PC7 : Spatially extended systems of equation Equilibria, traveling waves and Turing patterns

1 Introduction

The Petite Classe is divided into four parts. The first part is devoted to the thermal explosion, within the framework of the Frank-Kamenetskii theory in one space dimension [2], as well as its link with what we have seen in previous PCs (PC1 and 6). The second part is devoted to flames, deflagrations, modeled through a traveling wave self-similar solution, which leads us to the resolution of an ODE on the full real line [9], and to a heteroclinic orbit joining two equilibrium points at infinity. Such a case has been encountered and presented in the course for the Nagumo equation [3], for which there is an analytic solution. We only prove the existence of solution, whereas the stability of such solutions [4, 8], as well as the numerical resolution in the phase space through shooting methods is beyond the scope of the course [6]. The third part is devoted to the numerical simulation of traveling waves of semi-discretized in space systems of PDEs leading to the resolution of large systems of ODEs. We focus on the Nagumo reaction-diffusion equation, conduct numerical simulations and draw conclusions on the results. The last part is devoted to the simulation of a 1D Turing pattern, where the homogeneous steady state becomes unstable because of the diffusion and non homogeneous steady states appear.

2 Thermal explosion - 1D problem

We consider inhomogeneous temperature and fuel mass fraction fields in space, which also depend on time. We consider a horizontal layer of height $2L$, homogeneous in the x and y directions as presented in the Figure in 2D, and inhomogeneous in space in the vertical z direction (see Figure 1). The problem is then mono-dimensional and the system of interest is a PDE system of equations reading:

$$\partial_t Y - D\,\partial_{zz} Y = -B\,e^{-\frac{E}{RT}}\,Y, \tag{1}$$

$$\partial_t T - D\,\partial_{zz} T = (T_b - T_0)\,B\,e^{-\frac{E}{RT}}\,Y, \tag{2}$$

where ∂_{zz} denotes the second order partial differential in space in the z direction, and ∂_t is the time derivative. The following initial conditions are considered: $Y(0,z) = 1$ and $T(0,z) = T_0$, for all $z \in [0, 2L]$ as well as the boundary conditions $T(t,0) = T(t,2L) = T_0$ and $\partial_z Y(t,0) = \partial_z Y(t,2L) = 0$. It can be shown mathematically that there exists a unique C^∞ solution in time $z \in [0, 2L]$, $t \in [0, +\infty[$, at least for some proper set of coefficients, such that $Y(t,z) \in [0,1]$, $T(t,z) \in [T_0, T_b[$ and such that $z \to T(t,z)$ is concave for all $t \in [0, +\infty[$.

2.1 Link with 0D problem studied in the PC1

2.1.1 Write an equation on the average quantity $\overline{Y}(t) = \frac{1}{2L}\int_0^{2L} Y(t,z)\mathrm{d}z$ of Y on the interval $[0, 2L]$, as well as for $\overline{T}(t) = \frac{1}{2L}\int_0^{2L} T(t,z)\mathrm{d}z$ of T.

2.1.2 Using the boundary conditions and the fact that $T(t,z) \geq T_0$, show that $\overline{Y}(t) \underset{t\to\infty}{\longrightarrow} 0$ and $\overline{T}(t) \underset{t\to\infty}{\longrightarrow} T_0$. *Hint for the second limit: you might want to use the following estimate. If f is a concave function on $[a,b]$ satisfying $f(a) = f(b) = f_0$, then*

$$\overline{f} - f_0 \leq \frac{f'(a) - f'(b)}{4}.$$

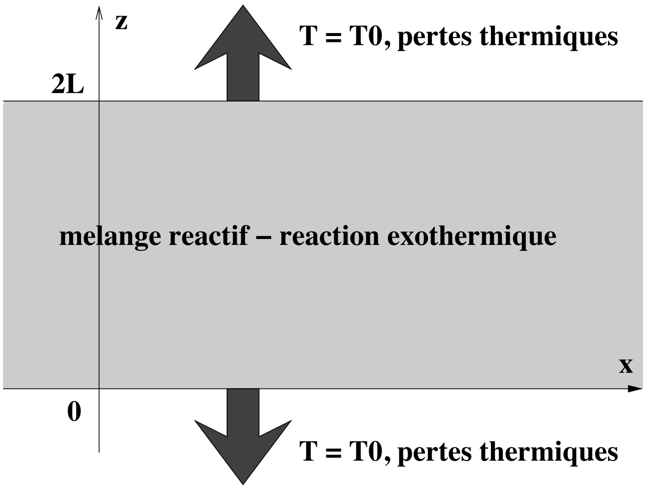

Figure 1: Schematic diagram of the configuration in the (x, z) plane.

