Pergamon

Appl. Math. Lett. Vol. 8, No. 2, pp. 39–44, 1995

0893-9659/95 $9.50 + 0.00

0893-9659(95)00008-9

Finite-Dimensional Model of Thermal Instability

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(Received and accepted October 1994)

Abstract—Using the collocation method, we derive a finite-dimensional (3-D) dynamical system whose dynamics mimic behavior of a free boundary problem for the heat equation that describes solid combustion and some phase transitions and has been shown to develop complex dynamical patterns. Numerical simulations on the 3-D system demonstrate a variety of dynamical scenarios depending on boundary kinetic functions inherited from the original problem. The multitude of nontrivial dynamical features as well as a clear physical origin of the system make it interesting in its own right.

Keywords—Free boundary problems, Pseudo-spectral approximation.

1. INTRODUCTION

In three recent papers, we studied rigorously [1,2] and numerically [3] a model free boundary problem capable of developing a number of nontrivial self-oscillatory regimes. The dynamics of the free boundary includes uniform motion, Hopf bifurcation and persistent simple periodic oscillations, Hopf bifurcation followed by a sequence of secondary period doubling resulting in a transition to chaos, reversed sequences, sequences followed by Shilnikov type trajectories, infinite period bifurcations, etc. [3]. It is rather remarkable that such a variety of patterns is exhibited by a relatively simple problem consisting of 1-D heat equation and (free) boundary conditions. This occurs essentially as a result of interaction between the heat transfer from the boundary and the boundary kinetics. It was argued in [1–3] that the model free boundary problem exhibits generic thermal instability peculiar to some nonequilibrium exothermal phase transitions such as solid-state combustion, laser induced evaporation from the surface of metals, etc. (see references in [3]).

Numerical experimentation with the one-phase problem demonstrates not only its remarkable dynamical wealth but also surprisingly clear-cut patterns that are well-known for the finite-dimensional dynamical systems. This leads to the suggestion that the dynamics generated by the free boundary problem may be essentially finite-dimensional. Thus, derivation of a justifiable low-dimensional qualitative approximation would present substantial, although indirect,

*Partially supported by NSF Grant No. DMS-9305228 and by the U.S. Department of Energy under Grant No. DE-FG02-88ER13822.
†Partially supported by NSF Grant No. 9311659.

evidence in favor of such a hypothesis. *The purpose of the present letter is to demonstrate such an approximation.* The derivation of the finite-dimensional model presented below is based on a rather straightforward approach. As a first step, by using an appropriate change of variables, the problem is reduced to a form with a stationary boundary and zero boundary conditions, while the unknown boundary (or rather its velocity) appears in a source term for the heat equation. Second, we employ a pseudo-spectral method with a natural basis for the problem: the Laguerre polynomials. The latter is due to the exponential decay of solutions at $-\infty$. The choice of the collocation method for the discrete approximation appears to be amazingly successful, especially taking into account that only two basis elements have been used.

2. DERIVATION OF THE 3-D SYSTEM

The free boundary model of thermal instability is given by

$$T_t = T_{xx}, \qquad \text{for } x < F(t),$$
$$T_{x=F(t)} = 1 + \nu K(-V), \quad \left.\frac{\partial T}{\partial x}\right|_{x=F(t)} = -V, \quad T(-\infty) = 0.$$

Here, $x = F(t)$ and $V = \frac{dF}{dt}$ are the location and the velocity of the free boundary, the function $K(-V)$ is the boundary kinetics with the normalization $K(1) = 0$, $K'(1) = 1$, ν is a positive parameter. The above problem has a (basic) solution in the form of a steadily propagating profile: $T_b = \exp(x+t)$, $F_b = -t$. It is convenient to consider the velocity perturbation $v = V + 1$ and deal with a fixed boundary and zero boundary conditions. We introduce $z = x - F(t)$. Then, for $w(z,t) = T - T_b + e^z[zv + \nu(z-1)k(v)]$, here $k(v) = K(1-v)$, we obtain

$$w_t = w_{zz} + (v-1)w_z + \Phi(v, \dot{v}, z), \qquad z \le 0, \tag{2.1}$$
$$w(0,t) = w_z(0,t) = w(-\infty) = 0. \tag{2.2}$$

The source $\Phi = e^z\{\dot{v}[z - \nu \frac{\partial k}{\partial v}(1-z)] - (zv+1)\nu k - (z+1)v^2\}$ "absorbs" the inhomogeneous boundary conditions.

