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Rubrique

Finite element modeling of exothermic reaction with convective boundary conditions

Sous-titre

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ABSTRACT. In this work, we used a finite element method for the boundary value problem governing the ignition of a solid reactant undergoing slow oxidation in an arbitrary domain. We also investigate the effect of various parameters on the temperature distribution profiles.

RÉSUMÉ. Dans ce travail, nous avons utilisé une méthode des éléments finis pour le problème de la valeur limite régissant l'allumage d'un réactif solide qui subit une oxydation lente dans un domaine quelconque. Nous étudions aussi l'effet de différents paramètres sur les profils de distribution de température.

KEYWORDS : Finite element method, exothermic reaction, Biot number, Arrhenius kinetics.

MOTS-CLÉS : méthode des éléments finis, réaction exothermique, nombre de Biot, la cinétique d'Arrhenius.

1. Introduction

The problem of self-ignition of energetic materials is of great importance in the field of safe use and storage of explosives and pyrotechnics. The self -ignition occurs when an explosive substance is heated to a temperature sufficient for the decomposition process begins to produce significant exothermic effects. Then there is a release of heat, accompanied by a rise in temperature and velocity of thermal decomposition. This causes a thermal runaway generating an explosion that can sometimes produce a devastating detonation wave. These phenomena were first studied analytically and Frank-Kamenetskii [1] has developed the quasi-stationary theory of thermal explosion for determining the critical conditions for self-ignition of explosives.

Many problems of practical importance in ignition theory involve the definition and determination of either the critical ambient temperature or the critical initial temperature. These phenomena were first subject to analytical studies and Frank-Kamenetskii [I] developed the theory of quasi-stationary thermal explosion, which identifies the critical conditions for self-ignition of explosive substances.

After the pioneer work of Frank-Kamenetskii [1], various aspects of these

phenomena were studied intensively by many authors, including [2-6]. The book [7] contains a part of these investigations and a large bibliography.

When reactant consumption is neglected, the equation for the heat balance in a bounded domain Ω, can be written as:

$$k\Delta T + C_0 Q A \exp(-\frac{E}{RT}) = c\frac{\partial T}{\partial t} \qquad in\ \Omega \tag{1}$$

with the boundary condition

$$k\frac{\partial T}{\partial n} + H(T - T_a) = 0\ on\ \partial\Omega \tag{2}$$

Where k is the thermal conductivity, c is the thermal capacity, C_0 is the initial concentration of the reactant species assumed constant, Q is the heat of reaction.

According to the Arrhenius law, the dependence of the rate constant on the absolute temperature has the form $A\exp(-\frac{E}{RT})$, where E is the activation energy, R the universal gas constant. T_a is the ambient temperature, H is the heat transfer coefficient. $\frac{\partial T}{\partial n}$ is the normal derivative of the temperature, n is the outward normal vector on the boundary .

Following Balakrishnan et al [4], we introduce the following dimensionless variables in Eq. 1:

$$u = (\tfrac{E}{RT_a^2})(T - T_a), \varepsilon = (\tfrac{RT_a}{E}), Bi = \tfrac{Ha_0}{k}, \delta = \tfrac{Q\sigma AEa_0^2}{kRT_a^2}\exp(-\tfrac{E}{RT_a}).$$

and obtain the dimensionless governing equation together with the corresponding boundary conditions as:

$$\Delta u + \delta\exp(\frac{u}{1+\varepsilon u}) = 0 \qquad on\ \Omega \tag{3}$$

$$\frac{\partial u}{\partial n} + Biu = 0 \qquad on\ \partial\Omega \tag{4}$$

δ is the Frank-Kamenetskii parameter, Bi is the Biot number and a_0 is some characteristic length scale of the problem.

