JOURNAL OF COMPUTATIONAL PHYSICS 17, 79–86 (1975)

Direct Evaluation of Branching Points for Equations Arising in the Theory of Explosions of Solid Explosives

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Received June 24, 1974

A novel method of evaluating the critical conditions of an explosive is suggested. The method is straightforward and can be used for any arbitrary geometry of the explosive body. The advantage of this method is that the technique can be easily applied to other branching problems arising in hydrodynamics, reaction kinetics, electronics, combustion, etc.

1. INTRODUCTION

Solid explosive materials undergo self-heating as a result of a spontaneous exothermic decomposition reaction. If the heat conduction within the solid material and the Newtonian cooling of the geometrical surface is sufficiently high to compensate the heat generated by the chemical reaction, a stable low-temperature profile within the explosives is established. If the explosive body is too thick, the heat liberated cannot be dissipated by heat conduction and Newtonian cooling, and the reaction is accelerated by self-heating effect until an explosion occurs. The limiting conditions for which the stable low-temperature regime can be maintained are referred to as the critical explosion conditions.

A number of methods have been described in the literature to establish the estimates for critical conditions. Usually these methods make use of analytical solutions which can be found for a simplified temperature dependence of the reaction rate and for plate [1] and cylinder geometry [2]. For a correct Arrhenius temperature dependence the strongly nonlinear differential equations cannot be integrated analytically [1] and the branching points have been found by interpolation [3, 4]. However, in the vicinity of branching points there are inherent difficulties connected with the numerical evaluation of the solutions because the calculated profiles during the iteration process can oscillate between two possible solutions.

The goal of this paper is to devise a straightforward method which can be

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easily adopted to calculate the branching conditions for a differential equation describing temperature profiles within the explosive body. The method will be developed for a single nonlinear second-order ordinary differential equation, and hence generalization to other similar physical problems is obvious.

2. The Method

The technique proposed is based on the GPM algorithm developed by us recently [10]. For simplicity, consider a single second-order ordinary differential equation:

$$y'' = f(x, y, y', \delta), \tag{1}$$

subject to boundary conditions

$$\begin{aligned} \alpha_0 y(0) + \beta_0 y'(0) &= \gamma_0 , \\ \alpha_1 y(1) + \beta_1 y'(1) &= \gamma_1 . \end{aligned} \tag{2}$$

To solve Eq. (1) by the shooting method,

$$y(0) = \eta \tag{3}$$

must be guessed. For $y'(0)$ we obtain ($\beta_0 \neq 0$)

$$y'(0) = (1/\beta_0)[\gamma_0 - \alpha_0 \eta]. \tag{4}$$

After denoting

$$\Omega_1 = \partial y / \partial \eta, \tag{5}$$

differentiation of Eq. (1) with respect to η yields:

$$\Omega_1'' = (\partial f / \partial y)\, \Omega_1 + (\partial f / \partial y')\, \Omega_1'. \tag{6}$$

Equations (3) and (4) yield for initial conditions $\Omega_1(0)$ and $\Omega_1'(0)$:

$$\Omega_1(0) = 1, \qquad \Omega_1'(0) = -(\alpha_0/\beta_0). \tag{7}$$

Using the notation

$$\psi = \partial y / \partial \delta, \tag{8}$$

differentiation of Eq. (1) with respect to δ gives rise to:

$$\psi'' = (\partial f / \partial y)\, \psi + (\partial f / \partial y')\, \psi' + (\partial f / \partial \delta). \tag{9}$$

The relevant initial conditions are

$$\psi(0) = \psi'(0) = 0. \tag{10}$$

For a correct guess $y(0) = \eta$ the marching integration of Eq. (1) yields:

$$F_1(\eta, \delta) = \alpha_1 y(1, \eta, \delta) + \beta_1 y'(1, \eta, \delta) - \gamma_1 = 0. \tag{11}$$

Obviously, the solution of the particular initial-value problem, $y(x, \eta, \delta)$, depends both on the guess η and on the value of the parameter δ.

