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Comment on intense shock waves in monatomic gases

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It is known that the wavefront of a shock wave in a shock tube becomes unstable at particular Mach numbers and unperturbed gas pressure. This instability leads to the distortion of the wave front, i.e. particular Mach numbers define a threshold beyond which the wavefront is no longer plane (see Annou and Ferhat 1997, and references therein). In a recent paper (Annou and Ferhat 1997, subsequently referred to as AF), the authors proposed a microscopic model based on an ionization mechanism described by a set of two reaction–diffusion equations in an effort to interpret the wavefront distortion. Using an analytical approach, they argued that their equations have a bifurcation point beyond which the wavefront instability occurs and that the solution thus obtained describes the distortion of the wavefront. In this brief comment, we present analytical and numerical arguments supporting the fact that the proposed model, although it has an instability point, is unable to explain the front behavior.

The proposed model (AF) is based on the reaction–diffusion equations

$$\left.\begin{aligned}\frac{\partial X}{\partial t} &= A - BX - XY,\\ \frac{\partial Y}{\partial t} &= BX - \delta XY^2 + XY - D\nabla^2 Y,\end{aligned}\right\} \tag{1}$$

where X and Y are the densities of the excited atoms and electrons, respectively, and A, δ, D and B are positive constants. It is worth noting that the cubic nonlinearity in the second equation can be responsible for the existence of nontrivial solutions. This model is somewhat similar to the well-known trimolecular model called the Brusselator (Nicolis and Prigogine 1977), described by the equations

$$\left.\begin{aligned}\frac{\partial X}{\partial t} &= A - (B+1)X + X^2Y + D_1\nabla^2 X,\\ \frac{\partial Y}{\partial t} &= BX - X^2Y + D_2\nabla^2 Y.\end{aligned}\right\} \tag{2}$$

For these equations, there exist two bifurcation points and B is the bifurcation parameter. After the first bifurcation, the system becomes unstable with respect to perturbations that oscillate in time, whereas after the second one, it is unstable with respect to perturbations that grow exponentially in time. The first bifurcation gives spatially varying structures: dissipative structures (Figs 1 and 2) that disappear when $D_1 = D_2$. If the AF model can develop such structures then the wavefront will be distorted. In fact, as the concentration of atoms X becomes space-dependent, the sound velocity, i.e. the velocity of the wavefront, will be space-varying. Guided by

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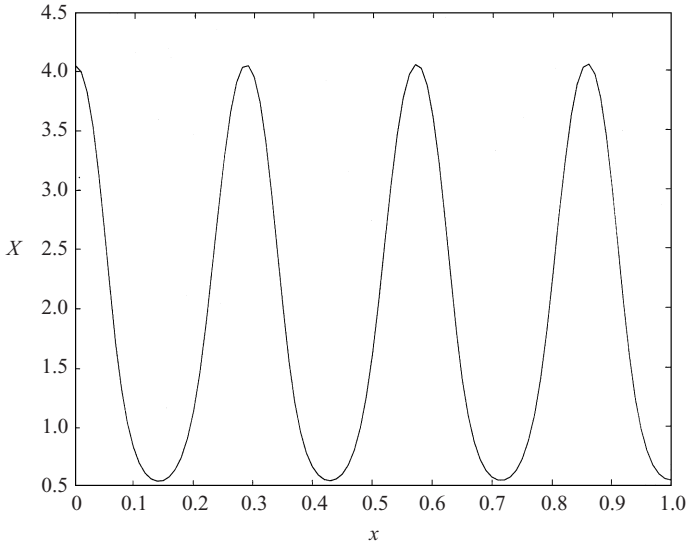


Figure 1. Steady-state dissipative structures (here for the variable X) of the Brusselator in one space dimension x, for no-flux boundary conditions and random initial conditions. $A = 2$, $B = 5.1$, $D_1 = 0.0016$ and $D_2 = 0.008$. This steady state is reached for $t \approx 100$. The dissipative structures for the variable Y are qualitatively the same.

