ fixed).

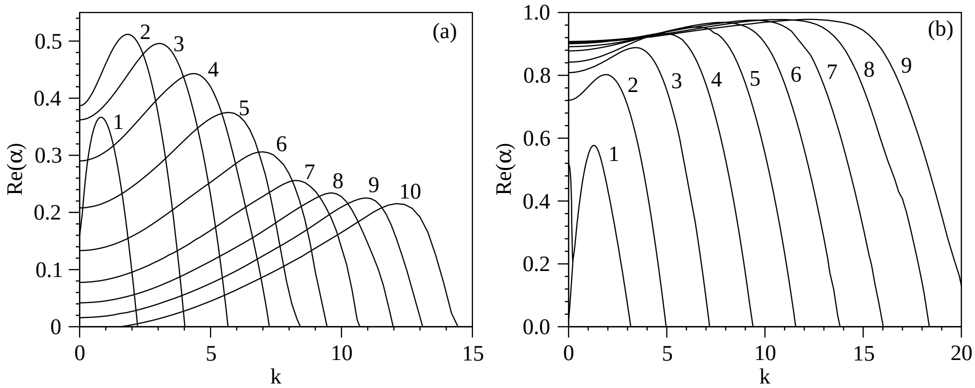

Figure 2. Growth rate $Re(\alpha)$ vs. wave number k for (a) $Q = 30$, the first ten unstable modes; (b) $Q = 10$, the first nine unstable modes (with $E = 30$, γ=1.2, $f = 1.2$ and $\nu = 0.5$ fixed).

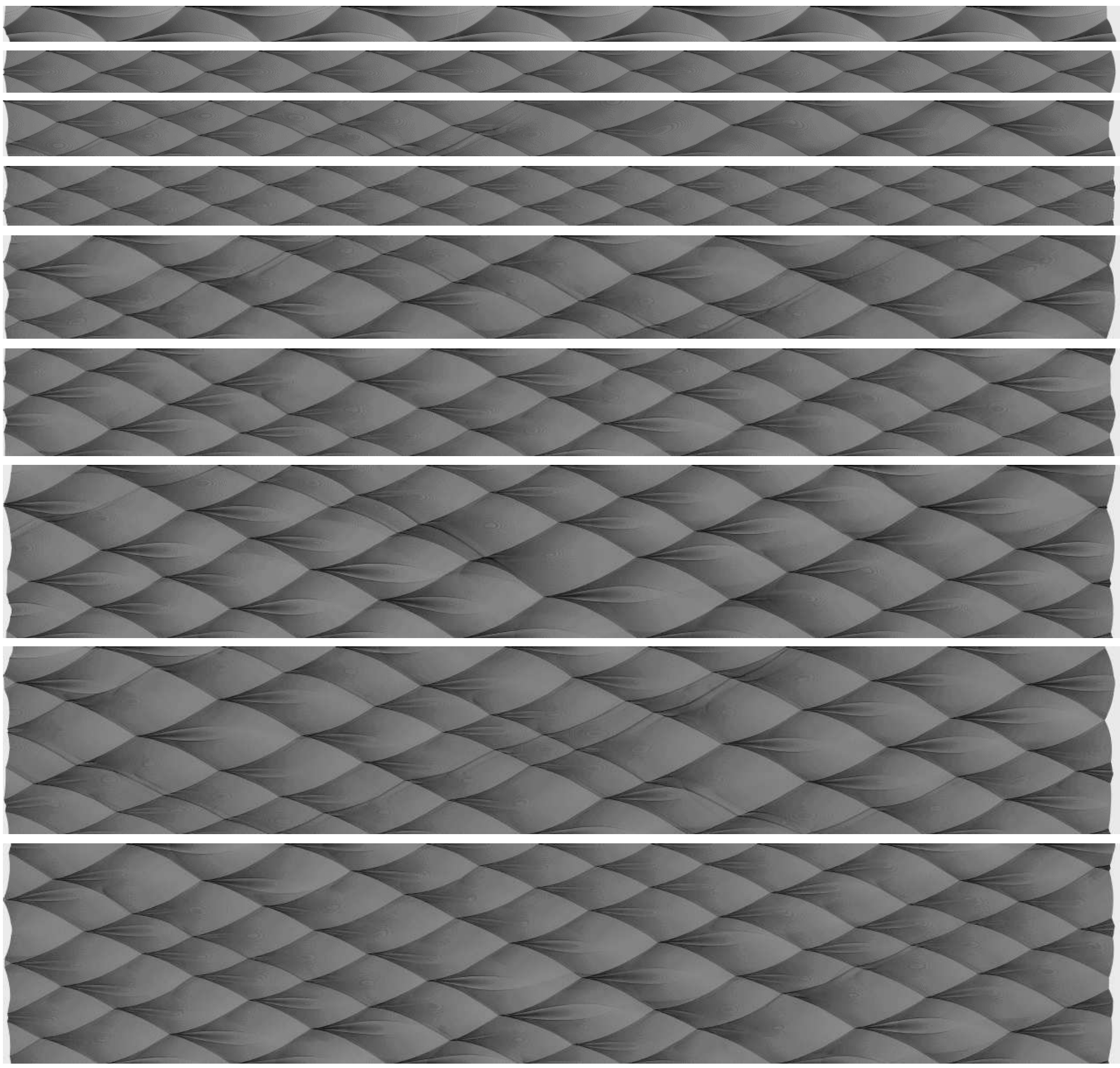

Figure 3. Smoke foils with the channel width changing from 9, 10, 13, 14, 24, 25, 40, 41, $50L_{1/2}$ for $E = 10$, $Q = 50$, γ=1.2, $f = 1.2$, $\nu = 0.5$ between time step 60000-90000.