

## MOVING BOUNDARIES - A NUMERICAL MODEL

S.-W. Kang

Lawrence Livermore National Laboratory  
P.O. Box 808  
Livermore, California 94550

FEMA Asilomar Conference  
May 30 - June 3, 1983

### ABSTRACT

A numerical model for time-dependent moving-boundary phenomena is constructed, with a view towards application of the method to calculation of the fire-spread characteristics in urban environments.

#### A. INTRODUCTION

Determination of the physical characteristics involved in the blast-propagation and the fire-spread phenomena during nuclear attack is important for civil defense programs in terms of planning and minimizing damages and casualties. A complete understanding of the phenomena will require concentrated and considerable time and effort. The enormous complexities involved in these phenomena have in the past necessitated a piece-meal approach to the problem.

The present paper investigates the possibility of a simplified approach on modelling the blast propagation and the fire-spread processes in terms of mathematical equations describing moving fronts. Across these fronts, there exist precipitous changes in the physico-chemical properties of the flow medium. The moving-boundary concepts have been previously applied to other situations, such as combustion problems, multi-phase problems and coal drying problems (Refs. 1-7). The present approach and the numerical code developed therefrom represent a first-approximation analysis, and hopefully these will be modified or expanded for a more detailed study in the future.

#### B. ANALYSIS

A time-dependent, one-dimensional (spherical, cylindrical, Cartesian) transport problem under the assumptions of "lumped" parameters in front of, and behind the moving fronts in the flow field is studied. These lumped physical parameters, such as thermal conductivity and density, need not be

constant with time. The governing equations describing the moving-front phenomena are the conservation equations of the global mass (or density), the constituent components, the momentum, and the thermal energy with appropriate boundary conditions (transient or steady).

The main thrust of the present analysis is to investigate the possibility of adapting the moving-front approach to the fire-spread and the blast-propagation history under nuclear-attack situations; therefore, the conservation equations mentioned above may not be directly applicable. Nevertheless, these equations form a basis for exploring the feasibility of model adaptation to the problems of present interest. For the sake of completeness and illustration, the relevant conservation equations specialized to the spherical coordinate system are included below.

Global mass conservation:

$$\frac{\partial \rho}{\partial t} = - \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 V_r \rho)$$

Component conservation:

$$\frac{\partial S_i}{\partial t} = - \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 V_r S_i) + \phi_i$$

Momentum conservation:

$$\rho \frac{DV_r}{Dt} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \bar{\mu} \frac{\partial V_r}{\partial r}) - \frac{\partial p}{\partial r}$$

Energy conservation:

$$\bar{\rho} \frac{\partial T}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} (r^2 \bar{k} \frac{\partial T}{\partial r}) - V_r (\sum_i S_i C_i) \frac{\partial T}{\partial r} + \sum_i \phi_i Q_i$$

where

$$\phi_i = \bar{W}_i - B_i/T.$$

The term  $\phi_i$  denotes the  $i$ -th component species production rate,  $\rho$  the global density of the medium,  $t$  the time,  $r$  the spherical radius,  $V_r$  the radial velocity,  $S_i$  the  $i$ -th component mass fraction,  $p$  the static pressure,  $T$  the temperature,  $\bar{k}$  the mean "thermal conductivity." This term may be regarded as one of the parameters to be appropriately used in considering fire-spread scenario. The term  $C_i$  denotes the specific heat of component  $i$ , and  $Q_i$  the heat release due to phase change of component  $i$ . The diffusion term in the component conservation equation is taken to be negligibly small in

comparison to the convective flux and the heat-generation effects in the present moving-front problem. In cases where the thermal-radiation effects are sizable, the radiation heat flux term can be added to the energy conservation equation. Other effects, where deemed important, can also be included in these equations.

In solving these equations, available numerical computer codes (Refs. 8-9) were utilized for describing a moving-front case in a semi-infinite region. This problem was chosen to demonstrate the versatility of the present approach in other coordinate systems in addition to the spherical conservation equations presented earlier. The results obtained are as follows.

