VAPORIZATION INTERFACE PROPAGATION THROUGH A ONE-DIMENSIONAL POROUS SLAB

By

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VAPORIZATION INTERFACE PROPAGATION

THROUGH A ONE-DIMENSIONAL

POROUS SLAB

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NOMENCLATURE

A	area
A_i	time dependent, Fourier cosine series coefficient i of the temperature approximation
a_i	rate constant for reaction i
C	mean specific heat
C_p	constant pressure specific heat
c	constant
E_i	activation energy for reaction i
G	heat flux parameter considered unity in this study (see Appendix I)
g	standard gravitational acceleration
g_c	gravitational dimension constant
h	enthalpy
h_{fg}	enthalpy of vaporization
K	thermal conductivity
L	slab thickness, between heated and insulated surfaces
ℓ	vaporization interface distance from insulated surface
N	one less than the number of coefficients used in the temperature approximation
P	pressure
Q	weighting function in x
q	heat flux

R	universal gas constant
T	temperature
t	time
u	internal energy
V	volume
v	velocity
$\hat{v}$	specific volume
x	slab distance from insulated surface
y_i	integrated value of derivative x_i

Greek Letters

α	thermal diffusivity
μ	integrating factor
ρ	density
τ_{xx}	viscous stress on the plane normal to the x axis in the x direction

Subscripts

A	actual
b	back (insulated) surface
D	dry region
i	index i = 0,1,2,...,N
ℓ	liquid
m	index m = 0,1,2,...,N
n	index n = 0,1,2,...,N
o	front (heated) surface
R	reference
s	solid
v	vapor

W wet region

z non-dimensionalization variable

Superscripts

′ differentiation with respect to x

‾ (bar) non-dimensional variable

- (minus) dry side of the vaporization interface

+ wet side of the vaporization interface

Note: A superscript bar is used to denote non-dimensional representation of the symbols as defined in Table I.

CHAPTER I

INTRODUCTION

For thousands of years man has known that wet logs do not burn as well as dry ones. He has also learned that liquids can be used effectively to douse certain unwanted fires. Man has thus studied the burning process for two opposing reasons. On one hand he has sought to improve this process as a tool for constructive uses and on the other hand he has sought to find ways to disrupt this process to protect himself from uncontrolled fires.

Since porous substances (such as wood, paper, fiber board, etc.) contain varying amounts of liquid when exposed to the natural environment, the burning of these materials is affected by the presence of this liquid. Yet, this extra-cellulosic liquid has been ignored in analytic studies of the thermal decomposition of porous materials. Considered as a fire retardant, the vaporization of a liquid possessing a high boiling point, a high latent heat of vaporization, and a relatively low thermal conductivity will reduce the overall temperature of the material in which it was saturated. Thereby the thermal decomposition will be retarded and the time to ignition of the substance will be increased.

It is advantageous, then, to study the effects caused by applying a heat flux to various substances initially saturated with some particular liquid. The calculation of the time required for the system to reach the temperature of vaporization of the liquid, the rate at which the

liquid-vapor interface propagates through the system, the temperature throughout the system, and time to ignition of the substance would aid considerably in the study of the burning process and fire retardation.

The Complete Problem

The time dependent temperature distribution within a saturated porous material (i.e. wood saturated with water) exposed to a heat flux may be calculated somewhat easily provided that the temperature distribution is not sufficiently high to cause vaporization of the liquid present or pyrolysis (thermal decomposition) of the material. If this condition on the temperature is not satisfied the problem of determining the temperature distribution becomes appreciably complicated and must include the endothermic process of vaporization and the endothermic or exothermic reactions of pyrolysis. A complete examination of the heating of a saturated porous material therefore would include determining the temperature distribution within the saturated material, the position and nature of the liquid-vapor interface as vaporization of the liquid progresses, the temperature distribution within the porous material after vaporization of the liquid initially present, and the pyrolysis and subsequent ignition of the material.

Division Into Cases of Study

Since wood is still one of the widest used porous materials and the thermal decomposition of wood closely follows that of cellulose, a reasonable choice of constitutents for this problem is cellulose and water. The thermal decomposition of cellulose has been shown to be minimal below 300° C (2,21). At standard pressure the vaporization of

water occurs at 100°C. Therefore, with the proper choice of material and liquid, decomposition of the porous material can be neglected below the temperature of vaporization of the liquid. The complete examination of the heating of a saturated porous material can then be divided into two cases, or areas, of investigation. The first case is the study of the temperature distribution within the porous material from the initial application of the heat flux up to and including the vaporization of the liquid and the propagation of the liquid-vapor interface through the material. The second case is comprised of the pyrolysis and ignition of the dried porous material remaining after vaporization of the liquid. The following sections briefly describe previous investigations of each case.

Pyrolysis and Ignition of a Porous Solid

The pyrolysis of wood has been studied both analytically and experimentally by Bamford, Crank and Malan (3). An infinite slab of wood was considered, symmetrically heated by a flame on each face. One exothermic reaction was included in the one-dimensional energy equation of the form

$$-q \frac{\partial \omega (x,t)}{\partial t}$$

where q is the heat liberated at constant pressure per gram of volatile products evolved, $\omega(x,t)$ is the weight of these products per cubic centimeter of wood. The rate of change of density (ω) with respect to time was represented by the Arrhenius expression

$$\frac{\partial \omega (x,t)}{\partial t} = k\omega \exp\ (-E/RT)$$

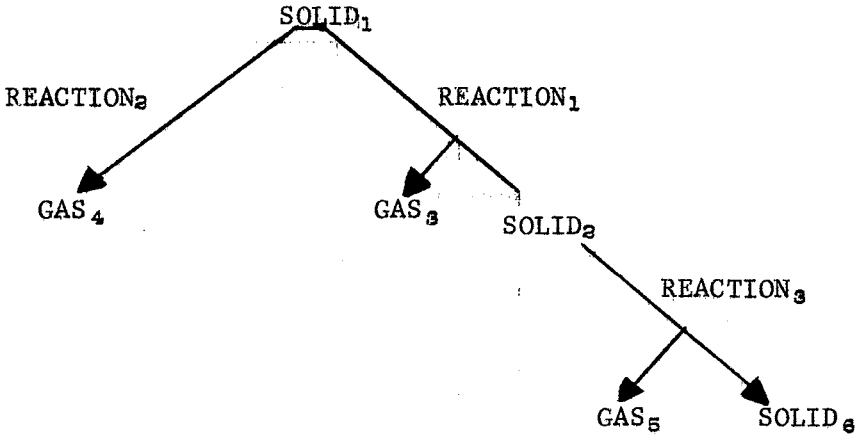
in which k is a frequency of molecular collision constant and E is the

activation energy of the reaction (assumed constant) (22). Although samples used in the experimental study contained moisture up to 11%, no additional endothermic reaction was included in the analytic study to represent the vaporization of extra-cellulosic moisture. The heat flux applied to the slab was considered a function of the surface temperature given by Fourier's Heat Conduction Law.

The analysis of a dry porous solid undergoing pyrolysis was substantially extended by Rittmann (21). Three chemical reactions were considered, two occurring simultaneously (competitive in nature) and two occurring consecutively (Figure 1). In the case of cellulose the first reaction is endothermic causing the pure cellulose to lose water and form a dehydrocellulose. This reaction was assumed to occur after vaporization of any extra-cellolosic moisture. Rittmann examined separately a time dependent, radiative heat flux and a constant, convective heat flux. Also the effect of a density dependent thermal conductivity was investigated.

One criteria for ignition of porous material (cellulose), which has been experimentally substantiated, is a temperature of approximately 600°C on the exposed surface of the slab. Martin (14) observed spontaneous-flaming ignition when the exposed surface of alpha-cellulose sheets reached a constant temperature in the range of 600° - 650° C. Alvares (1) employed optical temperature measurement techniques and obtained consistent temperatures of approximately 600° C on the exposed surface of alpha-cellulose at the onset of ignition regardless of the magnitude of the radiant heat flux.

Weatherford and Sheppard (25) examined the overall effects of various ignition criteria and the surface temperature histories of



Reactions 1 and 2 are competitive.

Reactions 1 and 3 are consecutive.

For Cellulose:

$Solid_1$	=	original cellulose
$Solid_2$	=	"dehydrocellulose"
Gas_3	=	water vapor
Gas_4	=	"tar" (levoglucosan)
Gas_5	=	CO, CO_2, H_2O, etc.
$Solid_6$	=	char

Figure 1. Pyrolysis Reactions in the Slab, Rittman (21)

finite-thickness slabs as opposed to the infinitely thick slab. The authors present a thermal feedback theory in which initial thermal energy received instantaneously at the surface of symmetry is visualized as moving back through the slab to the heated surface by a random self-diffusion process. This criteria is correlated with sustained ignitions which are dependent on the thickness of the slab. Alvares and Martin (2), conducting pyrolysis experiments on cellulose in "artificial airs" composed of different combinations of nitrogen, helium and carbon dipxide, have ruled out the concept that spontaneous ignition is triggered by the appearance of reactive species in the pyrolysis. Their hypothesis is one of thermal autoignition dependent on total pressure, oxidant concentration and inert diluent used.

The Change of Phase Phenomena

The change of phase phenomena is manifest in many physical processes involving heat transfer. The solidification of castings, freezing and thawing of soils and food stuffs, burning of liquid fuels, fusing of various metals, and the ablation process are a few examples. Literature pertaining to the analytic study of vaporization with consideration given to the location of the liquid-vapor interface is not readily available. Much work, however, has been done on the freezing and melting problem involving the location of the solid-liquid interface.

Muehlbauer and Sunderland (15) offer a comprehensive survey of publications dealing with the melting and freezing of infinite and semi-infinite slabs from Stephen's initial discussion of the problem

up to Moon and Keeler who use quantum mechanics to explain the electronics and phonon heat conduction between regions in contact.

Murray and Landis (16) review various methods of solution for the melting or freezing problem and propose two schemes for solution by finite difference approximations. One scheme is to divide the solid region into r equally sized space increments of

$$\Delta x_s = \frac{\epsilon}{r}$$

(where ϵ is the position of the interface) which increases as the freezing front progresses and a liquid region divided into N-r equally spaced intervals

$$\Delta x_L = \frac{E - \epsilon}{N - r}$$

(E being the length of the slab) which shrink with time. The second scheme is to have fixed "lump" sizes where the interface is in the q^{th} lump at some intermediate time. Two temperatures are calculated by interpolation from temperatures in the solid and liquid regions, respectively, using the fusion temperature and the fusion front location. The authors state that the variable space network is preferable for evaluation of the fusion front travel while the fixed space network is more convenient for temperature representation.