Making use of these variables, the branching points can be readily evaluated. The condition for branching is:

$$\frac{d\delta}{d\eta} = -\frac{\partial F_1/\partial\eta}{\partial F_1/\partial\delta} = -\frac{\alpha_1\Omega_1(1, \eta, \delta) + \beta_1\Omega_1'(1, \eta, \delta)}{\alpha_1\psi(1, \eta, \delta) + \beta_1\psi'(1, \eta, \delta)} = 0. \tag{12}$$

Equation (12) can be rewritten to:

$$F_2(\eta, \delta) = \alpha_1\Omega_1(1, \eta, \delta) + \beta_1\Omega_1'(1, \eta, \delta) = 0. \tag{13}$$

Evidently, to establish the branching points two nonlinear equations, Eqs. (11) and (13), must be solved simultaneously. Using the Newton–Raphson method we have:

$$\begin{pmatrix}\eta^{k+1}\\ \delta^{k+1}\end{pmatrix} = \begin{pmatrix}\eta^{k}\\ \delta^{k}\end{pmatrix} - \Gamma_F^{-1}(\eta^k, \delta^k)\, F(\eta^k, \delta^k), \tag{14}$$

where $F = (F_1, F_2)^T$ and Γ_F is the Jacobian matrix

$$\Gamma_F = \begin{pmatrix} \dfrac{\partial F_1}{\partial\eta} & \dfrac{\partial F_1}{\partial\delta} \\ \dfrac{\partial F_2}{\partial\eta} & \dfrac{\partial F_2}{\partial\delta} \end{pmatrix}. \tag{15}$$

Clearly,

$$\partial F_1/\partial\eta = \alpha_1\Omega_1(1, \eta, \delta) + \beta_1\Omega_1'(1, \eta, \delta), \tag{16a}$$

$$\partial F_1/\partial\delta = \alpha_1\psi(1, \eta, \delta) + \beta_1\psi'(1, \eta, \delta). \tag{16b}$$

To evaluate the derivatives $\partial F_2/\partial\eta$ and $\partial F_2/\partial\delta$ the relevant auxiliary differential equations must be developed.

On denoting

$$\Omega_2 = \partial^2 y/\partial\eta^2 \qquad \text{and} \qquad \varphi = \partial^2 y/\partial\eta\,\partial\delta,$$

differentiation of Eq. (6) with respect to η yields

$$\Omega_2'' = (\partial f/\partial y)\,\Omega_2 + (\partial^2 f/\partial y^2)(\Omega_1)^2 + 2(\partial^2 f/\partial y\,\partial y')\,\Omega_1\Omega_1' + (\partial f/\partial y')\,\Omega_2' + (\partial^2 f/\partial(y')^2)(\Omega_1')^2, \tag{17}$$

$$\Omega_2(0) = \Omega_2'(0) = 0, \tag{18}$$

and differentiation of Eq. (6) with respect to δ gives rise to

$$\varphi'' = (\partial f/\partial y)\,\varphi + (\partial^2 f/\partial y^2)\,\psi\Omega_1 + (\partial^2 f/\partial y\,\partial y')[\psi'\Omega_1 + \Omega_1'\psi] + (\partial^2 f/\partial y\,\partial\delta)\,\Omega_1 + (\partial f/\partial y')\,\varphi' + (\partial^2 f/\partial(y')^2)\,\Omega_1'\psi' + (\partial^2 f/\partial y'\,\partial\delta)\,\Omega_1', \tag{19}$$

$$\varphi(0) = \varphi'(0) = 0. \tag{20}$$

Differentiation of Eq. (13) yields

$$\partial F_2/\partial\eta = \alpha_1\Omega_2(1, \eta, \delta) + \beta_1\Omega_2'(1, \eta, \delta), \tag{21a}$$

$$\partial F_2/\partial\delta = \alpha_1\varphi(1, \eta, \delta) + \beta_1\varphi'(1, \eta, \delta). \tag{21b}$$

3. Evaluation of Critical Conditions of Explosion

The method described above may be easily used to establish the conditions of explosion.