2.1.3 Make the link with the homogeneous model we have already studied, in particular in PC1.

2.2 Stationary solution as equilibria of the infinite dimensional dynamical system - qualitative analysis

Recalling the quantities

$$T_{FK} = \frac{RT_0^2}{E}, \quad \tau_I = \frac{T_{FK}}{T_b - T_0} \frac{\exp(E/(RT_0))}{B}, \quad \epsilon = T_{FK}/(T_b - T_0)$$

and assuming [H1] + [H2] (see PC1), introducing $\tau_{\text{dif}} = L^2/D$, $\lambda = \tau_{\text{dif}}/\tau_I$ and using the new scales $\xi = z/L$ and $\tau = t/\tau_I$, we obtain a non-dimensional form of the PDE on $\theta = (T - T_0)/T_{FK}$ and Y:

$$\partial_\tau \theta - \frac{1}{\lambda} \partial_{\xi\xi} \theta = \exp(\theta)\, Y, \tag{3}$$

$$\partial_\tau Y - \frac{1}{\lambda} \partial_{\xi\xi} Y = -\epsilon \, \exp(\theta) Y. \tag{4}$$

If we also make the assumption that fuel consumption is neglected, that is $Y \equiv 1$, we get an independent equation on θ:

$$\partial_\tau \theta - \frac{1}{\lambda} \partial_{\xi\xi} \theta = \exp(\theta). \tag{5}$$

2.2.1 BONUS: The goal of this question is to find a stationary temperature profile $\theta^{\text{st}}(\xi)$ of (5) which is smooth, concave, symmetric (i.e. $\theta^{\text{st}}(\xi) = \theta^{\text{st}}(2 - \xi)$) and has an analytic formula.

2.2.1.a Find a first integral of $\theta^{\text{st}}(\xi)$, and compare its value for an arbitrary ξ with the value for $\xi = 1$. *Hint: multiply the stationary equation by* $\frac{d}{d\xi}\theta^{\text{st}}$.

2.2.1.b Consider the change of variable $\phi^2(\xi) = \exp(\theta_m^{\text{st}}) - \exp(\theta^{\text{st}}(\xi))$, where $\theta_m^{\text{st}} = \theta^{\text{st}}(1)$ denotes the maximum value of θ^{st}, and get and ODE for ϕ having θ_m^{st} as a parameter.

2.2.1.c Derive an analytic formula for $\theta^{\text{st}}(\xi)$, depending on θ_m^{st}, as well as a relation of the form

$$\Psi(\theta_m^{\text{st}}) = \sqrt{\lambda/2},$$

that must be satisfied between λ and the maximal temperature θ_m^{st}.

2.2.2 Plot the function Ψ, given by

$$\Psi(x) = e^{-x/2} \cosh^{-1} e^{x/2} = e^{-x/2} \frac{1}{2} \ln \frac{1 + \sqrt{1 - e^{-x}}}{1 - \sqrt{1 - e^{-x}}}.$$

Show that it admits a maximum as well as a related critical parameter $\sqrt{\lambda_{\rm cr}/2} = \Psi^{\max}$. Deduce that there are three scenarios on the existence or not of smooth, concave and symmetric stationary temperature profiles, depending on $\lambda < \lambda_{\rm cr}$, $\lambda = \lambda_{\rm cr}$ or $\lambda > \lambda_{\rm cr}$.

2.2.3 When $\lambda < \lambda_{\rm cr}$, how many profiles do you think there are? Referring to the last PC, propose a conjecture on their stability.

2.3 Numerical resolution of the semi-discretized in space problem

2.3.1 Semi-discretize the two sets of PDEs on θ and Y on the one side (3)-(4) and purely on θ on the other side (5) using a central second order finite difference approximation as already done previously. Explain what is the form of the system of ODEs resulting from the semi-discretization in space.