### C. RESULTS AND DISCUSSION

The time-dependent moving front problem in a semi-infinite flow medium was solved with the following initial and boundary conditions and lumped property values. The term  $F(t)$  signifies the location of the moving front measured from  $X = 0$ , a boundary where we prescribe a sudden increase in temperature and maintains it at  $T_0$ . This high temperature, taken to be 1273 K in the present example, represents a source of thermal transport potential for the medium ( $0 \leq x < \infty$ ), generating a moving front and changes in the property values as the front (called "havoc front") moves inward from  $X = 0$  as a function of time. Other conditions used in the example are:

$0 \leq x \leq F(t)$ , i.e., behind the moving front;

$$\bar{k} = 1.1(10^3) \text{ [J/m - Sec - K]}$$

$$\overline{\rho c} = 1.3(10^6) \text{ [J/m}^3 \text{ - K]}$$

$F(t) < x < \infty$ , i.e., undisturbed region:

$$\bar{k} = 2.1(10^6) \text{ [J/m - Sec - K]}$$

$$\overline{\rho c} = 2.6(10^6) \text{ [J/m}^3 \text{ - K]}$$

$X = 0$ ;  $T = T_0 = 1273 \text{ K}$ ,  $Z = 0$

$$X \rightarrow \infty; T = T_\infty = 273 \text{ K}, Z = 1.0,$$

and the  $Q_i = 2(10^6) \text{ [J/kg]}$ , denoting the "latent" heat of phase change of the medium  $z$ . The "activation-energy barrier"  $B$  used was  $8(10^3) \text{ K}$  and the "reaction-rate coefficient"  $W$  was taken to be 10.0. The results obtained on LLL CRAY Computer are presented.

Figure 1 describes the temperature distributions as a function of time in a semi-infinite region, in which the boundary condition used was a constantly maintained temperature at a prescribed location in the field, (i.e.,  $X = 0$ ). At a certain critical value ( $T_c$ ) at  $400^\circ \text{ C}$ , the thermal properties were assumed to undergo precipitous changes, such as ablation, releasing or absorbing latent thermal energy in the process. This then delineates the "havoc front" characterizing the moving boundary in the field creating vastly

different transport phenomena in front of and behind the demarkation. The movement history of this havoc front ( $S_1$ ) is shown in Fig. 2.

In the present illustration, the havoc front may be considered to represent the fire-spread front, moving inward at a certain speed whose magnitude depends upon various thermodynamic properties and initial conditions used in the problem.

The present analysis can also generate a second havoc front along with the first front. This has potential application in the fire-spread studies where some materials may undergo radical property changes at a higher critical temperature ( $T_2$ ) than the lower critical temperature ( $T_C$ ) at which some fraction of the medium has already experienced drastic changes. Solutions were obtained for  $W = 90.0$ , and  $B = 3(10^4)$  K. This is shown in Fig. 3.

These results indicate that the moving front speed under prescribed boundary conditions (such as the temperature differential between  $X = 0$  boundary and  $X = \infty$ ) is a function of various thermodynamic properties of the medium. Of these, a dominant dependence of the movement speed on the "reaction term" in the component conservation equation was observed. In particular, the parameters  $W_i$  and  $B_i$  are identified as significant factors in determining the movement speed of the  $i$ -th component. This is illustrated in Fig. 4. The figure shows that a certain  $B_i - W_i$  combination exists for which the speed of the havoc front (i.e., fire spread front) is identical, but that change in either  $W_i$  or  $B_i$  produces change in the movement behavior. Specifically, increasing  $W_i$  for constant  $B_i$  brings about an increase in the front speeds. The magnitude of  $B_i$  (which may be regarded as an activation energy barrier) is indirectly related to the magnitude of the critical temperature, a thresh hold temperature for drastic change in the medium. Thus, Fig. 4 may be used as a guide in calibrating the movement speed for a given problem, where the critical temperature--and, therefore, the value of  $B$ --is inferred based on the makeup of the medium and the magnitude of  $W$  can be adjusted to fit experimental data. This  $W$ - $B$  pair then may be applied to other problems with comparable medium compositions in calculating the havoc-front movement history. It goes without saying that judicious choice of the various lumped property values is required in utilizing the approximate approach taken in the present analysis.