Both of the above methods produce two singularities within the finite difference equations when $\epsilon = 0$ and $E = \epsilon$. Therefore the problem must be started with an assumed initial value of ϵ and an assumed temperature distribution in the solid region. This procedure can lead to instability of the solution caused by very small numerical values or by a step input condition as a result of improper choice of initial temperatures. Lazaridis (12) presents a method to extend the finite

difference technique to multidimensional configurations. Longwell (13) developed a unique extention to the Schmidt graphical method. In solving the freezing problem the time for the interface to move a distance Δx is calculated by moving the interface a distance Δx , and then performing Schmidt constructions in each phase. The Newmann problem is solved by this method and compared to the exact solution with good agreement.

Goodman and Shea (10) assumed the applied heat flux at one surface of a semi-infinite slab was not immediately felt throughout the slab. A time dependent region extending from the surface into the slab was defined as the thermal-layer thickness. The heat conduction equation was then reduced by integrating over this defined region. This method of integral solution will only satisfy the original heat conduction equation on the average and is dependent on the time required for the thermal-layer to develop.

Scope of the Present Study

The object of this study is to develop an analytic model of the vaporization interface propagation and the temperature distribution within a semi-infinite, porous slab prior to pyrolysis. A constant, radiative heat flux is applied to the slab which is initially saturated with a liquid.

The semi-infinite slab is divided into two regions by the vaporization interface. Three energy balance equations are developed by application of the first law of thermodynamics to a differential volume in each region and at the interface then taking the limit as the thickness approaches zero. The integral method of reducing partial

differential equations is employed enabling the combination of the three energy equations into one.

By choosing $\cos n\pi\bar{x}$ for the weighting function and the Fourier cosine series to approximate the temperature, a system of ordinary first order differential equations is developed. This system of equations yields valid temperatures for any location within the slab. Hamming's modified predictor-corrector method of numerical integration is then used to solve this system of equations for the temperature coefficients and the interface distance.

As explained in Chapter II, the kinetic and potential energies of the system are assumed negligible. The densities and thermodynamic properties are assumed to be constant with the density and thermodynamic properties for the two component region calculated on a percent unit volume basis.

The analysis is developed for an idealized liquid and solid. The assumption is made that the thermodynamic properties of the liquid and solid are equal in each region as discussed in Chapter II. Complexities of solution and enhancements which might be incorporated in future investigations are mentioned. The resulting temperature profiles and the interface velocity are physically realistic. The coupling of this study with the analysis of chemical reactions can then be employed to solve the complete pyrolysis problem.

CHAPTER II

PROBLEM ANALYSIS

Physical Model

To model the heating of a saturated porous material without simplification is an extremely difficult task. The following factors might be considered in the analysis:

1. Environment of the model
2. Nature of the applied heat flux
3. Size and shape of the material
4. Variations in the thermodynamic properties
5. Representation of the pyrolysis reactions
6. Criteria to determine ignition
7. Representation of the vaporization process.

The model presented here is assumed to be of a semi-infinite, homogeneous (with respect to density and thermodynamic properties), porous slab of thickness L, initially saturated with a homogeneous liquid in thermodynamic equilibrium at a reference temperature (T_R). The front surface (x = L) is exposed to a constant, radiative heat flux (q_o) with the back surface (x = 0) insulated against heat transfer (Figure 2). This is similar to one-half a slab of thickness 2L symmetrically heated. Heat is transferred into the saturated slab from the surface by conduction. None of the radiant energy striking the slab is assumed to penetrate below the surface.

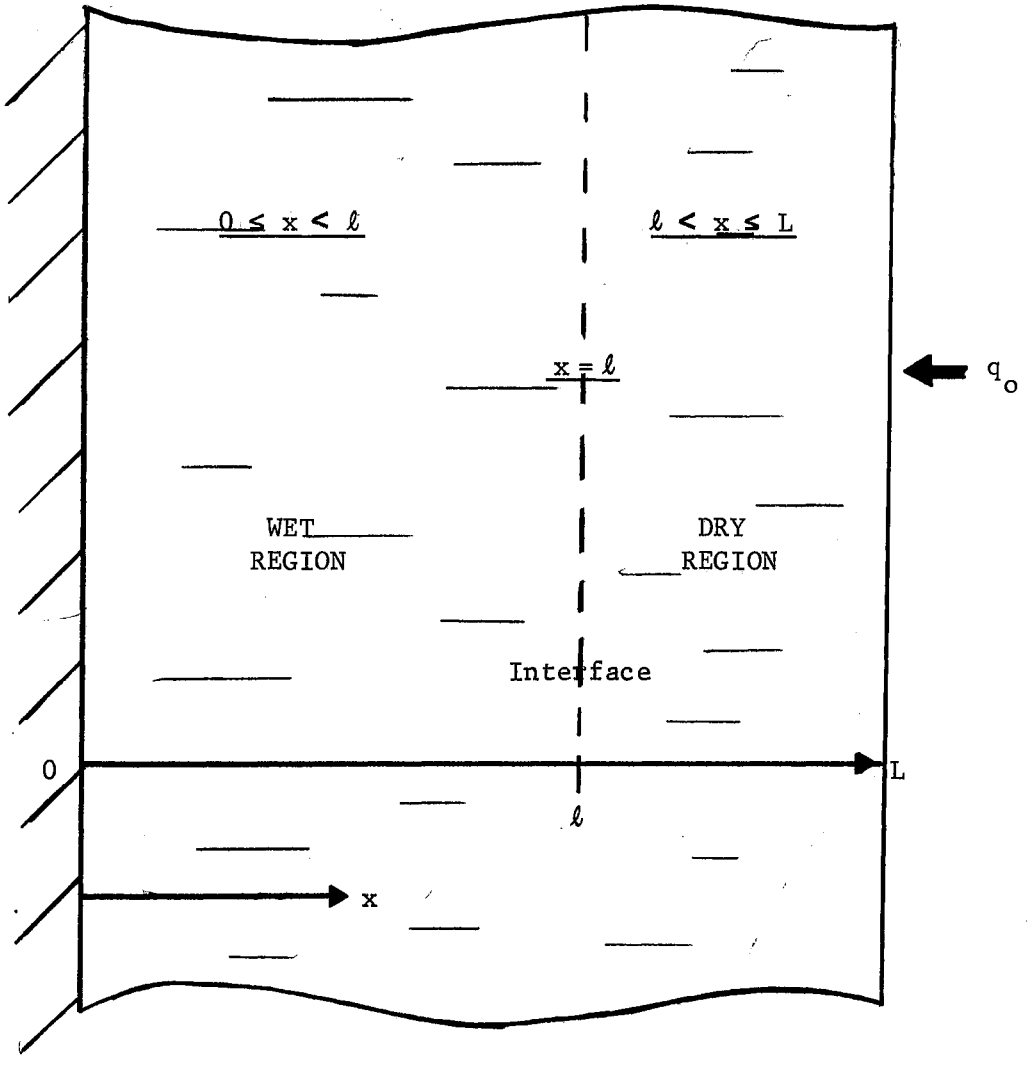


Figure 2. Physical Model

No ignition or chemical reaction of the porous slab is considered. Vaporization of the liquid is considered when the front surface has reached the temperature of vaporization (T_v) of the liquid. At this point in time, vaporization of the liquid is assumed to commence. Heat transfer from and the thermal capacitance of the vapor thus produced is neglected as it flows out through the pores of the slab.[1]

As the heat flux is continually applied the time dependent liquid-vapor interface proceeds into the slab in the -x direction, thereby dividing the slab into regions, a wetted region preceeding the interface and a dry region behind. The wetted region consequently shrinks with increasing time as the dry region expands. As stated previously the wetted region is considered non-reactant since its temperature will remain well below that which is necessary to cause significant chemical reaction provided the proper choice of solid and liquid is made.

The pyrolysis of the dry region (second case investigation) can be modeled after the extensive work of Rittmann (21). If the overall effects of pyrolysis leading to the ignition of the solid is of main interest a single endothermic or exothermic reaction will suffice in representing a lumped form of the pyrolysis as done by Bamford, Crank, and Malan (3).

Experimental and analytic research indicates that the ignition of the porous solid can be approximated as the point in time at which the front surface of the semi-infinite slab exceeds 600°C. Thus the effects, caused by the initial presence of a liquid, on the ignition

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[1] For a discussion of this assumption see Appendix A.

time of a porous solid can be directly related to the surface temperature. This investigation is left to future studies.

Energy Equation

The energy equation for a semi-infinite saturated slab is developed by writing an energy balance over a volume element $\Delta x \Delta y \Delta z$ in the x direction then taking the limit as these dimensions approach zero. Considering only the fluid, the following equation evolves from Figure 3.

$$\underset{\text{I}}{\frac{\partial}{\partial t}\rho_\ell\left[u_\ell + \tfrac{1}{2}v_\ell^2 + \frac{g}{g_c}z\right]} = \underset{\text{II}}{-\frac{\partial}{\partial x}\left(\rho_\ell v_\ell u_\ell\right)} \underset{\text{III}}{-\frac{\partial}{\partial x}\left(v_\ell \rho_\ell \frac{v_\ell^2}{2}\right)}$$

$$\underset{\text{IV}}{-\frac{\partial}{\partial x}q_\ell} + \underset{\text{V}}{\frac{\partial}{\partial x}\left(\rho_\ell \frac{g}{g_c} v_\ell z\right)}$$

$$\underset{\text{VI}}{-\frac{\partial}{\partial x}\left(\rho_\ell v_\ell\right)} \underset{\text{VII}}{-\frac{\partial}{\partial x}\left(\tau_{xx} v_\ell\right)} \qquad (2.1)$$

where

Term I = Rate of change of energy per unit volume.

Term II = Net rate of internal energy input per unit volume by convection.

Term III = Net rate of kinetic energy input per unit volume by convection.

Term IV = Net rate of energy input per unit volume by conduction.

Term V = Rate of work done on the fluid per unit volume by gravitational forces.

