# Note

# Application of a Semi-implicit Finite Difference Scheme to Heat Generation in Explosives

## 1. INTRODUCTION

Materials that undergo exothermic chemical decomposition reactions can exhibit self-heating phenomena. At steady state the heat lost by conduction and/or convection is just balanced by the heat generated; however, above a certain critical temperature more heat will be generated than can be removed by these means and the temperature will increase to ignition or explosion [1–5]. When the primary heat loss mechanism is conduction and the chemical reaction is first-order the paper of Frank-Kamenetzky [1] is the definitive work for determination of the critical temperature. Zinn and Mader [6] carried out numerical calculations on the time dependent problem to determine the induction time (time to explosion) for slab, cylindrical, and spherical geometries exposed to a surrounding temperature above critical, however their procedure is not applicable to situations involving nonlinear thermal properties, phase changes, or time dependent boundary conditions. In the present note the application of a recently introduced symmetric semi-implicit (SSI) finite difference scheme [7] to the problems of internal heat generation and thermal initiation of explosion is reported.

## 2. THE SSI SCHEME

The heat conduction equation with internal heat generation is given by

$$\rho C(\partial u/\partial t) = \lambda \nabla^2 u + H(u) \tag{1}$$

where $u$ is the temperature, $\lambda$ the thermal conductivity, $\rho$ the density, $C$ the heat capacity, and $H(u)$ the rate of heat generation. Writing (1) in the SSI scheme of Livne and Glasner [7] for the cell $(i)$.

$$\rho C V_i(u_i^{j+1} - u_i^j)/\Delta t = -\sum_k J_{ik} A_{ik} + H(u_i^j) V_i + q_i \tag{2}$$

where $J_{ik}$ is the heat flux from cell $(i)$ to $(k)$, $A_{ik}$ is the area bounding the $(i)$ and $(k)$ cells, $V_i$ is the volume of cell $(i)$, $u_i^{j+1}$ is its temperature at the end of the time step $\Delta t$ and $u_i^j$ its temperature at the beginning of the time step. The term $q_i$ is needed to

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exactly conserve energy [7] at the interface between cell $(i)$ and its neighbors. For one independent spacial variable in plane, cylindrical or spherical symmetry,

$$J_{i,k} = -\lambda(u_k^j - u_i^{j+1})/\Delta x \qquad (3)$$

and after summing over cells $(k)$ adjacent to $(i)$ as indicated in Eq. (2),

$$q_i = (\lambda/2\,\Delta x)[(u_{i+1}^j + u_i^j - u_{i+1}^{j-1} - u_i^{j-1})\,A_{i,i+1} + (u_{i-1}^j + u_i^j - u_{i-1}^{j-1} - u_i^{j-1})\,A_{i,i-1}] \qquad (4)$$

where $u_k^{j-1}$ is the temperature of the cell $(k)$ at the time step prior to that indicated by $u_k^j$. Defining the geometric factors

$$G_{i\pm} = A_{i,i\pm1}\,\Delta x/V_i$$

and the Fourier number

$$F = \lambda\,\Delta t/\rho C\,\Delta x^2$$

some algebra yields,

$$u_i^{j+1} = \frac{F(u_{i+1}^j G_{i+} + u_{i-1}^j G_{i-}) + h_i + Q_i + u_i^j}{1 + F(G_{i+} + G_{i-})} \qquad (5)$$

where the thermal properties are considered constant,

$$h_i = (\Delta t/\rho C)\,H(u_i^j)$$

and

$$Q_i = (F/2)[u_{i+1}^j + u_i^j - u_{i+1}^{j-1} - u_i^{j-1})\,G_{i+} + (u_{i-1}^j + u_i^j - u_{i-1}^{j-1} - u_i^{j-1})\,G_{i-}].$$