2.3.2 Starting from an initial profil $\theta \equiv 0$ for the single equation on θ neglecting the fuel consumption, and for $\lambda < \lambda_{\rm cr}$, describe the dynamics of the system as well as the final state towards which the dynamics is converging. Check that it is coherent with the analytic solution obtained previously. You will use the ROCK4 or RADAU5 solvers provided in the notebook in order to conduct the integration in time of the system.

2.3.3 Taking into account the fuel consumption, and taking any positive Y profile at $t = 0$, which has the same average as $Y \equiv 1$, show that the diffusion of the fuel mass fraction is so quick that its initial spatial distribution has no influence on the dynamics of the problem for $\lambda < \lambda_{\rm cr}$, and even in the neighborhood of the critical λ parameter (try $\lambda = 0.9$).

2.3.4 Propose a synthesis of the results in connection with the original problem of PC1 and with the analytical results obtained above.

3 Study of Combustion waves

One way of modeling combustion fronts or deflagration fronts is to consider systems of reaction-diffusion equations, modeling the coupling between a diffusive process and a reaction one, and to prove that they admit “traveling waves” solution, which are self-similar spatial profiles traveling at constant speed. The combustion process is once again described through a system of partial differential equations on the fuel mass fraction Y and the (rescaled) temperature Θ, with a non linear, monotone and non negative function $\widetilde{\psi}$, which will be clarified later

$$\begin{cases} \partial_t Y - D\,\partial_{xx} Y = -\widetilde{\psi}(\Theta)\,Y, \\ \partial_t \Theta - D\,\partial_{xx}\Theta = \widetilde{\psi}(\Theta)\,Y, \end{cases} \tag{6}$$

for $Y \in [0,1]$ and $\Theta \in [0,1]$. The notation are similar to the thermal explosion problem and, for simplicity, we assume the same diffusion coefficients for mass and temperature (unit Lewis number).

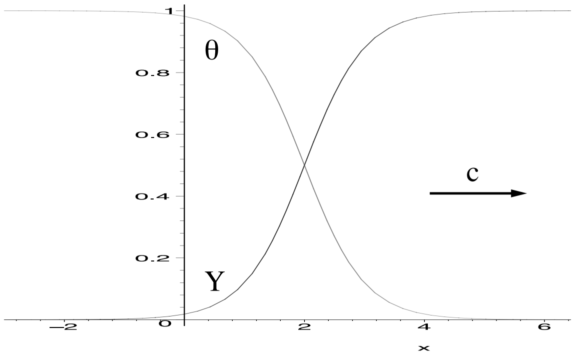

Figure 2: Traveling wave representing a deflagration front.

3.1 Traveling waves

We are looking for self-similar profiles $\phi(y)$ and $\theta(y)$, $y \in \mathbb{R}$ as well as a velocity of the wave c (c is part of the unknowns of the problem), such that, when $y = x - ct$, $Y(t,x) = \phi(y)$ and $\Theta(t,x) = \theta(y)$ are solutions of the previous system (6). The special character of this problem is that we have to impose boundaries at infinity. We look for profiles ϕ and θ satisfying $\lim\limits_{y\to-\infty} \phi(y) = 0$, $\lim\limits_{y\to+\infty} \phi(y) = 1$ and $\lim\limits_{y\to-\infty} \theta(y) = 1$, $\lim\limits_{y\to+\infty} \theta(y) = 0$. The unburnt gases are then on the "$+\infty$" side and the burnt gases on the "$-\infty$" one. We suppose that $\theta(y) \in]0,1[$ and $\phi(y) \in]0,1[$. The flame is moving from the burnt gases toward the unburnt gases at the unknown velocity c (Figure 2).

3.1.1 First, setting a positive velocity c, write the system of ODEs satisfied by the two functions $\phi(y)$ and $\theta(y)$.

3.1.2 We note $\mathcal{H} = \phi + \theta$. Show that if we have a traveling wave, this quantity is constant. *Hint: solve the differential equation satisfied by $\mathcal{H}$ and use the conditions at infinity.*

3.1.3 Show that the problem can be reduced to an equation on $\theta(y)$

$$c\,\theta' + D\,\theta'' + \psi(\theta) = 0, \tag{7}$$

and give an explicit expression for the non-linearity ψ (in terms of $\tilde{\psi}$).