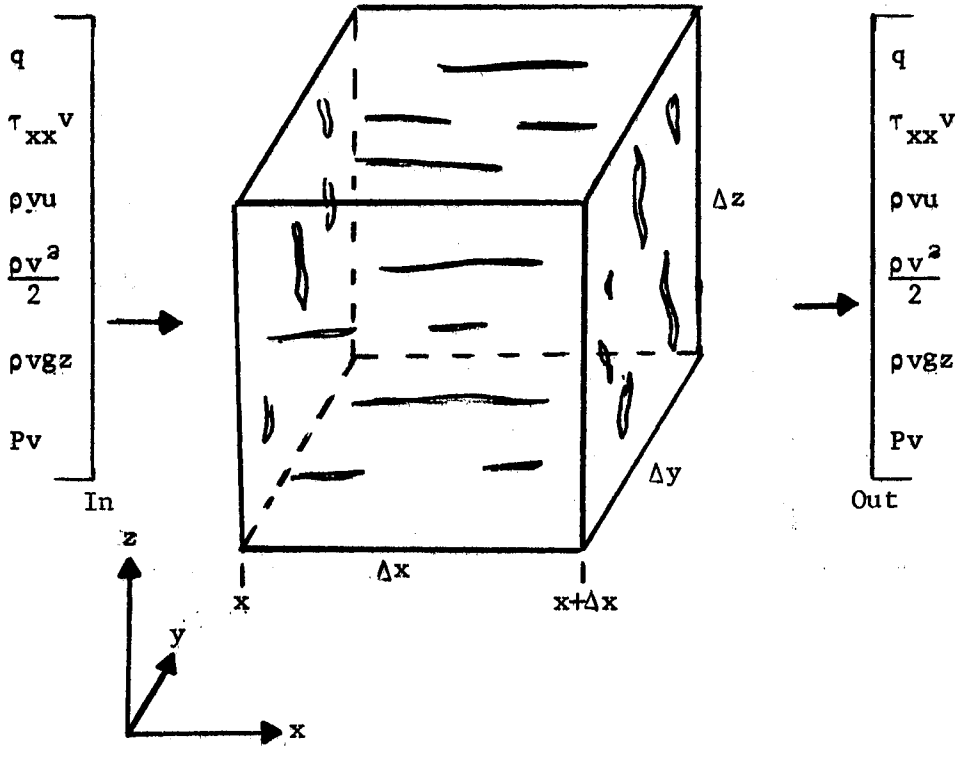

Figure 3. Volume Element of the Saturated Slab

Term VI = Rate of work done on the fluid per unit volume by pressure forces.

Term VII = Rate of work done on the fluid per unit volume by viscous forces.

The fluid flows in the x direction only, thus the potential energy is constant with a rate of change consequently equal to zero. The viscous forces are assumed to be negligible with the fluid velocity considered small. By combining pressure work, or flow work, with the internal energy term the differential equation of energy for the fluid is

$$\frac{\partial}{\partial t} \rho_\ell \left[u_\ell + \tfrac{1}{2} v_\ell^2 \right] = - \frac{\partial}{\partial x} \rho_\ell v_\ell \left[u_\ell + \frac{1}{\rho_\ell} P_\ell \right] - \frac{\partial}{\partial x} \rho_\ell v_\ell \frac{v_\ell^2}{2}$$

$$- \frac{\partial}{\partial x} q_\ell \qquad (2.2)$$

The solid being fixed in space gives rise to the following energy equation.

$$\underset{\text{I}}{\frac{\partial}{\partial t} \rho_s u_s} = \underset{\text{II}}{- \frac{\partial}{\partial x} q_s} \qquad (2.3)$$

Since again gravitational forces are constant and the solid is stationary.

Term I = Rate of change of the internal energy of the solid per unit volume.

Term II = Net rate of energy input per unit volume by conduction.

Combining the fluid and solid the composite energy equation is

$$\underset{\text{I}}{\frac{\partial}{\partial t} \rho_T u_T} + \underset{\text{II}}{\frac{\partial}{\partial t} \rho_\ell \tfrac{1}{2} v_\ell^2} = \underset{\text{III}}{- \frac{\partial}{\partial x} q_T} \underset{\text{IV}}{- \frac{\partial}{\partial x} \rho_\ell v_\ell \left[u_\ell + \frac{1}{\rho_\ell} P_\ell \right]}$$

$$\underset{\text{V}}{- \frac{\partial}{\partial x} \rho_\ell v_\ell \frac{v_\ell^2}{2}} \qquad (2.4)$$

Letting the internal energy be a function of temperature only

$$u = u(T)$$

Then

$$du = \left(\frac{\partial u}{\partial T}\right) dT = CdT$$

Differentiation of term I yields

$$\underset{\text{I}}{\rho_T c_T \frac{\partial T}{\partial t}} + \underset{\text{II}}{u_T \frac{\partial \rho_T}{\partial t}} + \underset{\text{III}}{\frac{\partial}{\partial t} \rho_\ell \tfrac{1}{2} v_\ell^2} = \underset{\text{IV}}{- \frac{\partial}{\partial x} q_T} \underset{\text{V}}{- \frac{\partial}{\partial x} \rho_\ell v_\ell \left[u_\ell + \frac{1}{\rho_\ell} P_\ell \right]}$$

$$\underset{\text{VI}}{- \frac{\partial}{\partial x} \rho_\ell v_\ell \frac{v_\ell^2}{2}} \qquad (2.5)$$

Term II in equation (2.5) the absorption or generation of thermal energy, is frequently represented by one or several chemical reactions of the form;

$$q_i \frac{\partial \rho_i}{\partial t} = q_i \rho_i a_i \exp \frac{-E_i}{RT}$$

where q_i is the latent heat liberated or absorbed, a_i is a maximum rate constant, E_i is the energy of activation required, and R is the universal gas constant. Many authors have shown this expression to closely approximate chemical reactions within the same order of magnitude as the energy change and conduction terms (I and III) of the energy equation (2.5).

If such a function is used to approximate the vaporization process the vaporization is then distributed throughout the slab (i.e. for any given temperature, some vaporization is attained). A plot of

$$q_v \frac{\partial \rho_\ell}{\partial t}$$

versus temperature (T_v) shows that the vaporization is distributed mainly between $T_v - \Delta T$ and $T_v + \Delta T$ (Figure 4).[a]

When vaporization is considered a surface occurrence, the density of the liquid becomes zero at some infinitely small distance Δx from the surface. Vaporization of a liquid also occurs at a constant temperature thus the vaporization process appears as plotted in Figure 5. To accomplish this the reaction rate of the function must be very high.

$$\lim_{\rho_\ell \to 0} \frac{\partial \rho_\ell}{\partial t} \to \infty$$

This would require the time associated with the approximation of

$$q_v \frac{\partial \rho_\ell}{\partial t}$$

to be very fast as compared to the time associated with the other reactions and terms in the energy equation.

In lieu of the above, the semi-infinite slab is modeled by dividing it into two regions separated by the liquid-vapor interface (Figure 2). The energy equation (2.5) is thus the summation of three energy balances, one applying to each region and one at the interface. The thermodynamic properties of each region considered constant within the range of temperatures to be encountered yields the following energy equations: For the wetted region ($0 \leq x < \ell$) the fluid is considered stationary with no generation or absorption of thermal energy. Therefore, energy equation (2.5) reduces to

$$\rho_W C_W \frac{\partial T}{\partial t} = - \frac{\partial}{\partial x} q_W$$

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[a] In this instance q_v represents the latent heat of vaporization, ρ_ℓ the density of the liquid, and T_v the temperature of vaporization.

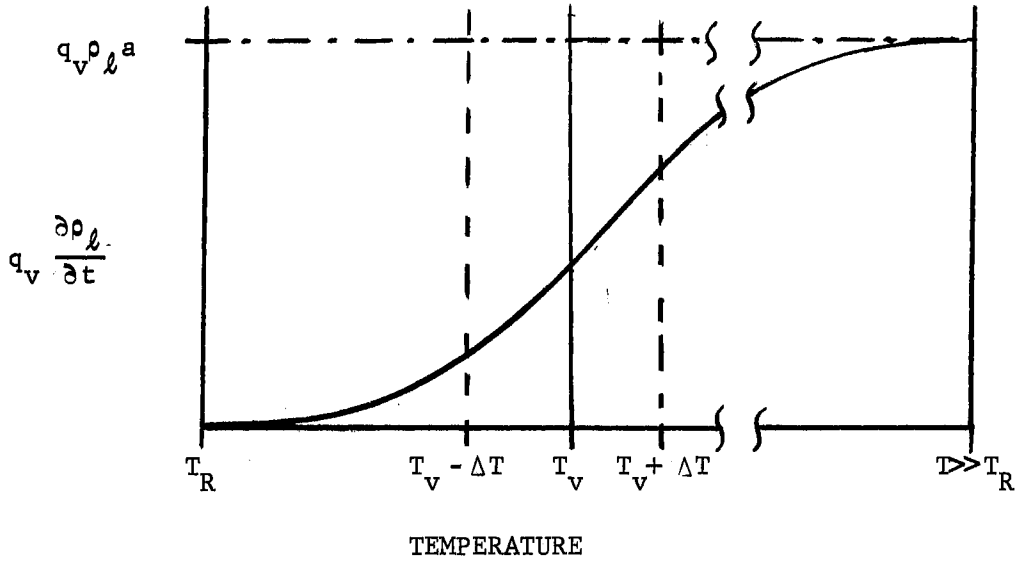

Figure 4. Vaporization Represented as a Chemical Reaction

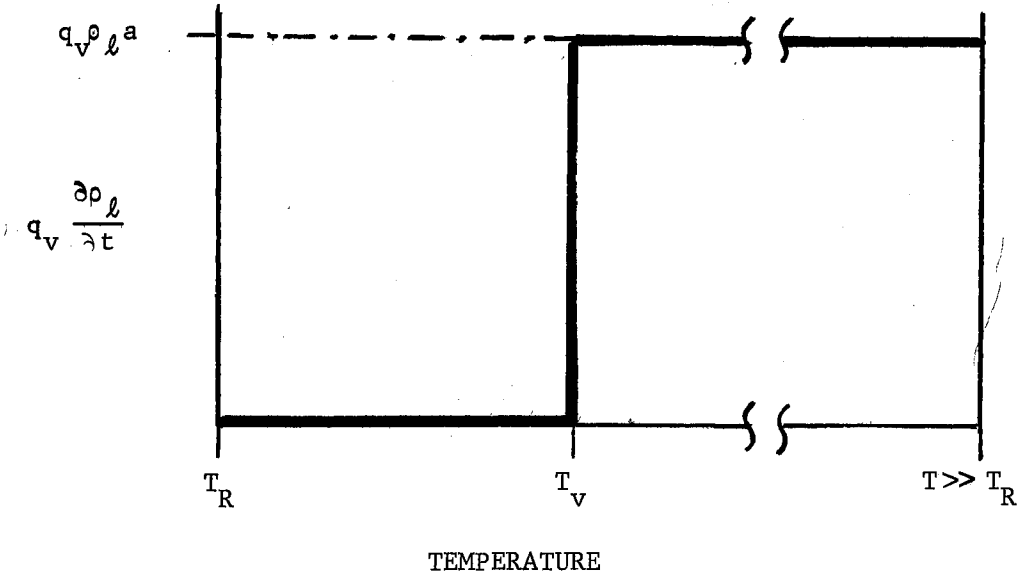

Figure 5. Vaporization Represented as a Surface Phenomena

Applying Fourier's Heat Conduction Law with the temperature gradient in the negative x direction yields

$$\rho_W C_W \frac{\partial T}{\partial t} = K_W \frac{\partial^2 T}{\partial x^2} \tag{2.6}$$