Problem (2.1)–(2.2) has a unique classical solution for any meaningful initial distribution provided that kinetics K satisfies certain conditions [1]. The solutions decay exponentially at $-\infty$, and, thus, Laguerre polynomials represent a natural basis for their expansion. Let us assume a rough approximation to the solution of the form

$$w(z,t) = \left[W(t)z^2 + U(t)z^3\right]e^z. \tag{2.3}$$

Note that in fact, the Laguerre polynomials of degrees 0 and 1 have already been used in reducing the problem to the form (2.1)–(2.2). We choose three collocation points: 0, $-a$, and $-b$ $(a, b > 0)$. The choice of 0 corresponds to the requirement that the equation is satisfied up to the boundary and appears to be necessary to produce a "well-behaved" finite-dimensional system.

Thus, we substitute (2.3) into (2.1) and demand (2.1) to be satisfied exactly at the collocation points. Then, we obtain the following system of o.d.e.'s:

$$\dot{v} = \frac{2W - \nu k - v^2}{\nu k'},$$
$$\dot{W} = \alpha\left[-2W - 3U - \frac{2W - \nu k - v^2}{2\nu k'} + \frac{\nu k}{2}(v+1) + v^2 - vW\right] + 3U(v+1) + vW,$$
$$\dot{U} = \beta\left[-2W - 3U - \frac{2W - \nu k - v^2}{2\nu k'} + \frac{\nu k}{2}(v+1) + v^2 - vW\right] + vU,$$

where dot stands for $\frac{d}{dt}$ and prime for $\frac{d}{dv}$, $\beta = 2/ab$ and $\alpha = (a+b)\beta$. In terms of the variables $\xi = 2((W/\alpha) - (U/\beta))$, $\eta = v + (2/\beta)U$, the system takes a somewhat simpler form

$$\dot{v} = \frac{\alpha(\xi + \eta - v) - \nu k - v^2}{\nu k'}, \tag{2.4}$$

$$\dot{\xi} = 3\frac{\beta}{\alpha}(\eta - v)(1+v) + v\xi, \tag{2.5}$$

$$\dot{\eta} = (2\alpha + 3\beta)(v - \eta) - 2\alpha\xi + \nu(v+1)k + 2v^2 + v\left[(1-\alpha)(\eta - v) - \alpha\xi\right]. \tag{2.6}$$

As one could expect, system (2.4)–(2.6) has an equilibrium at (0,0,0). We should now choose some collocation points for the numerical solution (for example, $a = 1$, $b = 2$ which produce $\alpha = 3$, $\beta = 1$). Linearization of (2.4)–(2.6) yields then the eigenvalue equation

$$\lambda^3 + \left(10 - \frac{3}{\nu}\right)\lambda^2 + \left(12 - \frac{3}{\nu}\right)\lambda + 3 = 0.$$

For the purely imaginary roots $\lambda = i\omega$, $(3/\nu - 10)(4 - 1/\nu) + 3 = 0$ yielding $\nu = 1/3$. The spectrum of the linearization at ν_{cr} consists of two complex conjugate eigenvalues crossing into the positive half-plane (*as ν decreases*) and a real one $\lambda = -1$. We note that the linearization of the original pde problem also possesses two complex conjugate eigenvalues crossing into the positive half-plane plus a continuous spectrum situated in the negative real part half-plane. By a coincidence, the threshold value is the same 1/3.