3.1.4 Show that a solution of (7) satisfying $\theta \in [0,1]$, $\lim\limits_{y\to-\infty} \theta(y) = 1$ and $\lim\limits_{y\to+\infty} \theta(y) = 0$ must be non increasing. *Hint: remember that $\tilde{\psi}$ is assumed to be non-negative, and argue by contradiction.* Prove that the solution must in fact be decreasing.

3.1.5 Introducing $\tilde{p} = -\theta'$, rewrite (7) as a system of first order ODEs.

3.1.6 Then, in order to compactify time, we change the "time variable" y to $s = \theta(y)$, and write $p(s) = \tilde{p}(y)$. Show that we get the following equation on p,

$$D\,p(s)\,p'(s) = c\,p(s) - \psi(s), \tag{8}$$

with the boundary conditions $p(0) = p(1) = 0$.

Our goal is now to study (8) with the condition $p(1) = 0$, and show that there exists a value of c for which the solution also satisfies $p(0) = 0$, as on Figure 4. To be able to do so, we make some further assumptions on the non-linear source term ψ. We assume there exists $\eta \in]0,1[$ such that $\psi(\theta) = 0$ for $\theta \in [0,\eta[$ and $\psi(\theta) > 0$ for $\theta \in [\eta,1[$, as well as $\psi(1) = 0$, $\psi'(1) = -\gamma$, with $\gamma > 0$ and finite. Such a function is represented in Figure 3. For the sake of simplicity, we will also take $D = 1$.

3.1.7 Using a Taylor expansion, determine $\alpha = p'(1)$ as a function of c and γ.

3.1.8 We first focus on the behavior of the solution on the interval $[\eta,1]$. For each given velocity c, can one find a profile p satisfying (8) on $[\eta,1]$? Show that p remains positive on $[\eta,1[$. Show

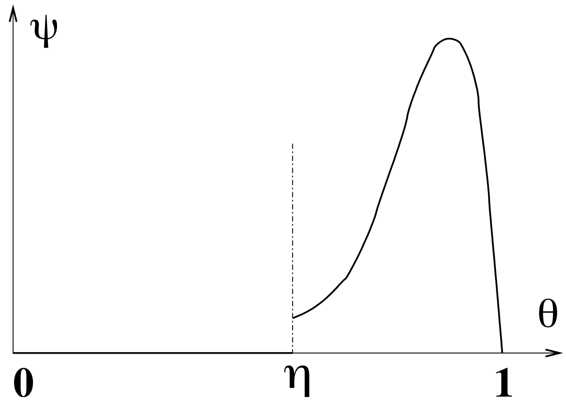

Figure 3: Structure of the non-linearity.

that the solution in this interval is a decreasing function of c. For $c = 0$, find an expression of the solution, denoted $\bar{p}$ as the value of $\bar{p}(\eta)$ as a function of $I = \int_0^1 \psi$.

3.1.9 Solve for the solution on the interval $[0, \eta[$. Prove the existence of a velocity c_0 such that there exist a continuous integral curve in the phase plane joining $(0, 0)$ and $(1, 0)$. This solution is denoted $p_0(\theta)$.

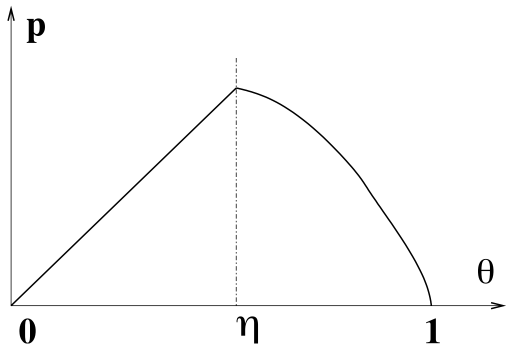

Figure 4: Phase space resolution of the wave profile.

3.2 BONUS: Flame speed and its limit

The purpose of this final subsection is to study the flame speed and obtain its limit in the case $\eta \to 1$ with fixed I. We first obtain upper and lower bounds on the flame speed c_0 as a function of η, starting from $c_0 = \frac{p_0(\eta)}{\eta}$.

3.2.1 Show that $c_0 \leq \frac{\sqrt{2I}}{\eta}$.

In order to obtain a lower bound on the flame speed, we consider the solution $\underline{p}$ of the ODE :

$$\underline{p}' = c_0 - \psi(\theta)/\bar{p}(\theta)$$

on $\theta \in [\eta, 1]$ with $\underline{p}(1) = 0$, where $\bar{p}$ is the solution for $c = 0$ studied previously.