The internal energy, being an extensive thermodynamic property, is additive for a composite system.

$$u_W = u_s + u_\ell$$

differentiating

$$C_W dT = C_s dT + C_\ell dT$$

or

$$\rho_W V_W C_W = \rho_s V_s C_s + \rho_\ell V_\ell C_\ell$$

$$\rho_W C_W = \rho_s \frac{V_s}{V_W} C_s + \rho_\ell \frac{V_\ell}{V_W} C_\ell$$

For the dry region ($\ell < x \leq L$) including the generation or absorption of thermal energy from equation (2.5)

$$\rho_D C_D \frac{\partial T}{\partial t} + u_D \frac{\partial \rho_D}{\partial t} + \frac{\partial}{\partial t} \rho_v \tfrac{1}{2} v_v^2 = K_D \frac{\partial^2 T}{\partial x^2} + \frac{\partial}{\partial x} \rho_v v_v \left[u_v + \frac{1}{\rho_v} P_v \right]$$

I II III IV V

$$+ \frac{\partial}{\partial x} \rho_v v_v \frac{v_v^2}{2} \tag{2.7}$$

VI

Terms III and VI are kinetic energy terms. If the velocity of the vapor escaping is assumed small in magnitude these kinetic energy terms can be neglected. Term V can be rearranged as follows; since

$$\frac{1}{\rho_v} = \hat{v}_v \qquad \text{(specific volume)}$$

$$\frac{\partial}{\partial x} \rho_v v_v \left[u_v + \frac{1}{\rho_v} P_v \right] = \frac{\partial}{\partial x} \rho_v v_v \left[u_v + P_v \hat{v}_v \right]$$

from the definition of enthalpy

$$h = u + P\hat{v}$$

and

$$\frac{\partial}{\partial x} \rho_v v_v \left[u_v + P_v \hat{v}_v \right] = \frac{\partial}{\partial x} \rho_v v_v (h_v)$$

This term is then the thermal energy convected by the vapor as it flows through the dry region. The magnitude of which is discussed in Appendix A. This convection term is assumed of minimum consequence in this study. The heat capacity of the vapor is also assumed to be negligible in the final energy equation of the dry region. Thus the heat capacity of the dry region is assumed equal to that of the solid alone. Therefore, equation (2.7) is reduced to

$$\rho_D C_D \frac{\partial T}{\partial t} + u_D \frac{\partial \rho_D}{\partial t} = K_D \frac{\partial^2 T}{\partial x^2} \tag{2.8}$$

At the liquid-vapor interface ($x = \ell$) the volume element (Figure 3) is considered to move in the negative x direction with a velocity $d\ell/dt$. The mass flow of fluid entering this moving volume equals the mass flow of vapor leaving, thus satisfying mass conservation. The time rate of change of kinetic energy is assumed zero. Within this elemental volume the temperature is constant and the densities of the liquid and vapor are also assumed constant. Thus equation (2.5) reduces to

$$\frac{\partial}{\partial x} \rho_\ell \frac{d\ell}{dt} \left[u_\ell + \hat{v}_\ell P_\ell \right] = \frac{\partial}{\partial x} q$$

Integrating with respect to x yields

$$\rho_\ell h_{fg} \frac{d\ell}{dt} \Bigg|_{\ell^+}^{\ell^-} = q \Bigg|_{\ell^+}^{\ell^-}$$

or

$$\rho_{\ell} h_{fg} \frac{d\ell}{dt} \Bigg|_{\ell^+}^{\ell^-} = K_D \frac{\partial T}{\partial x} \Bigg|_{\ell^-} - K_W \frac{\partial T}{\partial x} \Bigg|_{\ell^+}$$

with the limit as the length $\Delta\ell$ approaches zero

$$\rho_{\ell} h_{fg} \frac{d\ell}{dt} = K_D \frac{\partial T}{\partial x} \Bigg|_{\ell^-} - K_W \frac{\partial T}{\partial x} \Bigg|_{\ell^+} \tag{2.9}$$

I II III

Term I = Rate of change of the internal energy of the liquid per unit volume plus the rate of work done on the fluid per unit volume by pressure forces.

Term II = Energy leaving the interface by conduction per unit volume.

Term III = Energy entering the interface by conduction per unit volume.

Initial and Boundary Conditions

Initially the saturated slab is at a constant temperature (T_R) throughout with an insulated boundary (back surface) at x = 0 and an exposed boundary (front surface) at x = L. The initial conditions at t = 0 are

$$T(x,0) = T_R \tag{2.10}$$

$$\rho_D C_D = \rho_s C_s \tag{2.11}$$

$$\rho_W C_W = \rho_s \frac{V_s}{V_W} C_s + \rho_{\ell} \frac{V_{\ell}}{V_W} C_{\ell} \tag{2.12}$$

$$\rho_i (x,0) = 0 \tag{2.13}$$

where $\rho_i(x,t)$ is the density of the substance remaining or the products produced after some amount of chemical reaction (i) has taken place when pyrolysis is considered (second case of study).

With the introduction of a heat flux (q_o) at the front surface the process is initiated. The entire slab is represented as the wetted region until the time (t_v) at which the front surface reaches the temperature of vaporization of the liquid (T_v). The boundary conditions imposed until vaporization commences ($0 < t < t_v$) are

at $x = 0$

$$q_b = K_W \frac{\partial T}{\partial x} = 0$$ [3]

Thus

$$\frac{\partial T}{\partial x} = 0 \qquad (2.14)$$

at $x = L$

$$q_o = K_D \frac{\partial T}{\partial x} = \text{constant} \qquad (2.15)$$

with the onset of vaporization ($t \geq t_v$) the slab is divided into two regions with the following conditions:

Wetted region ($0 \leq x \leq \ell$) at $x = 0$

$$q_b = K_W \frac{\partial T}{\partial x} = 0$$

or as above

$$\frac{\partial T}{\partial x} = 0$$

at $x = \ell$

$$T(x,t) = T_v = \text{constant} \qquad (2.16)$$

---

[3] The signs of q_b and q_o are negative as a result of the problem being oriented in the negative x direction.

Dry region ($\ell \leq x \leq L$) at $x = \ell$

$T(x,t) = T_v = \text{constant}$

at $x = L$

$q_o = K_D \frac{\partial T}{\partial x} = \text{constant}$

The boundary conditions (2.14) and (2.15) with respect to the front and back surfaces, therefore remain throughout the entire process with the addition of a third condition (2.16) when vaporization begins. The complete problem is thus defined by equations (2.6), (2.8) and (2.9) with initial conditions (2.10) through (2.13) and boundary conditions (2.14) through (2.16) for all time $t \geq 0$. The assumptions made thus far can be summarized as follows: A constant, radiative heat flux was applied to a semi-infinite slab. No ingition or chemical reaction of the slab was considered. The slab was divided into two regions by the vaporization interface. The changes in potential and kinetic energies were neglected in the application of the first law of thermodynamics to each region and at the vaporization interface. Work done on the fluid by viscous forces was neglected. The internal energy was assumed to be a function of temperature only. The mass flow rate of the fluid entering the moving vaporization interface was assumed equal to the mass flow of the vapor leaving. Within the vaporization interface the temperature and the densities of the liquid and vapor were considered constant. The dry region was considered as an infinite sink with respect to the vapor. Therefore the heat capacity of the vapor and the thermal energy convected away from the solid as a result of the flow of vapor through it were eliminated from the energy equation of the dry region.

Non-Dimensionalization

All variables in the aforementioned equations and conditions may be non-dimensionalized by some chosen characteristic dimension of the problem. The analysis is thus freed of dimensional dependency and allows the problem to be specified by relatively few pertinent parameters. The independent variable x and the dependent variable $\ell(t)$ are non-dimensionalized by the characteristic length L (slab thickness). The independent variable t (time) is non-dimensionalized by the characteristic conduction time L^2/α to yield the Fourier number. The temperature, measured from some reference temperature T_R, is made dimensionless by considering the boundary conditions at the front and back surfaces. The remaining variables are rendered dimensionless after division by their initial values. Table I presents a list of the resulting non-dimensional variables.

When the non-dimensional variables are substituted into the energy equations (2.6), (2.8) and (2.9) and the boundary conditions (2.14) through (2.16) it is possible to form dimensionless groups which simplify computation.[4] The new parameters thus formed are used to characterize the solution of the problem in place of the non-dimensional variables separately. These incurred parameters are given in Table II.

The resulting non-dimensional energy equations are;

wetted region $(0 \leq \bar{x} < \bar{\ell}(\bar{t}_W))$

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} = \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^2} \qquad (2.17)$$

---

[4] See Appendix B.