One of the commonly used formulation is the exponential approximation of Frank-Kamenetskii, in which ε is supposed so small to be neglected. So the problem (3-4) is reduced to the following nonlinear eigenvalue problem:

$$\begin{cases} \Delta u + \delta \exp(u) = 0 & x \in \Omega \\ \frac{\partial u}{\partial n} + Biu = 0 & x \in \partial\Omega \end{cases} \tag{5}$$

The problem (5) have been studied both analytically and numerically, for simple class A geometries (infinite cylinder, infinite slab, and a sphere) and also for some non class A geometries [4]. Thermal ignition in all these geometries can be formulated using a single variable [1, 4, 8-9].

Thermal stability analysis in the theory of thermal ignition, with or without consideration of consumption and diffusion of the reactant, has generally been performed using the Frank-Kamenetskii number as a parameter of bifurcation, ε is kept fixed. But this number dissimulates the role of the most practically significant control variable, namely the ambient temperature. Several authors [10-13] have assessed thermal ignition models with regard to multiplicity and stability of these steady states using the dimensionless ambient temperature.

In terms of the following dimensionless quantities:

$$u = \frac{RT}{E}, U = \frac{RT_a}{E}, \lambda = \frac{Ra_0^2 QC_0 A}{KE}$$

the governing steady state of heat balance are reduced to:

$$\begin{cases} \Delta u + \lambda \exp(-\frac{1}{u}) = 0 & x \in \Omega \\ \frac{\partial u}{\partial n} + Bi(u - U) = 0 & x \in \partial\Omega \end{cases} \tag{6}$$

The aim is to determine the critical value of U, say U_{crit}, beyond which multiple solutions of the problem (6) occur.

In this paper we first show how to use the finite element method to find an approximation of the solution of the problem (6). This can be done using a fixed point iteration method that we will describe below. Then, we deal with the study of the stability and bifurcation using the block Lanczos algorithm.

2. Computational method

2.1. Variational Formulation :

In this section we first derive a variational formulation of the boundary value problem (6) subject to Robin boundary condition.

We multiply the equation (6.1) by a test function $v \epsilon H^1(\Omega)$ multiply, integrate and use Green's formula to obtain:

$$\int_\Omega \nabla u \nabla v \, dx + Bi \int_{\partial\Omega} uv dS + \int_\Omega \lambda \exp(-\frac{1}{u}) \, v dx = BiU \int_{\partial\Omega} v dS \quad , \quad \forall v \in H^1(\Omega) [7]$$

It is obvious that the left term of this expression is not a bilinear form. Therefore the Lax-Milgram theorem cannot be applied here.

To solve this problem, we must linearize the problem in order to bring the solution to a series of linear problem converging to the solution of the initial nonlinear problem. We have several approaches to deal with such problems in particular Picard method or Newton method.

2.2. Picard's method :

We briefly recall the principle of Picard's method (or successive iterations), which is a variant of the fixed-point method.

Let the matrix system:

$$Ku = f \qquad [8]$$

as a result of the finite element discretization of a non-linear problem, where K is the stiffness matrix, u the unknown vector and f the 'load vector'. K may be linear or not.

The residue R, which is defined by: $R = f - Ku$ is a measure of the distance from the solution.

The methods of solving nonlinear systems are all iterative. At every step, they calculate du , the solution increment defined by: $du = u^{i+1} - u^i$, where i is the index of the iteration.

One seeks the convergence of the system by successive approximations. This convergence can be measured by a standard of the increment or a norm of R. du residue, the solution increment can also be seen as a descent direction, down to the zero residue, i.e. to the solution.

The method of Picard is a fixed point method [14]. It is defined by:

$$K(u^i)u^{i+1} = f(u^i) \qquad given\, u^0 \qquad [9]$$

which can also be written as:

$$K(u^i)du = R(u^i)$$

for the solution increment du.

an accuracy of ε is required the process may be terminated by setting a criterion:

$$\max \|u^{i+} - u^i\| \prec \varepsilon$$

With $\| \, . \, \|$ is the Euclidian norm.

Rather than being recalculated at each iteration, the matrix K can be maintained constant over a number of sub-iterations.