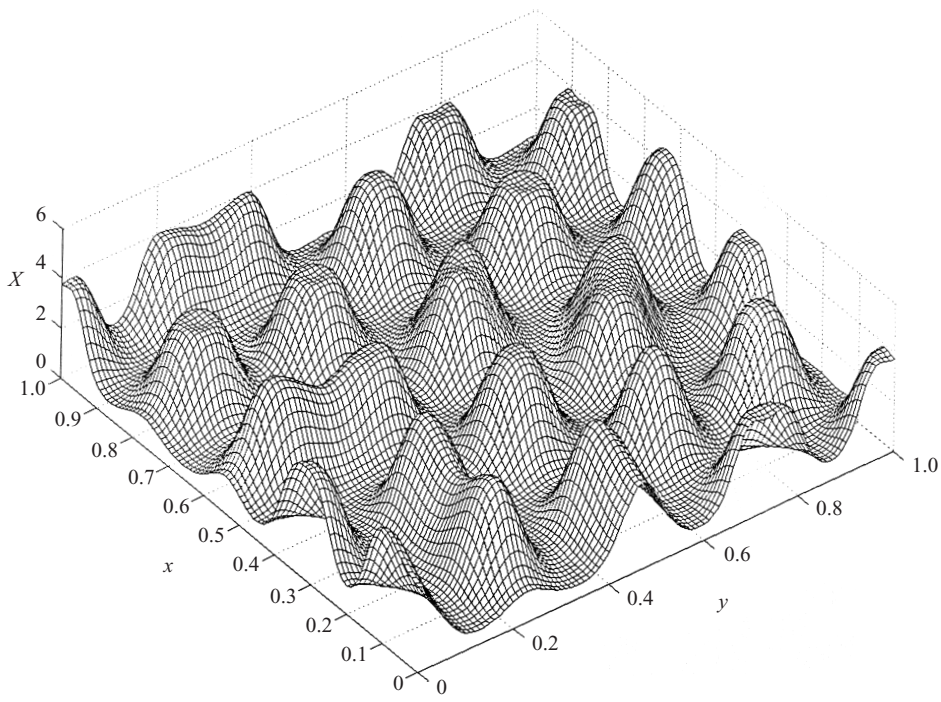


Figure 2. Steady-state dissipative structures of the Brusselator in two space dimensions x and y, for no-flux boundary conditions and random initial conditions. $A = 2$, $B = 5.1$, $D_1 = 0.0016$ and $D_2 = 0.008$. This steady state is reached for $t \approx 1000$.

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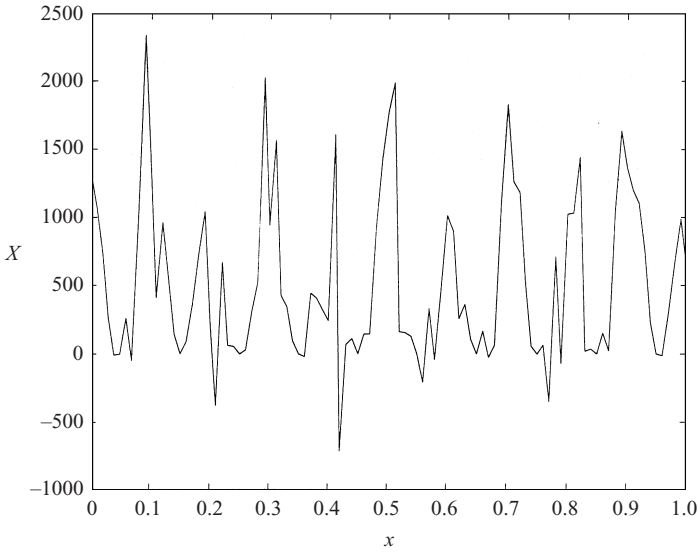


Figure 3. The case with $A = 4$, $B = 1$, $\delta = 0.1$, $D = 0.01$ and $t = 0.3$ for the system (1) in one space dimension. The maximum amplitude of the random initial condition for X is 0.67.