TABLE I

NON-DIMENSIONAL VARIABLES

Dependent	Independent
$\bar{T}(\bar{x},\bar{t}_W) = \frac{T_A - T_R}{q_o L/K_W}$	$\bar{x} = \frac{x}{L}$
$\bar{\ell}(\bar{t}_W) = \frac{\ell(t)}{L}$	$\bar{t}_W = \frac{\alpha_W t}{L^2}$
$\bar{\rho}_W(\bar{x},\bar{t}_W) = \frac{\rho_W(x,t)}{\rho_W(x,0)}$	
$\bar{\rho}_D(\bar{x},\bar{t}_W) = \frac{\rho_D(x,t)}{\rho_W(x,0)}$	

TABLE II

NON-DIMENSIONAL PARAMETERS

$\bar{H} = \frac{h_{fg}\rho_\ell \alpha_W}{q_o L}$
$\bar{K} = \frac{K_D}{K_W}$
$\bar{A} = \frac{\alpha_D}{\alpha_W} = \frac{K_D}{K_W}\frac{\rho_W C_W}{\rho_D C_D} = \bar{K}\frac{\rho_W C_W}{\rho_D C_D}$

dry region ($\bar{\ell}(\bar{t}_W) < \bar{x} \leq 1$)

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} + \frac{\bar{T}(\bar{x},\bar{t}_W)}{\bar{\rho}_D(\bar{x},\bar{t}_W)} \frac{\partial \rho_D(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} = \bar{A} \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^2} \tag{2.18}$$

liquid-vapor interface ($\bar{x} = \bar{\ell}(\bar{t}_W)$)

$$\bar{H} \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} = \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\bigg|_{\ell^-} - \bar{K} \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\bigg|_{\ell^+} \tag{2.19}$$

The non-dimensional initial conditions become

$$\bar{T}(\bar{x},o) = 0 \tag{2.20}$$

$$\bar{C}_D\bar{\rho}_D(\bar{x},0) = \frac{C_D\rho_D(x,0)}{C_W\rho_W(x,0)} \tag{2.21}$$

$$\bar{C}_W\bar{\rho}_W(\bar{x},0) = 1 \tag{2.22}$$

$$\bar{\rho}_i(\bar{x},0) = \frac{\rho_i(x,0)}{\rho_W(x,0)} = 0 \tag{2.23}$$

with the non-dimensional boundary conditions

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\bigg|_{\bar{x}=0} = 0 \tag{2.24}$$

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\bigg|_{\bar{x}=1} = 1 \tag{2.25}$$

$$\bar{T}(\bar{x},\bar{t}_W)\Big|_{\bar{x}=\bar{\ell}(\bar{t}_W)} = \bar{T}_v \tag{2.26}$$

CHAPTER III

MATHEMATICAL SOLUTION

Background

Except in limiting cases non-linear partial differential equations are not readily amenable to solution by analytic means. Complicated geometries, boundary conditions or laborious calculations lead to the use of the digital computer to calculate approximate solutions by numerical methods. Most methods of solution either approximate the derivatives and solve the resulting system of algebraic equations or reduce the non-linear partial differential equations to linear ordinary differential equations and integrate this resulting set of equations by some method of numerical quadrature.

The finite-difference approach is used quite extensively in the solution of boundary value problems. The derivatives are approximated at given nodal points by various difference schemes, many of which are described by Özisik (18). The resulting system of algebraic equations must be solved at each step (increment of the independent variable), which becomes cumbersome when many equations are involved requiring considerable amounts of core storage and computational time. The repeated solution of these equations over a period of time may lead to an accumulative round-off error within the order of magnitude of the coefficients involved. The accuracy of the finite-difference method is controlled by the number of nodal points, or the grid spacing chosen.

Therefore, as accuracy is increased, computer storage, execution time, and possibly round-off error are increased.

With the development of highly sophisticated computer routines for the simultaneous integration of ordinary differential equations, the integral method, in which partial differential equations are reduced to ordinary differential equations, has become quite popular. The method of integral relations described by Belotserkovskii and Chushkin (4) and the procedure used by Goodman and Shea (10) to obtain their heat balance integral are two examples of the integral method. Basically, the partial differential equation is multiplied by a weighting function of the spacial coordinate and then integrated with respect to this variable. The remaining functions within the integrals are then approximated by some interpolation formula. The integrals are then evaluated and the resulting system of ordinary differential equations can be integrated by any number of numerical methods. Care must be taken in the selection of the formulas used to approximate these integrals (e.g. polynomials, spline functions, trigonometric series, geometric series). If a polynomial is chosen, the ordinary differential equation which results will be dependent on the selection of nodes with respect to the spacial coordinate much like the finite-difference method. Also at each step, simultaneous algebraic equations must be solved where in some cases, (i.e. coefficients with very small values) the accumulation of round-off error or the singularity of a matrix will lead to unpredictable integration results.

Some numerical methods for integrating ordinary differential equations incorporate a weighting function (chosen by the user) which is a factor in determining the accuracy of each integration step.

Therefore, if the weighting function utilized in reducing the partial differential equation weights certain areas of the problem for higher accuracy, care must be taken in applying integration methods to avoid additive or canceling weights.

The dependence on nodal selective and possible additive round-off errors can be eliminated by electing the weighting function and the approximation function to be orthogonal. The calculations required to solve the problem are also reduced since the integral of the product of two orthogonal functions, i.e.

$$\int_a^b f_m(x)\ g_n(x)$$

is zero except when m and n are equal. With the proper choice of functions, the heat conduction equation is transformed into an equation satisfying the original only approximately. This technique or the weak solution is employed in this study.

The extension of the Schmidt graphical method of solution suggested by Longwell (13), while of interest, is tedious and its accuracy depends on the exactness of construction. This method can be used, however, to show trends and gross effects within the magnitude of more detailed solutions if so desired.

Application of the Integral Method

The primary concern of this study is the first of the limiting cases discussed in Chapter I. Accordingly the following equations are considered:

equation (2.17)

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{t}_w} = \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{x}^2}$$

equation (2.18) minus the energy generation or absorption term

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{t}_w} = \bar{A} \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{x}^2}$$

and equation (2.19)

$$\bar{H} \frac{d\bar{\ell}(\bar{t}_w)}{d\bar{t}_w} = \frac{\partial \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{x}}\bigg|_{\bar{\ell}^-} - \bar{K} \frac{\partial \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{x}}\bigg|_{\bar{\ell}^+}$$

$\bar{A}$ and $\bar{K}$ are given in Table II.

Solving for $\bar{t}_w > \bar{t}_v$ (after vaporization commences) equation (2.17) is multiplied by the weighting function $Q(\bar{x})$ and integrated with respect to $\bar{x}$ over the interval $[0,\bar{\ell}]$

$$\int_0^{\bar{\ell}(\bar{t}_w)} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{t}_w} d\bar{x} = \int_0^{\bar{\ell}(\bar{t}_w)} Q(\bar{x}) \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_w)}{\partial \bar{x}^2} d\bar{x} \qquad (3.1)$$

Applying Leibnitz's forumla for differentiating an integral and integration by parts yields [5]

[5] See Appendix C.

$$\frac{d}{d\bar{t}_W}\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\ d\bar{x} - Q(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\ \frac{\partial\bar{\ell}(\bar{t}_W)}{\ell\bar{t}_W}\Bigg|_{x=\ell} =$$

$$Q(\bar{x})\ \frac{\partial\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Bigg|_0^{\bar{\ell}(\bar{t}_W)} - Q'(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\Big|_0^{\bar{\ell}(\bar{t}_W)}$$

$$+\int_0^{\bar{\ell}(\bar{t}_W)} Q''(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\ d\bar{x} \tag{3.2}$$

Similarly multiplying equation (2.18) by $Q(\bar{x})$ and integrating with respect to $\bar{x}$ over the interval $[\bar{\ell},1]$.

$$\int_{\bar{\ell}(\bar{t}_W)}^1 Q(\bar{x})\ \frac{\partial\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{t}_W}\ d\bar{x} = \overline{A}\int_{\bar{\ell}(\bar{t}_W)}^1 Q(\bar{x})\ \frac{\partial^2\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}^2}\ d\bar{x} \tag{3.3}$$

Applying Leibnitz's formula for differentiating an integral and integrating by parts yields[6]

$$\frac{d}{d\bar{t}_W}\int_0^1 Q(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\ d\bar{x} + Q(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\ \frac{\partial\bar{\ell}(\bar{t}_W)}{\partial\bar{t}_W}\Bigg|_{\bar{x}=\bar{\ell}(\bar{t}_W)} =$$

$$\overline{A}\ Q(\bar{x})\ \frac{\partial\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Bigg|_{\ell(t_W)}^1 - \overline{A}\ Q'(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\Big|_{\bar{\ell}(\bar{t}_W)}^1$$

$$+\overline{A}\int_{\bar{\ell}(\bar{t}_W)}^1 Q''(\bar{x})\ \overline{T}(\bar{x},\bar{t}_W)\ d\bar{x} \tag{3.4}$$

---

[6] See Appendix D.

To obtain the integral over the entire slab $[0,1]$ equations (3.2) and (3.4) are added to produce when further simplified,

$$\frac{d}{d\bar{t}_W}\int_0^1 Q(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x} = \underset{\text{I}}{Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Big|_{\bar{x}=\bar{\ell}^-}}$$

$$\underset{\text{II}}{-\bar{A}\,Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Big|_{\bar{x}=\bar{\ell}^+}} \underset{\text{III}}{-\,Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Big|_{\bar{x}=0}}$$

$$\underset{\text{IV}}{+\bar{A}\,Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Big|_{\bar{x}=1}} \underset{\text{V}}{-\,Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,\Big|_{\bar{x}=\bar{\ell}}}$$

$$\underset{\text{VI}}{+\,Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,\Big|_{\bar{x}=0}} \underset{\text{VII}}{-\,\bar{A}\,Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,\Big|_{\bar{x}=1}}$$

$$\underset{\text{VIII}}{+\,\bar{A}\,Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,\Big|_{\bar{x}=\bar{\ell}}}$$

$$\underset{\text{IX}}{+\int_0^{\bar{\ell}(\bar{t}_W)} Q''(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x}} \underset{\text{X}}{+\int_{\bar{\ell}(\bar{t}_W)}^1 Q''(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x}} \qquad (3.5)$$

Term I is the heat flux exiting the interface in the -x direction and Term II is the heat flux entering the interface in the -x direction. In this initial study for simplification $\bar{A}$ and $\bar{K}$ are chosen to be unity and equation (2.19) can be substituted for Terms I and II. Terms V and VIII will then add out and the resulting equation is

$$\frac{d}{d\bar{t}_W}\int_0^1 Q(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x} = Q(\bar{x})\,\bar{H}\,\frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W}$$

$$\text{I}$$

$$- Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\bigg|_{\bar{x}=0} + Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\bigg|_{\bar{x}=1}$$

$$\text{II} \qquad\qquad \text{III}$$

$$+Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,\big|_{\bar{x}=0} - Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,\big|_{\bar{x}=1}$$

$$\text{IV} \qquad\qquad \text{V}$$

$$+\int_0^1 Q''(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x} \qquad (3.6)$$

$$\text{VI}$$

Substituting boundary conditions (2.24) and (2.25) into Terms II and III respectively, and rearranging

$$\frac{d}{d\bar{t}_W}\int_0^1 Q(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x} = Q(\bar{x})\,\bar{H}\,\frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W}$$

$$- Q(\bar{x})\,(0) + Q(\bar{x})\,(1) + Q'(\bar{x})\,\bar{T}(0,\bar{t}_W) - Q'(\bar{x})\,\bar{T}(1,\bar{t}_W)$$

$$+\int_0^1 Q''(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x} \qquad (3.7)$$

The functions chosen for the weighting function ($Q(\bar{x})$) and the temperature approximation function ($\bar{T}(\bar{x},\bar{t}_W)$) must be continuous, complete and have at least continuous second derivatives on the interval of interest ($0 \le \bar{x} \le 1$). Equation (3.7) is void of all derivatives of temperature with respect to $\bar{x}$. The discontinuity of this derivative of temperature at the interface was removed by substitution of equation (2.19). Thus the weighting and approximation functions are not required to satisfy the derivative of temperature with respect to $\bar{x}$. The temperature

throughout the slab and at the boundaries is then the primary requirement which these functions must satisfy. The cosine function (i.e. $\cos n\pi\bar{x}$) is chosen for two reasons. First, $\cos n\pi\bar{x}$ exists within the region $0 < \bar{x} < 1$ and at the boundaries of the semi-infinite slab ($\bar{x} = 0,1$), therefore, the temperature requirement is satisfied. Secondly, the cosine function ($\cos n\pi\bar{x}$) is orthogonal with respect to itself which greatly reduces computations. The derivative of $\cos n\pi\bar{x}$ matches the boundary condition at the back wall (2.24) but does not match the boundary condition at the surface (2.25). Again this is of no consequence since the boundary conditions (2.24) and (2.25) along with equation (2.19) are substituted into the energy equation (3.6) thus eliminating all derivatives of temperature with respect to $\bar{x}$.