At convergence, and if the solution exists, then it satisfies (8). The advantage of this method lies in the existence of a large enough radius of convergence that allows us not to worry too much about the initial approximation. In return, its convergence rate remains often too slow for practical applications of interest. We can then use a relaxation method speeding a little bit the scheme (9). The latter is defined as follows:

$$\begin{cases} K(u^i)u^* = f(u^i)\,, u^0 given \\ u^{i+1} = \alpha u^{i+1} + (1-\alpha)u^* \quad , 0 \leq \alpha \leq 1 \end{cases} \qquad [10]$$

2.3. Method of solution

After the choice of appropriate finite elements by a method adapted from discretization in space, the system of nonlinear equations resulting system (7) is solved using techniques such as Newton's method or the method of Picard.

The discrete problem arises as usual by restricting $V = H^1(\Omega)$ to a discrete space V_h according to some mesh with some element type. Similarly, we let u_d be the discrete solution, so the discrete nonlinear problem is then written as: find u_d such that:

$$F(u_d, v) = L(v).$$

with $u_d = \sum_{j=1}^{N} \alpha_j \Phi_j$. Since F is a nonlinear function of u_d, the variational statement gives rise to a system of nonlinear algebraic equations. Picard's method can be used in alternative way for solving a nonlinear PDE problem.

We simply use a known, previous solution in the nonlinear terms so that these terms become linear in the unknown u_d.For our particular problem, we use a known, previous solution in the coefficient $e^{-\frac{1}{u}}$.

More precisely, given a solution u^k from iteration k, we seek a new (hopefully improved) solution u^{k+1} in iteration $k+1$ such that u^{k+1} solves the linear problem,

$$\begin{cases} \Delta u^{k+1} + \lambda \exp(-\frac{1}{u^k}) = 0 \qquad x \in \Omega \\ \frac{\partial u^{k+1}}{\partial n} + Bi(u^{k+1} - U) = 0 \quad x \in \partial\Omega \end{cases} \qquad [11]$$

The iterations require an initial guess u^0. The hope is that $u^k \longrightarrow u_d$ as $k \to \infty$, and that u^{k+1} is sufficiently close to the exact solution u_d of the discrete problem after just a few iterations.

We can easily formulate a variational problem for u^{k+1} from the last equation. Equivalently, we can approximate $e^{-\frac{1}{u}}$ to obtain the same linear variational problem. Therefore, the problem consists of seeking $u^{k+1} \epsilon V_h$ such that :

$$\text{a(u}^{k+1}, v) = L(v)\,, \quad \forall v \in V_h \qquad [12]$$

whith :

$$\begin{aligned} a(u^{k+1}, v) &= \int_\Omega \nabla u^{k+1} \nabla v \, dx + Bi \int_{\partial\Omega} u^{k+1} v dS \\ L(v) &= BiU \int_{\partial\Omega} v dS - \lambda \int_\Omega v \exp(-\tfrac{1}{u^k}) \, dx \end{aligned}$$

The iterations can be stopped when $\varepsilon = \| u^{k+1} - u^k \| \prec tol$ where tol is a small tolerance, or when the number of iterations exceed some critical limit. The latter case will pick up divergence of the method or unacceptable slow convergence.

Note that the existence and uniqueness of the solution of problem (12) is established through the Lax-Milgram theorem [15].

Thus, Picard's linearization reads as follows:

Find u^{k+1} such that :

$$\int_\Omega \nabla u^{k+1} \nabla v \, dx + Bi \int_{\partial\Omega} u^{k+1} \, v dS = BiU \int_{\partial\Omega} v dS - \lambda \int_\Omega v \exp(-\frac{1}{u^k}) \, dx \quad , \\ given \; u^0$$

2.4. Numerical results

In this section we first present the spatial discretization using finite element method with P1 continuous piecewise linear functions. Then we develop all the steps of the FreeFem++ code to solve the problem by using the technique of mesh adaptation and at the end we present some numerical results.