## 3. NUMERICAL EXAMPLE: CONSTANT HEAT ADDITION

The SSI scheme (5) was tested for the case of constant heat addition in a slab of RDX with half-thickness 1 cm. The physical properties of RDX are taken from [6]. The initial temperature of the slab was 300° K and the wall temperature was fixed at 300° K. The heat generation term was calculated from the data in [6] for a constant reaction temperature of 500° K. The temporal and spacial temperature distributions calculated by the SSI method are shown in Fig. 1 for Fourier Numbers of 1.56 and 3.90. The exact solution for this constant heat addition problem given by Carslaw and Jaeger [8] is also shown in Fig. 1 for comparison.
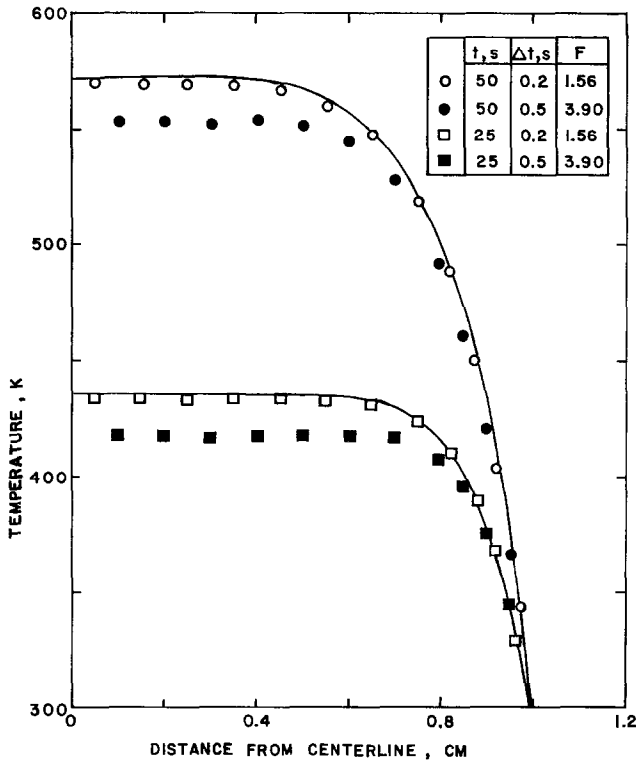
FIG. 1. Temperature profiles in a 1 cm half-thickness RDX slab with constant heat generation. Curves are exact solutions, symbols are present SSI scheme calculations.

## 4. NUMERICAL EXAMPLE: HEAT GENERATION BY FIRST-ORDER CHEMICAL REACTION

The SSI difference scheme was also tested for heat generation by first-order chemical reaction. For this case

$$H(u) = Q\rho Z \exp(-E/Ru)$$

where $Q$ is the heat of reaction, $Z$ is the Arrhenius pre-exponential frequency constant, $E$ is the activation energy, and $R$ the gas constant. Equation (5) was used to calculate the temperature profiles in 2.54 cm thick slabs and 2.54 cm diameter spheres of RDX beginning with the RDX uniformly at 300° K and the wall temperature $u_w$. The calculation advanced by time steps until a temperature reached 5000° K, at which point an explosion was considered to have been initiated and the induction time, $t_i$ recorded. The results are shown in Fig. 2, where they are compared with the numerical calculation of Zinn and Mader [6]. An explicit finite dif-
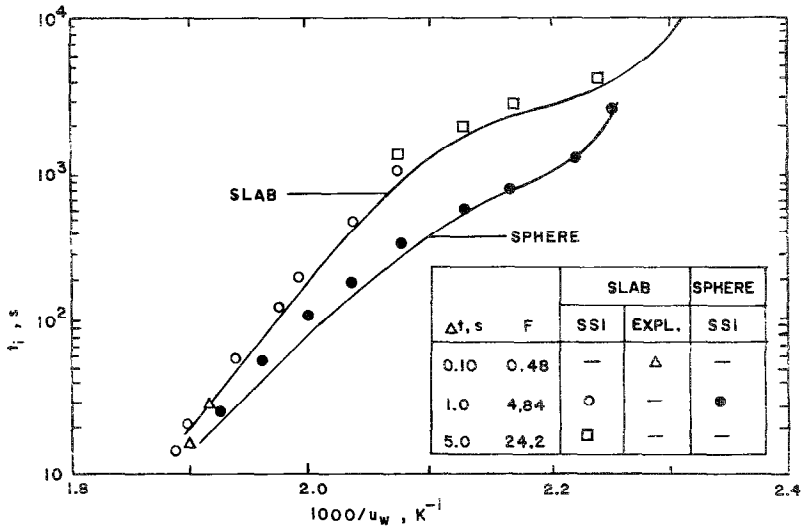
FIG 2. Induction time to explosion in 2.54 cm slabs and 2.54 cm diameter spheres of RDX. Curves are calculations of [6], symbols are present calculations.

ference scheme was also used to compute $t_i$ over the limited range for which it was practical. These results are also displayed on Fig. 2.

## 5. CONCLUSIONS

Experience with the SSI scheme has shown that the time step is limited in practice by the nature of the heat generation term. While the time step must, of course, be small compared to the induction time, steps up to 50 times greater than allowed for the explicit scheme can give sufficient accuracy. The SSI results compare well with the results of exact calculations, calculations using the explicit scheme, and with other work employing less flexible methods [6]. Even better results could be achieved if the heat addition term in Eq. (2) were forward centered in time by using $H(u_i^{j+1/2})$, where $u_i^{j+1/2} = (u_i^j + u_i^{j+1})/2$.

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JOHN W. SHELDON

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JOHN W. SHELDON

*Physics Department,*
*Florida International University,*
*Miami, Florida 33199*