Choosing then the weighting function $Q(\bar{x})$ to be

$$Q(\bar{x}) = \cos m\pi\bar{x} \qquad m = 0,1,2,\ldots,N \tag{3.8}$$

and approximating the temperature by

$$\bar{T}(\bar{x},\bar{t}_W) = \sum_{n=0}^{N} A_n(\bar{t}_W) \cos n\pi\bar{x} \qquad n = 0,1,2,\ldots,N \tag{3.9}$$

equation (3.7) produces N equations of the form[7]

$$\frac{dA_n(\bar{t}_W)}{d\bar{t}_W} = 2\cos(n\pi\bar{\ell})\,\bar{H}\,\frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} + 2\cos(n\pi) - (n\pi)^2 A_n(\bar{t}_W) \qquad (n > 0) \tag{3.10}$$

and for $n = 0$

$$\frac{dA_o(\bar{t}_W)}{d\bar{t}_W} = \bar{H}\,\frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} + 1 \tag{3.11}$$

---

[7] See Appendix E.

In deriving the (N+1) equations (3.10) and (3.11) above, equations (2.17) through (2.19) were used with boundary conditions (2.24) and (2.25). The remaining condition at the interface ($\bar{x} = \bar{\ell}(\bar{t}_W)$) is boundary condition (2.26).

$$\bar{T}(\bar{\ell}, \bar{t}_W) = \bar{T}_v = \text{constant}$$

The total derivative of $\bar{T}_v$ is zero. Then

$$d\bar{T}_v = 0 = \frac{\partial \bar{T}_v}{\partial \bar{t}_W}\Big)_{\bar{x}} d\bar{t}_W + \frac{\partial \bar{T}_v}{\partial \bar{x}}\Big)_{\bar{t}_W} d\bar{x}$$

By equation (3.9)

$$\bar{T}_v = \sum_{n=0}^{N} A_n(\bar{t}_W) \cos(n\pi \bar{\ell})$$

Therefore, the additional equation produced becomes

$$0 = \sum_{j=0}^{N} \frac{dA_j(\bar{t}_W)}{d\bar{t}_W} \cos(j\pi \bar{\ell}) - \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} \sum_{j=0}^{N} (j\pi) A_j(\bar{t}_W) \sin(j\pi \bar{\ell}) \quad j = 0,1,2..,N \qquad (3.12)$$

This yields (N+2) equations with (N+2) unknowns. The problem is reduced then to the simultaneous solution of equations (3.10) through (3.12) to obtain values of

$$\frac{dA_j}{d\bar{t}_W} \qquad j = 0,1,2,\ldots,N$$

then integrating these values with respect to time by some numerical method resulting in the N+1 coefficients A_j, $j = 0,1,2,\ldots,N$.

As a consequence of utilizing orthogonal functions the set of N+2 simultaneous algebraic equations (3.10) through (3.12) may be solved

once for all time. Thereby the need to solve this set of equations simultaneously at each step in the problem solution is eliminated. Solving for the derivative of the interface location with respect to time yields[8]

$$\frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} = - \frac{\left\{1+2\sum_{j=1}^{N}\left[\cos(j\pi)\cos(j\pi\bar{\ell})\right]\right\} - \sum_{j=1}^{N}(j\pi)^2 A_j \cos(j\pi\bar{\ell})}{H\left\{1+2\sum_{j=1}^{N}\cos^2(j\pi\bar{\ell})\right\} - \sum_{j=1}^{N}(j\pi) A_j \sin(j\pi\bar{\ell})} \qquad (3.13)$$

Substituting the solution of equation (3.13) into equations (3.10) and (3.11) at each step will yield the values of the coefficient derivatives

$$\frac{dA_j(\bar{t}_W)}{d\bar{t}_W} \qquad j = 0,1,2,\ldots,N$$

to be integrated.

The solution of the problem before vaporization (i.e. $\bar{\ell} = 1$) can be accomplished analytically.

For $0 < \bar{t}_W < \bar{t}_v$, $\bar{\ell} = 1$ = constant

$$\frac{d\bar{\ell}}{d\bar{t}_W} = 0$$

Equation (3.10) reduces to

$$\frac{dA_n(\bar{t}_W)}{d\bar{t}_W} = 2\cos(n\pi) - (n\pi)^2 A_n(\bar{t}_W) \qquad (3.14)$$

for $n > 0$, with equation (3,11) being

$$\frac{dA_o(\bar{t}_W)}{d\bar{t}_W} = 1 \qquad (3.15)$$

---

[8] See Appendix F.

Integrating equations (3.14) and (3.15) results in[9]

$$A_o(\bar{t}_W) = \bar{t}_W \tag{3.16}$$

$$A_n(\bar{t}_W) = \frac{2(-1)^n}{(n\pi)^2}\left[\exp\{-(n\pi)^2\,\bar{t}_W\} - 1\right] \qquad (n > 0) \tag{3.17}$$

The problem is therefore solved algebraically for any increment of time between zero and the time vaporization commences at the front surface (i.e. $0 < \bar{t}_W < \bar{t}_v$).

Initial Conditions

Of the non-dimensional initial conditions given in Chapter II, only condition (2.20) is pertinent to the vaporization study.

At $\bar{t}_W = 0$, condition (2.20) states

$$\bar{T}(\bar{x},0) = 0$$

Applying the temperature approximation (3.9) to condition (2.20) yields

$$\bar{T}(\bar{x},0) = \sum_{n=0}^{N} A_n(0)\cos(n\pi\bar{x}) \qquad n = 0,1,2,\ldots,N$$

$\cos(n\pi\bar{x})$ will be zero for $\bar{x} = \frac{1}{2}$ only. Therefore $A_n(0)$ must be zero. The initial temperature coefficients are then

$$A_o = 0$$

$$A_1 = 0$$

$$\vdots$$

$$A_N = 0$$

---

[9] See Appendix G.

Computer Technique

The computer program developed to solve the first case or vaporization problem described by equations (3.10) through (3.17) consists of four sections or subroutines. The main or executive section (MAIN) initiates all control parameters, non-dimensional parameters, and equation coefficients. This section solves the algebraic equations (3.16) and (3.17) for the heating of the saturated porous slab prior to vaporization (i.e. $0 < \bar{t}_W < \bar{t}_v$) and initiates the integration of equations (3.10), (3.11), and (3.13).

The output section (DEROUT) prints and/or punches any desired temperatures along with the vaporization position and velocity for various increments of time.

The derivative function subroutine (DERFUN) calculates the derivatives of the coefficients, using equations (3.10), (3.11), and (3.13) for each successive time step employing previous values of the coefficients obtained from the integration routine.

The integration routine (DHPCG) integrates the calculated values of the derivatives given by the derivative function and passes the new values of the coefficients to the output and derivative function routines. A complete listing of each program section is given in Appendix I. Table III presents the basic steps followed by the computer program.

Method of Numerical Integration

Numerical techniques for solving first order ordinary differential equations with given conditions $y_i(x_o)$ are usually based on the direct or indirect use of Taylor's expansion or on the employment of open or

TABLE III

COMPUTER PROGRAM CYCLE

I. Main Section

1. Read summation limit (N), dimensional constants, output and integration routine control parameters.
2. Initialize numerical constants and non-dimensional parameters.
3. Calculate coefficients for the temperature approximation function by the analytic solution ($0 < \bar{t}_W < \bar{t}_v$). Call output routine.
4. Repeat step 3 until vaporization commences ($\bar{t}_W = \bar{t}_v$).
5. Initialize constants required for numerical integration.
6. Call integration routine (II).

II. Integration Routine

1. Apply one-step integration method.
2. Call derivative function and output routines.
3. Apply multistep integration method.
4. Call derivative function (III) and output (IV) routines.
5. Repeat steps 3 and 4 until the entire interval specified is integrated over or an unresolvable error is encountered.
6. Return to main section (I).

III. Derivative Function Routine

1. Using coefficient values received from the integration routine (II) calculate the temperature coefficient derivatives for the next integration step.

TABLE III (Continued)

2. Return to the integration routine (II).

IV. Output Routine

1. Determine if output is desired for this step.
2. Calculate temperatures at specified locations throughout slab.
3. Determine when vaporization begins.
4. Print or punch time, interface velocity, interface position and desired temperature profiles.
5. Return to calling routine.

closed integration formulas. Carnahan, Luther, and Wildes (7) group these techniques into two classes, one-step methods which calculate the value y_{i+1} given only y_i and the multistep methods requiring y_i plus several other values y_i's outside the integral of integration.

One disadvantage of the multistep methods is that they are not self-starting and require a one-step method to calculate the initial values of the solution y_i (i.e., $y(x_1)$, $y(x_2)$, etc.). Also with multistep methods it is cumbersome to change the integration step size once the calculation is initiated. The major advantage of multistep methods is the fact that less computation is required than comparable one-step methods while producing results of similar accuracy.