To discretize (12), let T_h denote a regular, quasi uniform triangulation of Ω with triangles of maximum size $h \prec 1$. Let $V_h = \left\{ v_h \in C^0(_\Omega), v_{h/T} \in P_1(T), \forall T \in T_h \right\}$ denote a finite dimensional subspace of $H^1(\Omega)$ where P_1 is the set of polynomials of degrees ≤ 1 .

Let Ω be the rectangle $[0,1] \times [0,1]$, the triangulation T_h of Ω is automatically generated by using a FreeFem command (Figure1) .

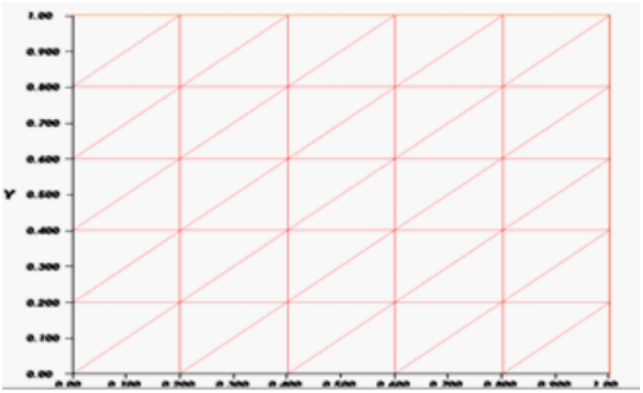


Figure 1 : mesh Th.

In Figures 2-4, we present the evolution of the temperature profiles according to different parameters (λ, U, Bi).

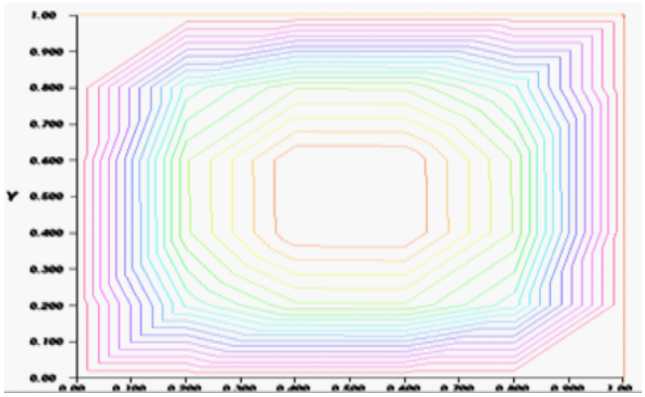


Figure 2 : Temperature distribution profile for λ = 1, U = 1, Bi = 1.

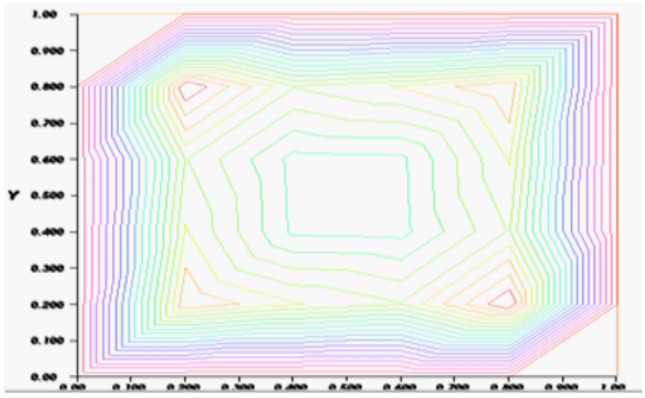


Figure 3 : Temperature distribution profile for λ =10, U = 10, Bi = 1000.