3. NUMERICAL RESULTS

Since our goal has been to evaluate the quality of imitation of the original free boundary problem by the 3-D system (2.4)–(2.6), we present numerical solutions of the latter for the same types of kinetics as in [3]. One of them has the form: $K_{p,q}(\zeta) = (\zeta^p - \zeta^q)/(p+q)$. Similar "artificial" kinetics can be easily constructed based on a variety of other functions. The specific form of $K_{p,q}$ was designed to control the growth of the kinetic function for $\zeta > 1$ and descend for $\zeta < 1$, with the normalization preserving the exact spectrum of the linearized problem. The behavior of $K_{p,q}$ is very similar (see [3]) to that of the Arrhenius kinetics reduced to the interface, $K_A(\zeta) = \ln(\zeta)/(1 - \gamma\ln(\zeta))$.

The first sequence obtained for $K_{3,1}$ demonstrates a clear-cut case of the infinite period bifurcation at ν_{cr}. Figure 1 depicts the velocity perturbation profiles $v(t) = V + 1$ and, respectively, the phase space projections onto the plane $(v(t), w(1,t))$ for several values of the parameter ν. We reconstruct $w(1,t) = (1.5\xi + \eta - v)/e$ from the assumed form of approximated solution and the assumed choice of collocation points. Just below the critical value ($\nu = .3325$), we observe a solution of a very large period $T \sim 200$ (Figure 1, A,a). For a somewhat more overcritical value of the parameter ($\nu = .33$), the total period becomes significantly shorter—about 60 time units (Figure 1, B,b). Note also that the characteristics of the bursts remain practically unchanged. One can observe a further degeneration of the "accumulation phase" as the parameter moves away from the instability threshold until it disappears entirely (Figure 1, C,c). We should mention that extremely large periods can indeed be achieved when ν gets close to ν_{cr}. The scenario of infinite period bifurcation never breaks down within the range of parameter ν that we were able to investigate.

The next sequence obtained for K_A exhibits a part of period doubling cascade leading to chaotic oscillations. Figures 2, A,a–B,b correspond to 4-periodic and 8-periodic solutions, respectively. Periodic solutions of greater 2^n multiplicities can be found as well but they attract much slower. Finally, Figures 2, C,c correspond to a chaotic orbit. We should mention that period doubling cascades occur for $K_{p,q}$ as well.

The last scenario (Figure 3) represents, in a way, a curious mixture of the first two. It begins from a period doubling sequence and enters the chaotic region. However, the appearance of the