The predictor-corrector methods, where an open integration formula is utilized to predict the integration and a closed integration formula is employed to correct this estimate, inherit the disadvantages of the multistep methods. But a considerable advantage of this method is that solutions can be produced with comparable accuracy and stability of a fourth order one-step method using as few as two derivative evaluations at each step. Hamming's modified predictor-corrector method represents the best compromise between stability and accuracy and is the most popular multistep method (7).

The numerical integration method used in this study is an IBM application program (DHPCL) (24) which employs Hamming's modified predictor-corrector method with a fourth order Runge-Kutta method, suggested by Ralston (20), to start the process. This routine incorporates an error weighting function and allows the user the option of changing the integration step size during execution.

CHAPTER IV

COMPUTATIONAL RESULTS

Inert Solution

By the nature of the problem presented in Chapters II and III, an algebraic solution is possible for the heating of the saturated porous slab from time zero till the time of vaporization at the front surface. To assess this analytic solution the condition of vaporization at the surface was relaxed and the problem became one of the heating of an inert slab. Carslaw and Jaeger (8) give the exact solution for an inert semi-infinite slab heated by a constant heat flux at the front surface with an adiabatic back surface.

Figure 6 presents a comparison of the computer generated approximate solution utilizing five coefficients with the exact solution. A good approximation at the front surface is obtained while the inert calculations match the exact solution precisely at the back surface. Increasingly the number of coefficients in the inert solution will cause the exact solution at the front surface to be more closely modeled.

Constant and Parameter Values

The dimensional constants in the series of computational runs discussed here, were chosen to match approximately those of wood and water. Since the examination of the entire problem will eventually encompass pyrolysis, the constants and parameters generally match those

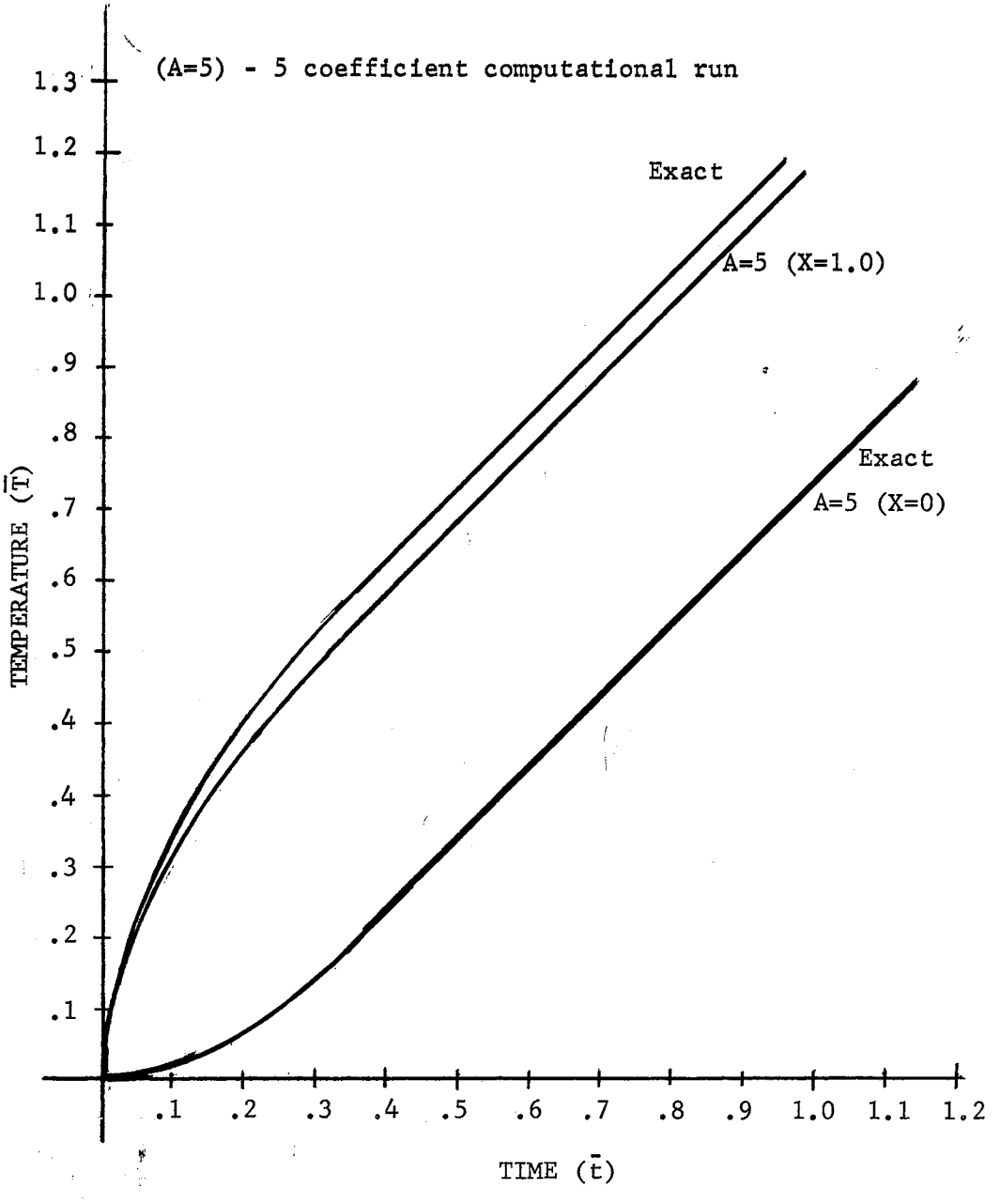

Figure 6. Comparison of Approximate Solution of Inert Slab With Exact Solution

of Rittmann (21) for future study. Table 4 lists the pertinent constants and parameters used.

Temperature Relations

Comparison of the temperatures obtained in this investigation with work previously done in the melting and freezing problem is difficult for two reasons. Firstly, the studies encountered consider the liquid or solid at a uniform temperature of solidification or melting before the process is initiated. Secondly, most previous studies use a step input of temperature to initiate the melting of solidification process. This study assumes the saturated slab is at a reference temperature well below that of vaporization and consequently when the constant heat flux is applied the temperature is no longer uniform throughout the slab. When vaporization commences the temperature profiles and the velocity of the interface are quite different than presented in other studies. Also the term containing the temperature at the front surface was deleted from the energy equation (3.7) as a result of the choice of cosine weighting and approximation functions. Therefore the application of a step input temperature is not possible.

A time history of temperatures at selected points within the slab is shown in Figure 7.[10] By comparison with Figure 6, the inert solution, it can be seen that when the front surface reaches vaporization ($\bar{t}_W$ = .05937) the temperature remains constant for some time. This is caused by the decrease in heat flux entering the remainder of the slab as a result of vaporization at and near the surface. The temperature

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[10] The graphs presented have been smoothed over discrete points to eliminate cosine fluctuations.

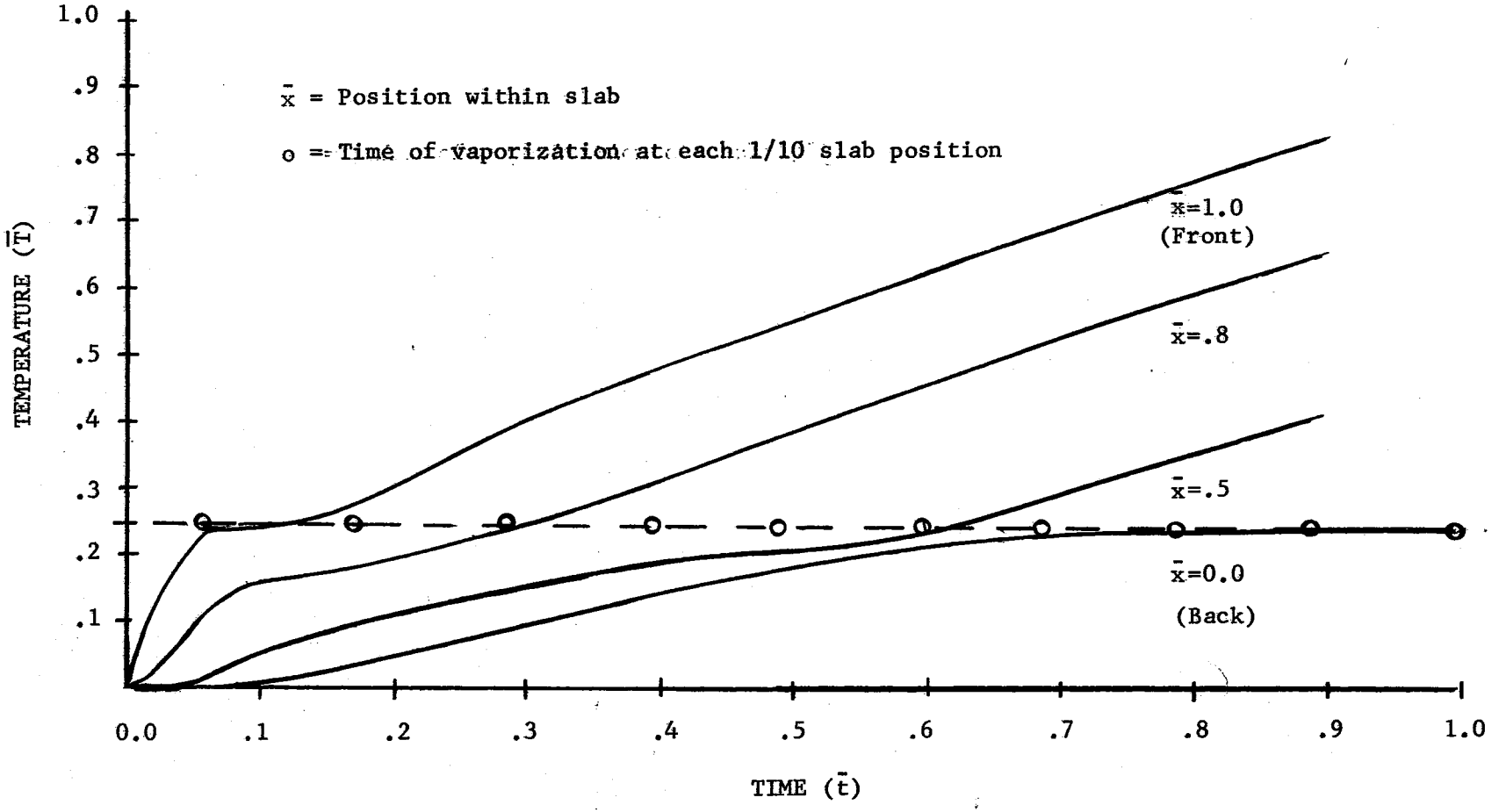

Figure 7. Selected Temperature Profiles With Respect to Time

TABLE IV

DIMENSIONAL CONSTANTS AND PARAMETERS

L	1.0 cm
T_R	300° K
q_o	0.081 cal/cm^2-sec
h_{fg}	539.05 cal/gm
T_v	373.15° K
C_W	.66 cal/gm-° K
K_W	2.7 × 10^{-4} cal-cm/cm^2-sec^2-° K
$\bar{T}_v$	.24383
$\bar{H}$	.544495
$\bar{\rho}_\ell$	.20
$\bar{A}$	1.0
$\bar{K}$	1.0

gradient throughout the slab is decreased as a result of the onset of vaporization. As time increases the points in the dry region, far enough from the interface, are no longer affected by the vaporization and approach a conduction dominated linear increase in temperature. The temperature at the back wall increases constantly throughout the entire process and has virtually reached the temperature of vaporization when the interface is at a point approximately .4 from the back wall.