the analogy between the two systems (2) and (1), we have tried to find the dissipative structures inherent to system (1), which were expected in AF to represent the wavefront form (the densities become dependent on spatial dimension, so the front is no longer plane). Using an implicit finite-difference algorithm (ADI scheme in two space dimensions), the numerical computation failed to find any dissipative structure (Figs 3–5). For any initial and boundary conditions, the solution diverges exponentially for any value of the parameter B, i.e. there is no bifurcation point. In fact, linear mode analysis about the equilibrium state (equations (12) and (14) of AF) gives the two real mode frequencies

$$\omega_1 = -B - \frac{1 + \sqrt{1 + 4\delta B}}{2\delta}, \tag{3}$$

$$\omega_m = \frac{-2\delta A\sqrt{1 + 4\delta B}}{1 + 2\delta B + \sqrt{1 + 4\delta B}} + m^2\pi^2 D, \tag{4}$$

where the perturbations about the equilibrium state for no-flux boundary conditions are of the form

$$\delta X(r, t) = \sum_{m=0}^{\infty} \delta X_m e^{\omega_m t} \cos m\pi r. \tag{5}$$

The first frequency leads always to stable modes ($\omega_1 < 0$) whereas the second one (4) is unstable for $B > B_m$, where B_m is given by equation (15) of AF.

$$B_m = \frac{1}{4\delta}\left\{\left[\frac{2}{m^2\pi^2 D}\left(\sqrt{A^2\delta^2 - A\delta D m^2\pi^2 + A\delta}\right) - 1\right]^2 - 1\right\}. \tag{6}$$

This was thought to be the bifurcation point in AF. We have two objections to this conclusion. First, the transition is from stable to unstable behavior with respect to exponentially growing perturbations in time; thus the instability does not lead

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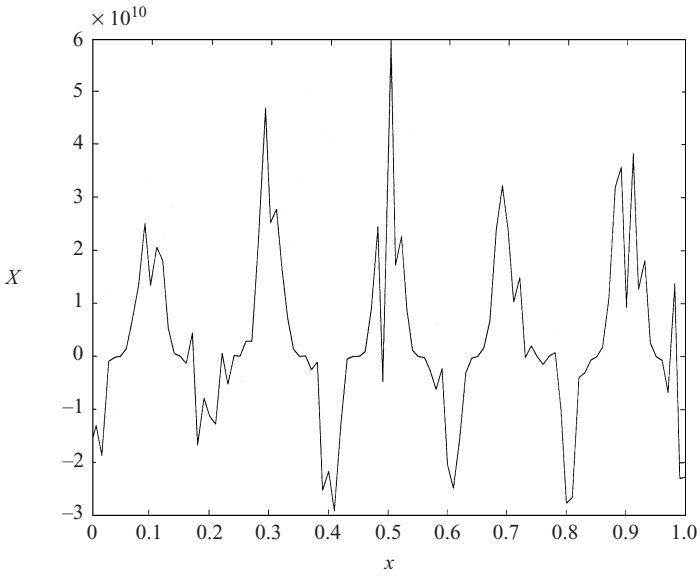


Figure 4. The same as Fig. 3, but for $t = 0.4$. The amplitude diverges exponentially.