#### REFERENCES

1. Wilson, D. G. Solomon, A. D. and Boggs, P. T. Moving Boundary Problems, Academic Press, N.Y. (1978).
2. Sikarskie, D. I. and Boley, B. A. "The Solution of a Class of Two-Dimensional Melting and Solidification Problems," *Int. J. Solids Structures*, Vol. 1, pp. 207-234 (1965).
3. Crank, J. and Gupta, R. S., "Isotherm Migration Method in Two Dimensions," *Int. J. Heat Mass Transfer*, Vol. 18, pp. 1101-1107, (1975).
4. Tsang, T. H., "Modeling of Heat and Mass Transfer During Coal Block Gasification," Ph.D. Thesis, Univ. of Texas (1980).

5. Gregg, M. L. Campbell, J. H. and Taylor, J. R., "Laboratory and Modelling Investigation of a Colorado Oil-Shale Block heated to 900° C," Fuel, Vol. 60, pp. 179-188 (1981).
6. Kashiwa, B. A. and Harlow, F. H., "An Investigation of Simultaneous Heat and Mass Transfer in Subbituminous Coal," Proc. 15th Intersociety Energy Conversion Eng'g Conf., AIAA, Vol. 2, pp. 1311-1314, (1980).
7. Kang, S.-W. and Levatin, J. L., "Transient Boundary-Layer Flows in Combustion Environments," AIAA Paper 81-0349, AIAA 19th Aerospace Sciences Conf., January (1981).
8. Madsen, N. K., "PDEPACK User's Guide" Lawrence Livermore Nat'l Laboratory Report, UCIR-1027, March (1975).
9. Sincovec, R. F. and Madsen, N. K., "Software for Nonlinear Partial Differential Equations," ACM Trans. on Math Software, Vol. 1, No. 3, pp. 232-260, Sept. (1975).

FIGURE 1.

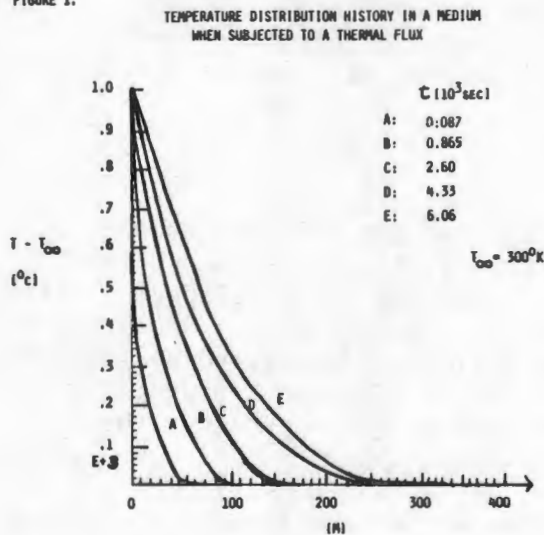


FIGURE 2.

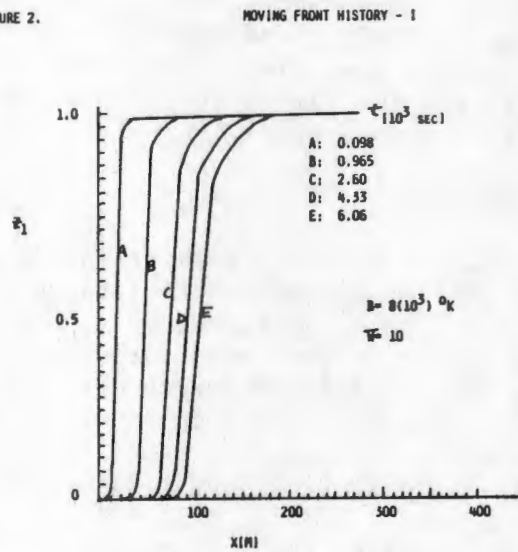


FIGURE 4. EFFECTS OF REACTION PARAMETERS ON MOVING FRONT SPEED

FIGURE 3.