The dimensionless steady state heat conduction equation with the zeroth order Arrhenius heat generation term is [1]:

$$\theta'' + (a/x)\,\theta' = -\delta\exp(\theta/(1 + \theta/\gamma)), \tag{1'}$$

$$x = 0 : \theta' = 0, \qquad x = 1 : \nu\theta + \theta' = 0. \tag{2'}$$

On denoting $R(\theta) = \exp(\theta/(1 + \theta/\gamma))$ and setting $y = \theta$, $\alpha_1 = \nu$, $\beta_1 = 1$, and $\gamma_1 = 0$ the following equations result.

$$\begin{aligned}\theta(0) &= \eta,\\ \theta'(0) &= 0,\end{aligned} \tag{3'}$$

$$\Omega_1'' + (a/x)\,\Omega_1' = -\delta R'(\theta)\,\Omega_1, \tag{6'}$$

$$\Omega_1(0) = 1, \qquad \Omega_1'(0) = 0, \tag{7'}$$

$$\psi'' + (a/x)\,\psi' = -R(\theta) - \delta R'(\theta)\,\psi, \tag{9'}$$

$$F_1(\eta, \delta) = \nu\theta(1, \eta, \delta) + \theta'(1, \eta, \delta) = 0, \tag{11'}$$

$$F_2(\eta, \delta) = \nu\Omega_1(1, \eta, \delta) + \Omega_1'(1, \eta, \delta) = 0, \tag{13'}$$

$$\Omega_2'' + (a/x)\,\Omega_2' = -\delta[R''(\theta)\,\Omega_1^2 + R'(\theta)\,\Omega_2], \tag{17'}$$

$$\varphi'' + (a/x)\,\varphi' = -R'(\theta)\,\Omega_1 - \delta[R''(\theta)\,\Omega_1\psi + R'(\theta)\,\varphi]. \tag{19'}$$

Equations (10), (14), (16), (18), (20), and (21) do not change. For the cylinder and sphere geometry, i.e., for $a = 1$ and $a = 2$, respectively, the ordinary differential equation (1′) contains a singular point for $x = 0$. The coefficient a/x, singular at $x = 0$, is cancelled by $\theta'(0) = 0$. At $x = 0$ Eq. (1′) must be written in the form $\theta'' = -\delta R(\theta)/(1 + a)$.

The initial-value problem given by (1′)–(3′), (6′), (9′), (17′), and (19′) can be integrated by the standard integration routines with the automatic step-size control, as e.g. Runge–Kutta–Merson, variable-order implicit Adams, etc.

The calculation of explosion conditions is as follows.

(1) Guess initial values of η^0 and δ^0, $k = 0$.

(2) Integrate a set of five second-order differential Eqs. (1′), (6′), (9′), (17′), and (19′) with initial conditions (3′), (7′), (10), (18), and (20) from $x = 0$ to $x = 1$. The values of $\theta(1, \eta^k, \delta^k)$, $\Omega_1(1, \eta^k, \delta^k)$, $\psi(1, \eta^k, \delta^k)$, $\Omega_2(1, \eta^k, \delta^k)$ and $\varphi(1, \eta^k, \delta^k)$ have been obtained.

(3) Evaluate the values of F_1, F_2 and Γ_F according to (11), (13), (16), and (21).

(4) Construct the next Newton approximation and test if the tolerance

$$|\eta^{k+1} - \eta^k| + |\delta^{k+1} - \delta^k| < \epsilon$$

is fulfilled. If not, set $k = k + 1$ and go to step 2.