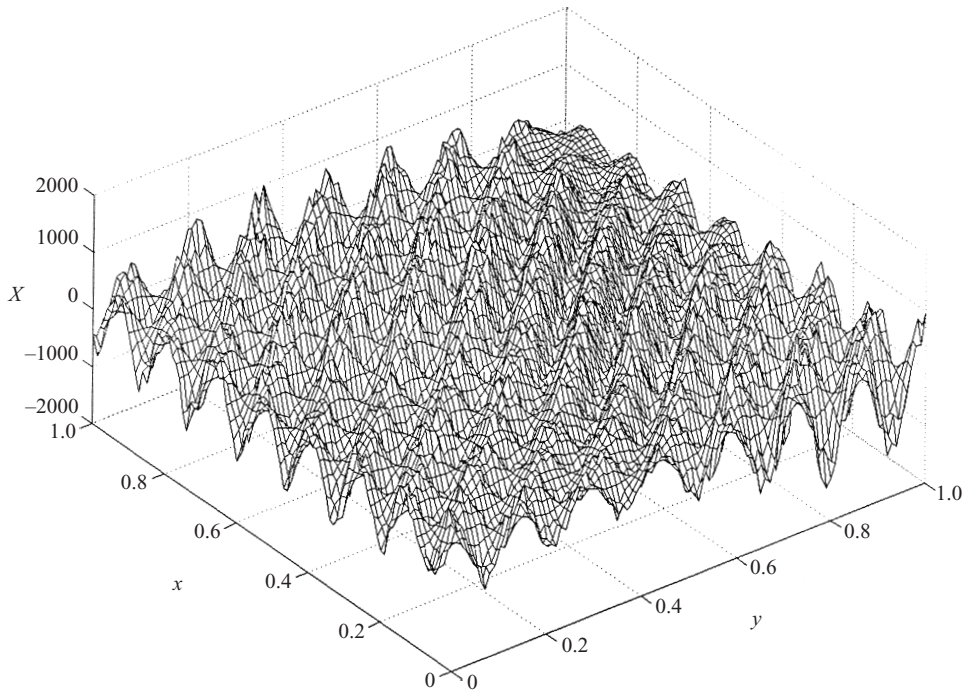


Figure 5. The case with $A = 4$, $B = 1$, $\delta = 0.1$, $D = 0.01$ and $t = 0.3$ for the system (1) in two space dimensions.

to a stable dissipative structure, as in the case of the system (2), but instead leads to the breaking of the wavefront. Second if $m > \bar{m} = \sqrt{\delta A/D}/\pi$, the expression (6) becomes singular and ω_m becomes positive. For instance, for typical parameter values ($A = 4, \delta = 0.1$ and $D = 0.01$), one finds $\bar{m} \approx 2$ (Fig. 6), and thus any

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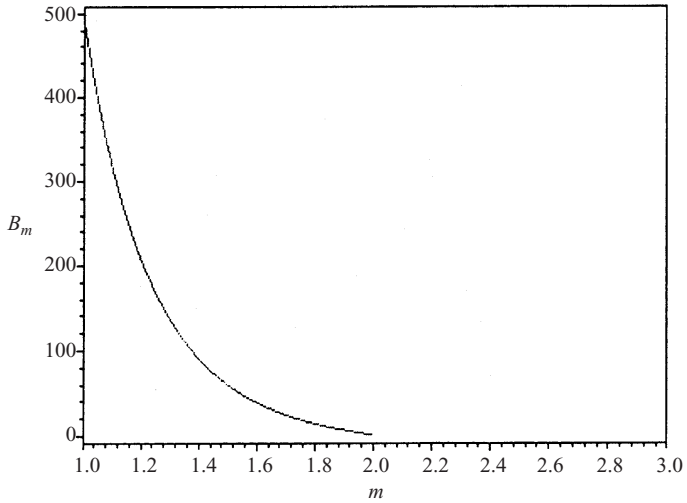


Figure 6. B_m as a function of m for $A = 4$, $B = 1$, $\delta = 0.1$ and $D = 0.01$. All the modes with $m \geqslant 2$ are unstable for any positive value of B.

perturbation with mode 3 in its spectrum will lead to an exponentially growing instability for any value of the 'bifurcation parameter' B. We thus conclude that the system (1) is unstable to exponentially growing perturbations for any value of the parameter B and there is no bifurcation point. In addition, in order to have dissipative structures, i.e. periodic structures in space and time, we must have complex eigenvalues of the linear operator (equation (14) in AF), which is not the case. These conclusions remain qualitatively unchanged if one introduces a diffusion term for the X species (excited atoms) or if one changes the sign of the diffusion term for the Y species and applies a nonzero-flux boundary condition to take into account electron escape to the wall. For this latter case, the equilibrium point of the system (1) is stable with respect to any perturbation, since the two real frequencies (3) and (4) are negative. As was noted above, these conclusions are corroborated by our numerical computation.

Thus, the system (1) is not suitable for the description of the wavefront in a shock-wave tube. However, we think that a deep understanding of the ionization process may improve the model by introducing other reaction terms or by increasing the number of equations. This work will be considered in a forthcoming paper.

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