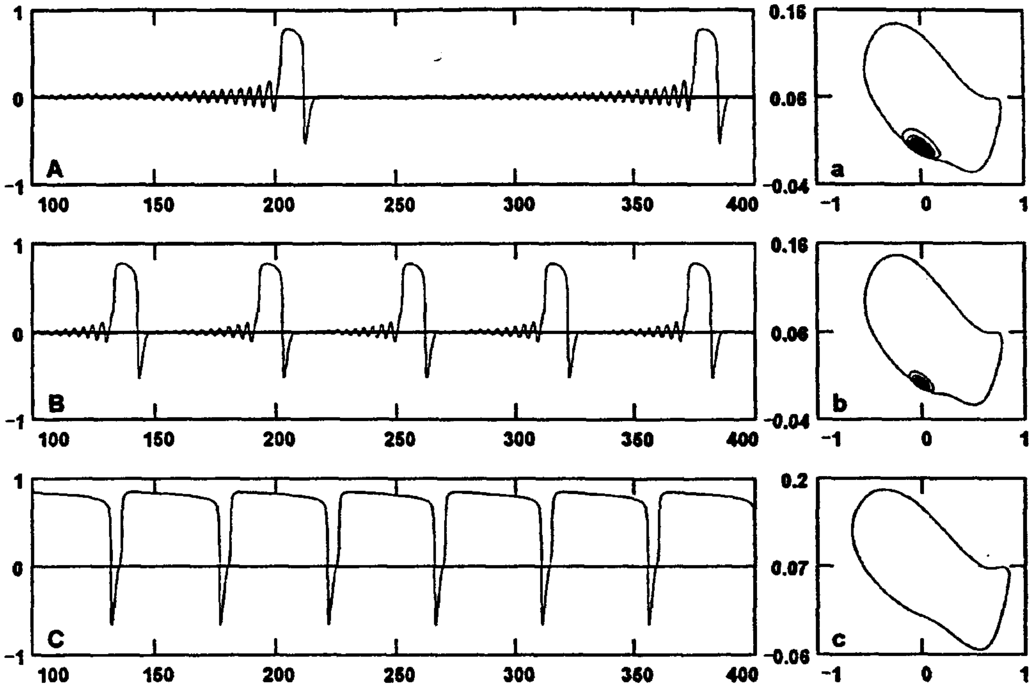

Figure 1. Velocity perturbation profiles $v(t)$ and projection of the orbits into the plane $(v, w|_{z=1})$ for $K_{3,1}$; $\nu = 0.3325, 0.33, 0.285$ (A,a–C,c, respectively).

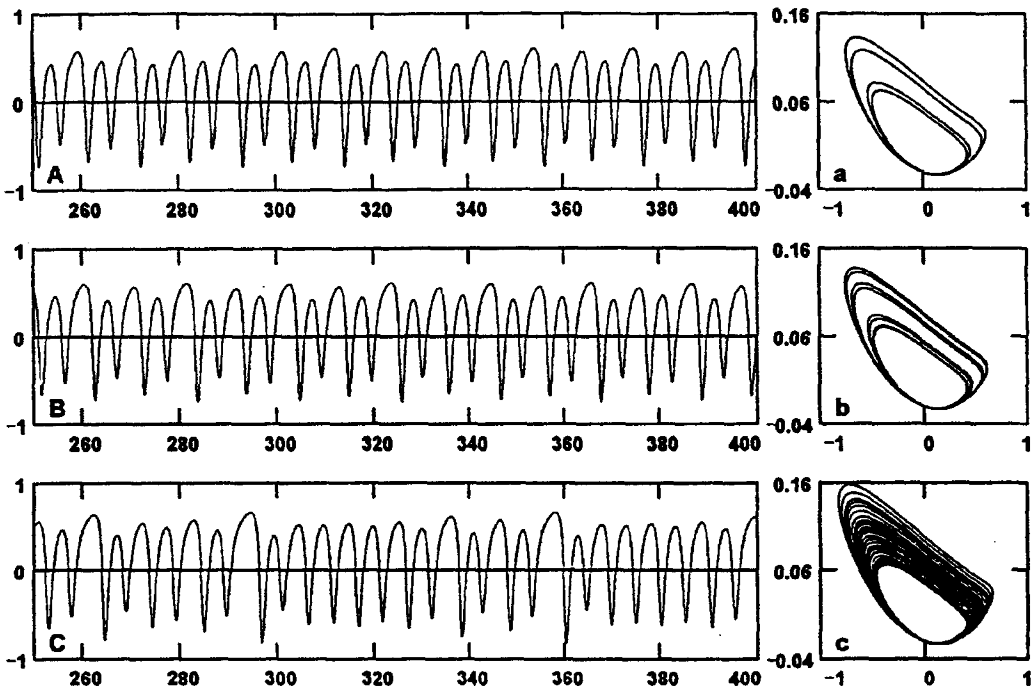

Figure 2. Velocity perturbation profiles $v(t)$ and projection of the orbits into the plane $(v, w|_{z=1})$ for K_A with $\gamma = 0.35$; $\nu = 0.33075, 0.330737, 0.33071$ (A,a–C,c, respectively).

chaotic solution changes drastically. One can see windows of accumulation-burst behavior appear on the velocity profile and birth of a "vortex" in the phase space projection. As ν continues to decrease, these windows widen gradually and at some point chaos is replaced by a periodic Shilnikov type solution of a finite winding number. To illustrate the above remark concerning the birth of the "vortex," in Figure 3 we present pictures in the (v, ξ, η) phase space obtained for $K_{2.3,1}$. Note that while the 8-periodic and the first chaotic solutions seem to be essentially two-dimensional (belonging to some smooth surface), the second chaotic and, even more obviously, the periodic Shilnikov type orbit develop a third dimension in the orthogonal direction. One can quite naturally speculate that this should be attributed to the birth of a homoclinic orbit for the values of ν somewhere between the two chaotic solutions.