A course of iteration is presented in Table I. The table reveals that from a relatively poor initial guess five iterations are sufficient to find the solution to four decimal places. Of course, the convergence properties of the Newton–Raphson method depend on the quality of the initial guess η^0 and δ^0. It can happen that for a very poor initial guess the first approximation to the solution, η^1 and δ^1, has no physical meaning, e.g., $\delta^1 < 0$, etc. Though the Newton method can also

TABLE I

Course of Iteration for $a = 2$, $\gamma = 10$, $\nu = 100$

k	0	1	2	3	4	5
η^k	1.5000	1.6760	2.0289	2.1160	2.1174	2.1174
δ^k	1.5000	3.3834	3.7697	3.6996	3.6997	3.6997
$\theta(1)$	0.7357	0.0993	0.0008	0.0254	0.0253	
$\theta'(1)$	−1.2719	−2.1305	−2.4815	−2.5327	−2.5337	
F_1	72.30	7.803	−2.4046	0.0023	−0.0000	
$\Omega_1(1)$	0.4972	0.1341	0.0174	0.0075	0.0072	
$\Omega_1'(1)$	−0.7156	−0.8030	−0.7299	−0.7210	−0.7208	
F_2	49.00	12.61	1.0113	0.0262	0.0001	
$\psi(1)$	−0.4240	−0.3148	−0.3291	−0.3423	−0.3424	
$\psi'(1)$	−0.5682	−0.2368	−0.1712	−0.1705	−0.1704	
$\Omega_2(1)$	−0.2096	−0.2287	−0.1948	−0.1894	−0.1893	
$\Omega_2'(1)$	−0.1686	0.0847	0.1729	0.1776	0.1777	
$\varphi(1)$	−0.2385	−0.1187	−0.0968	−0.0974	−0.0974	
$\varphi'(1)$	−0.1895	0.0461	0.0881	0.0936	0.0937	

TABLE II

Results for a Sequence of Values of ν, $a = 2$, $\gamma = 10$

	ν							
	100	50	20	10	5	2	1	0.5
η^0	1.5000	2.1174	2.1166	2.1109	2.0920	2.0282	1.8087	1.5992
δ^0	1.5000	3.6997	3.6270	3.4196	3.1076	2.5947	1.6639	1.0096
Number of iterations	5	3	3	3	4	4	4	4
η	2.1174	2.1166	2.1109	2.0920	2.0292	1.8087	1.5992	1.4489
δ	3.6997	3.6270	3.4196	3.1076	2.5947	1.6639	1.0096	0.5582

TABLE III

Critical Values for $\gamma = 40$

	plate ($a = 0$)		cylinder ($a = 1$)		sphere ($a = 2$)	
ν	δ	η	δ	η	δ	η
100	0.885	1.253	2.016	1.467	3.352	1.706
50	0.868	1.253	1.977	1.467	3.287	1.705
20	0.819	1.252	1.866	1.465	3.100	1.702
10	0.748	1.249	1.700	1.458	2.819	1.689
5	0.636	1.240	1.433	1.435	2.359	1.646
2	0.432	1.207	0.947	1.350	1.520	1.486
1	0.278	1.165	0.591	1.252	0.925	1.322
0.5	0.161	1.123	0.333	1.169	0.512	1.201

find in this event the domain of physically reasonable parameters it seems more convenient to select a new starting point. To enhance the economy of the method, the calculated values for a given value of ν can be used as the starting point for a new value of ν. Table II presents results calculated for a sequence of values of ν. Results for $\gamma = 40$ are summarized in Table III. Note that the value of η corresponds to the parameter $(\gamma\beta)^*$ in [3].

4. Conclusions

The method of direct evaluation of branching points can be easily used for a number of physically important equations. Let us mention a few of them: heat conduction, mass diffusion and a strong exothermic reaction occurring in a porous catalyst [5], axial heat and mass dispersion and a strong exothermic reaction in tubular reactors [6], equilibrium of neighboring drops at different potentials [7], breakdown of dielectrics [8], spiral flow in a porous pipe [11], combustion problems [12–14], evaluation of semiconductor device current characteristics [15], viscous heating in flow between moving surfaces [16], determination of the energy released in the nuclear reactor as a result of power excursion [17], etc. The method can be readily generalized to a set of ordinary differential equations. Since the "method of lines" [9] is capable of converting the elliptic partial differential equations to a set of ordinary differential equations, the method proposed can be used in a straightforward way to locate branching points in nonlinear elliptic equations.

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