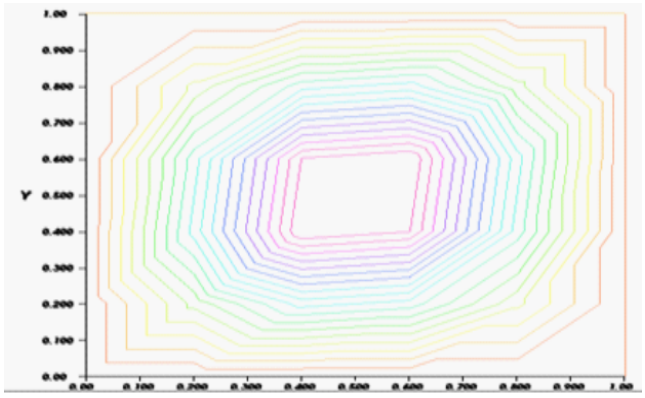


Figure 4 : Temperature distribution profile for λ= 9, U = 1, Bi = 1.

These solutions are in agreement with those obtaind by Balakrishnan et al. [4] by means of the shape factor method based on finite difference approximation.

3. Conclusion

Analysis has been carried out for steady state of exothermic chemical reaction of combustible material, in an arbitrary domain, with convective boundary conditions. The nonlinear PDE governing the problem are solved numerically using a FEM approach based on Picard's method. We have presented a numerical approach with FreeFem software, and we established the adequacy of the chosen finite element discretization by comparing the results with those of Balakrishnan et al. [4]. Thermal stability of such problems remains to be investigated. This can be undertaken using methods such as block Lanczos algorithm or Hermite-Padé approximations.

4. References

[1] FRANK-KAMENETSKII, D.A, "Diffusion and heat transfer in chemical kinetics", *Plenum Press, New York*, 1969.

[2] BODDINGTON T., GRAY P., HARVEY D.I., "Thermal theory of spontaneous ignition: Criticality in bodies of arbitary shape", *Philos. l+uns. Royal Sot. of London A270, 467-506*, 1971.

[3] BODDINGTON T., GRAY P., WAKE G.C., "Criteria for thermal explosions with and without reactant consumption", *Proceedings of the Royal Soc. of London A367, 403-422*, 1977.

[4] BALAKRISHNAN, E., SWIFT, A., WAKE G.C., " Critical values for some nonclass A geometries in thermal ignition theory", *Math. Comput. Model. 24 (8), 1–10*, 1996.

[5] MAKINDE O.D., "Strongly exothermic explosions in a cylindrical pipe:a case study of series summation technique", *Mechanics Research Communications 32, 191–195*, 2005.

[6] ER-RIANI M., CHETEHOUNA K., "On the Critical behaviour of exothermic explosions in class A geometries", *Mathematical Problems in Engineering Vol 2011, Article ID 536056*, 2011.

[7] BEBERNES J., EBERLY D., "Mathematical problems from combustion theory", *Springer-Verlag, New York*, 1989.

[8] CHAMBRÉ P.L., "On the solution of the Poisson-Boltzmann equation with application to the theory of thermal explosions", *J. Chem. Phys. 20*, 1795.

[9] SCATTER M.., SWIFT A. , "Path following, critical points and shape factors", *Annals of Numerical Mathematics 1, 491-500*, 1994.

[10] BURNELL J.G., GRAHAM-EAGLE J.G., GRAY B. F., WAKE G.C. , "Determination of critical ambient temperatures for thermal ignition", *IMA J Appl Math 42 (2):147-154*, 1989.

[11] GRAY B.F., WAKE G.C. , "Critical initial conditions for thermal ignition", *Mathematical and Computer Modelling, 18 (8), 65-75*, 1993.

[12] GRAY B.F., WAKE G.C. , "Critical initial conditions for spontaneous thermal ignition.", *J. Chem. Soc., Faraday Trans., 94, 3613-3617*, 1998.

[13] SEXTON M.J., MACASKILL C., GRAY B.F. , "Thermal ignition in rectangular and triangular regions", *ANZIAM J. 42, C1283–C1304*, 2000.

[14] REDDY J.N., GARTLING D.K. , "The Finite Element Method in Heat Transfer and Fluid Dynamics", *CRC Press*, 2010.

[15] DANERS D. "Robin boundary value problems on arbitrary domains, Trans", *Amer. Math Soc. 352, (9), 4207–4236*, 2000.