3.2.2 Show that $\underline{p}(\theta) \leq p_0(\theta)$ on $[\eta, 1]$.

3.2.3 Show that $\underline{p}(\eta) = \bar{p}(\eta) - (1 - \eta)c_0$. *Hint: in the equation for* $\underline{p}$*, use that* $\bar{p}\bar{p}' = -\psi$.

3.2.4 Putting together the results of the previous questions, show that

$$\sqrt{2I} \leq c_0 \leq \frac{\sqrt{2I}}{\eta}$$

3.2.4 Assuming that I remains constant as a function of η, can you describe the velocity of the flame as $\eta \to 1$? What can be said about the temperature profile? Does the temperature profile remain smooth? Plot it.

4 Simulation of traveling waves: Nagumo

In their original paper [4], the authors introduced a model describing the propagation of a virus through a reaction-diffusion PDE, and the first rigorous analysis of a stable traveling wave solution of a nonlinear reaction-diffusion equation. This equation, also called the Fisher equation was at the origin of several studies in the field and is related to a nonlinearity of monostable character [8]. Here we rather focus on a bistable case, with a cubic nonlinear term of as a limit of Nagumo type [3]:

$$\partial_t u - D\,\partial_x^2 u = k\,u^2(1-u), \tag{9}$$

for which we have presented a resolution during the course. We consider a 1D discretization with $N+1$ points on a $[-50, 50]$ region with homogeneous Neumann boundary conditions, for which we have negligible spatial discretization errors with respect to the ones coming from the numerical time integration.
The description of the dimensionless model and the structure of the exact solution can be found in [3], where a change of variable

$$\tau = kt, \qquad r = (k/D)^{1/2}x, \tag{10}$$

allows to characterize the velocity of the wavefront:

$$c \propto (Dk)^{1/2}, \tag{11}$$

whereas the sharpness of the wave profile is measured by

$$\mathrm{d}_x u|_{\max} \propto (k/D)^{1/2}. \tag{12}$$

In the case of $D = 1$ and $k = 1$, the velocity of the self-similar traveling wave is $c = 1/\sqrt{2}$ in (11) and the maximum gradient value reaches $1/\sqrt{32}$ in (12). The key point of this illustration is that the velocity of the traveling wave is proportional to $(k\,D)^{1/2}$, whereas the maximum gradient is proportional to $(k/D)^{1/2}$. Hence, we consider the case $kD = 1$, for which one may obtain steeper gradients with the same speed of propagation. The resolution of the semi-discretized version of the PDE in space is conducted using a combination of operator splitting with Strang formula, and of ROCK4 and RADAU5 for the various sub-steps dedicated to respectively diffusion and source.

4.1 Explain the influence of the two coefficients k and D on the stiffness of the system itself, and on the sharpness of the solution.

4.1 Propose a simulation, where the initial condition is taken as the exact traveling wave solution (without boundary condition nor space discretization), for a time interval of $[0, 50]$. In order to conduct a analysis of the splitting error, to what profile do you compare your simulation? Explain why you will have to propose a very fine simulation of the full coupled dynamics using RADAU5 for the whole system versus comparing to the exact solution of the original PDE on the full real line.

4.3 Evaluate the wave speed and wave profile in the phase space compared to the exact one, for several splitting time steps, whereas the evaluation through ROCK4 and RADAU5 of the various sub-steps are resolved with a small tolerance, so as to obtain a pure splitting error. Conduct this experiment for $D = 1$ and $k = 1$ and for $D = 0.1$ and $k = 10$. What is the influence of this parameters on the results?