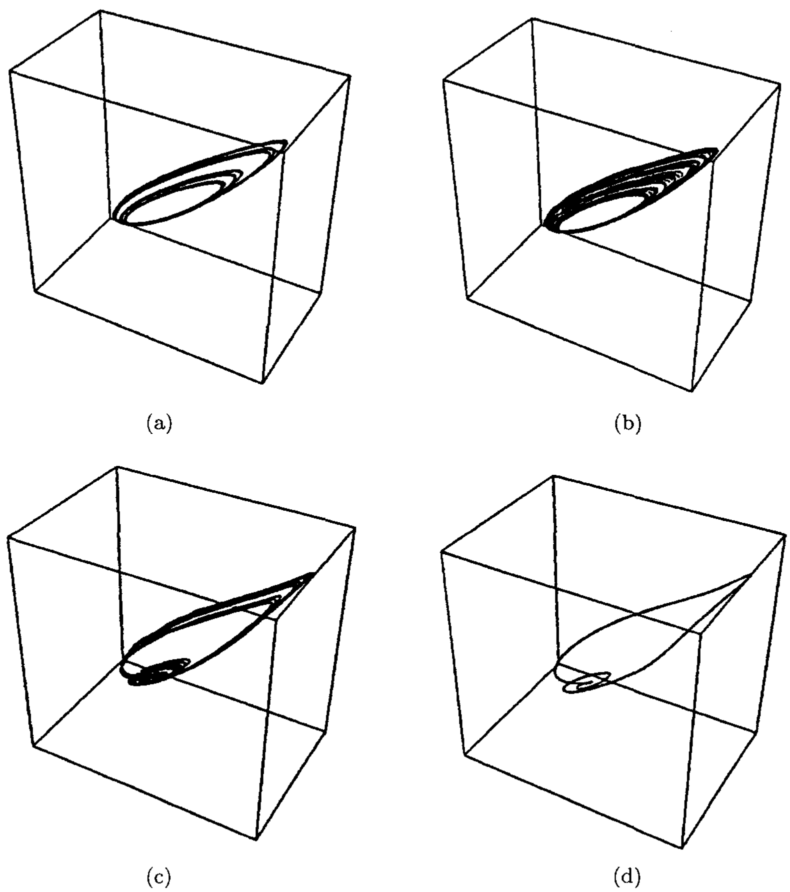

Figure 3. Projection of the orbits onto the (v, ξ, η) subspace for $K_{2.3,1}$ and $\nu =$ 0.32845, 0.3283, 0.324, and 0.315 (a–d, respectively).

Comparison of the results of numerical solution of the 3-D dynamical system with those in [3] presents convincing evidence that the system provides a sufficiently good imitation of the original free boundary problem. This imitation goes beyond mere reproduction of a single dynamical phenomenon, but in fact represents an adequate model of its physical source for a multitude of behavior patterns with a number of kinetics of appropriate type: numerical results here and in [3] are in uniform qualitative agreement practically throughout the entire parameter space. Such a success in modeling of a wide spectrum of dynamical features of the free boundary problem by a 3-D dynamical system is due to two important circumstances.

First of all, as our observations on the numerical simulations of such problems show, the spatial distributions of the temperature profiles remain essentially indifferent to the complexity of the interface motion due, apparently, to the powerful smoothing action of the heat operator. Thus, the spatial distribution can be roughly modeled by a very few (only two in the case of the one-phase model) basis elements. Second, the use of a relatively simple one-sided free boundary problem presents a clear advantage. Indeed, should we attempt to use a two-phase model, at least two additional collocation points in the "product" phase (and a new basis) would have been required, and, consequently, the derivation procedure becomes more complicated, and, more importantly, the finite-dimensional model less transparent and of greater dimensionality.

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