4.4 Conclude on the ability of the proposed strategy to resolve the wave.

5 Simulation of Turing pattern

In this section we focus on the simulation of Turing patterns [7, 1, 5], using again the Brusselator model as an example. Incorporating a spatial component into the ODE model we have studied up to now naturally gives the following reaction-diffusion system:

$$\begin{cases} \partial_t y_1 = d_1 \partial_x^2 y_1 + a - (b+1)y_1 + y_1^2 y_2 \\ \partial_t y_2 = d_2 \partial_x^2 y_2 + b\, y_1 - y_1^2 y_2, \end{cases} \tag{13}$$

where the space variable x is one-dimensional an belongs to the interval $[0, L]$. This system is complemented with Neumann boundary conditions and initial data at $t = 0$. It will be convenient to use the following notations

$$y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad D = \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix}, \quad f(y) = \begin{pmatrix} a - (b+1)y_1 + y_1^2 y_2 \\ b\, y_1 - y_1^2 y_2 \end{pmatrix},$$

which allows us to rewrite the system in a more compact form

$$\partial_t y = D \partial_x^2 y + f(y).$$

5.1 Recall the stability analysis that was done, for the homogeneous system (i.e. when solutions do not depend on x), in the previous PC around the equilibrium $y_{eq} = (a, b/a)$. In particular, under what condition on a and b was this equilibrium stable? We assume that this condition is satisfied for the rest of this exercise.

5.2 Consider a perturbation of the form

$$y(t,x) = y_{eq} + z(t) \cos \frac{n\pi}{L} x, \quad n \in \mathbb{N}, \quad z(t) = \begin{pmatrix} z_1(t) \\ z_2(t) \end{pmatrix}, \quad \|z\| \ll 1,$$

and show that z approximately satisfies a linear ODE of the form $z'(t) = A_n z(t)$ (find A_n).

5.3 Study the spectrum of A_n, and give a pair of necessary and sufficient conditions on a, b, d_1 and d_2 under which A_n can have a positive eigenvalue (assuming n and L are well chosen). *You may want to introduce* $X = \left(\frac{n\pi}{L}\right)^2$.

5.4 For the rest of this exercise, we take $a = 2$ and $b = 3$. What is the stability of the homogeneous equilibrium y_{eq} in the ODE case? Check that if we also take $d_2 = 8d_1$, $d_1 > 0$, the conditions obtained in the previous question are satisfied, and show that the perturbation is then unstable if

$$\frac{L}{\pi\sqrt{2d_1}} < n < \frac{L}{\pi\sqrt{d_1}}. \tag{14}$$

5.5 We now make some experiments with $a = 2$, $b = 3$, $d_1 = 1$ and $d_2 = 8$. For $L = 3$, take as initial condition a small random perturbation of the equilibrium, and integrate (13) using the notebook. Interpret what you observe in term of the stability analysis that we just performed. Repeat the experiment with $L = 4$, and then with $L = 7$. Explain what you observe (change the final time if needed). For $L = 20$, which modes are supposed to be unstable? Experiment with initial data containing all the unstable frequencies and comment on the obtained results.

References

[1] I.R. Epstein and J.A. Pojman. *An Introduction to Nonlinear Chemical Dynamics.* Oxford University Press, 1998. Oscillations, Waves, Patterns and Chaos.

[2] D. A. Frank-Kamenetskii. Towards temperature distributions in a reaction vessel and the stationary theory of thermal explosion. *Doklady Akad. Nauk SSSR*, 18, 1938.

[3] P. Gray and S.K. Scott. *Chemical Oscillations and Instabilities.* Oxford Univ. Press, 1994.

[4] A.N. Kolmogoroff, I.G. Petrovsky, and N.S. Piscounoff. Etude de l'équation de la diffusion avec croissance de la quantité de matière et son application a un problème biologique. *Bulletin de l'Université d'état Moscou, Série Internationale Section A Mathématiques et Mécanique*, 1:1–25, 1937.

[5] H. Meinhardt. *The algorithmic beauty of sea shells.* The Virtual Laboratory. Springer-Verlag, Berlin, 1995.

[6] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery. *Numerical recipes.* Cambridge University Press, Cambridge, third edition, 2007. The art of scientific computing.

[7] A. M. Turing. The chemical basis of morphogenesis. *Philosophical Transactions of the Royal Society of London B: Biological Sciences*, 237(641):37–72, 1952.

[8] A.I. Volpert, V.A. Volpert, and V.A. Volpert. *Traveling Wave Solutions of Parabolic Systems.* American Mathematical Society, Providence, RI, 1994.

[9] Ya. B. Zel'dovich, G. I. Barenblatt, V. B. Librovich, and G. M. Makhviladze. *The mathematical theory of combustion and explosions.* Consultants Bureau [Plenum], New York, 1985. Translated from the Russian by Donald H. McNeill.