The temperature profile through the slab at selected times is shown in Figure 8. Here again it can be seen that the temperatures in the area preceding the vaporization interface (i.e. wetted region) increase very slowly, but the temperatures within the area aft of the interface (i.e. dry region) are unaffected. The temperature gradient on the wetted side of the interface decreases with time and eventually reaches zero at the back surface (boundary condition). This is physically realistic since the wetted region slowly reaches the temperature of vaporization as the interface moves into the slab. Therefore, the temperature gradient is significant with the onset of vaporization and then must decrease as the temperature increases in the region ahead of the interface.

Interface Velocity

Figure 9 contains discrete points plotted from computational runs of five and seven coefficients. The oscillations observed are attributed to the representation of an infinite series, i.e.

$$\sum_{n=0}^{\infty} A_n \cos n\pi\bar{x}$$

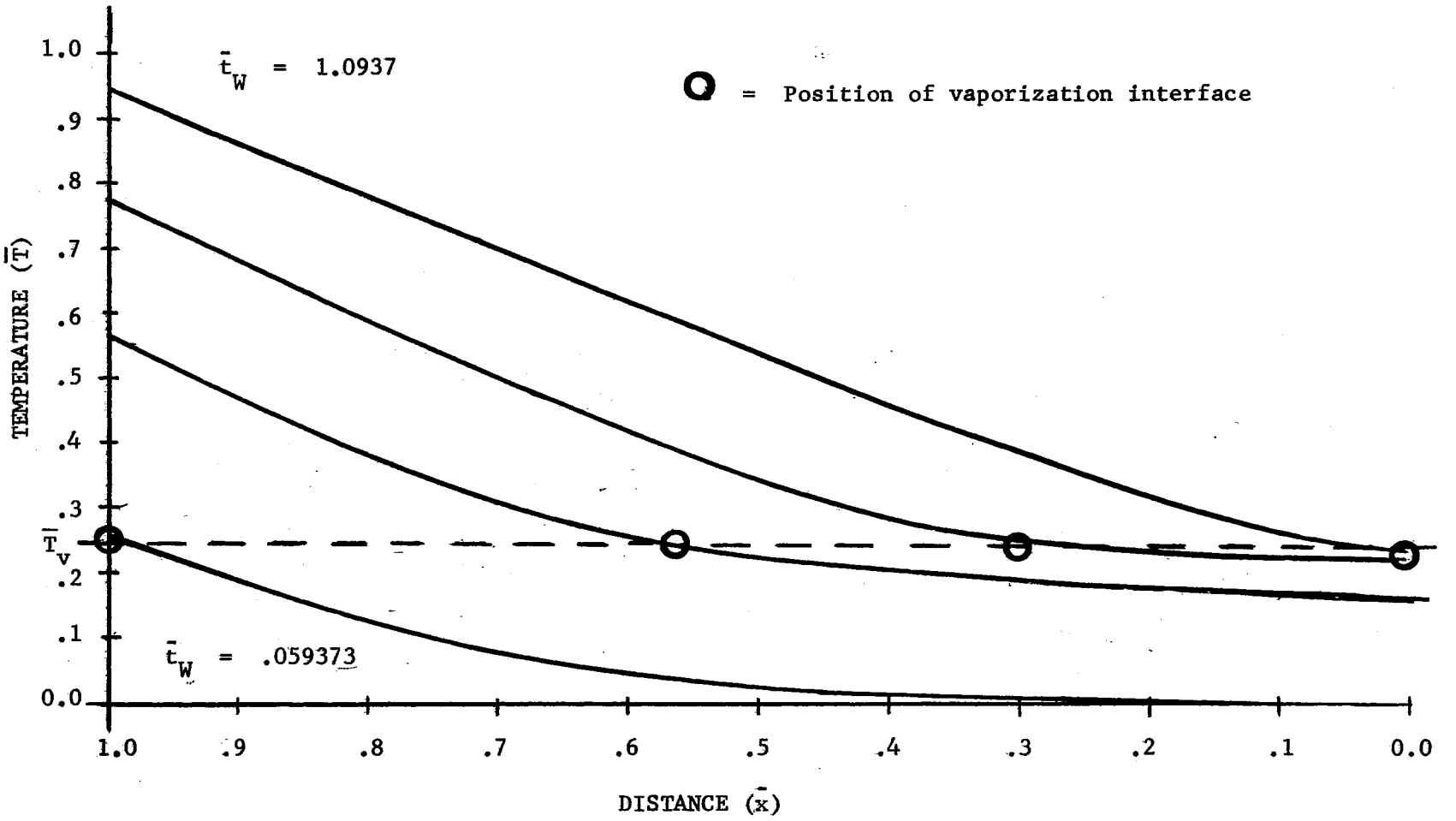

Figure 8. Temperature Profile of Slab at Selected Time Intervals

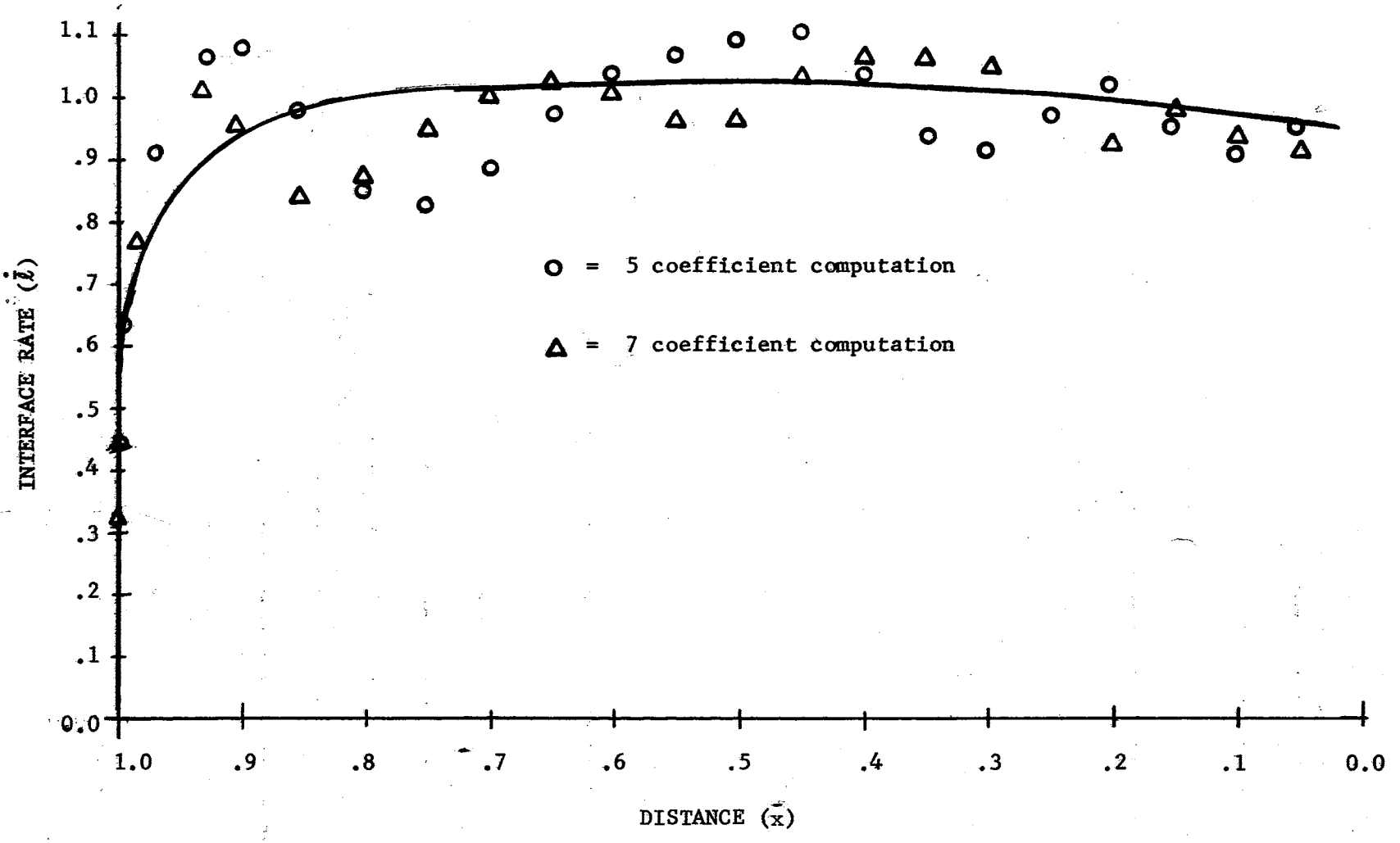

Figure 9. Interface Velocity With Respect to Distance

by a finite number of coefficients. Approximation of a mean value curve through these points shows the interface velocity starting at zero and rapidly increasing to a value in the neighborhood of .9. The velocity then increases slowly to a maximum somewhere in the vicinity of the center of the slab. From this point on the velocity drops off slowly through the remainder of the slab.

The interface velocity obtained appears to be physically realistic since at the onset of vaporization the surface and immediate area behind it are at the vaporization temperature. The rate of vaporization assumed starting at zero increases rapidly as the liquid in this area is vaporized. Once this initial area is vaporized a certain amount of flux must be used to heat the area immediately ahead of the interface to bring it to the temperature of vaporization. As the temperature in the wetted region increases the interface velocity increases slowly until a maximum is reached. At this point, the temperature gradient in the dry region is such that more and more energy is required in raising the temperature in this region. Thus the interface velocity decreases and continues decreasing throughout the remainder of the slab as the temperature gradient in the dry region increases.

The initial velocity as shown starts at definite rates of approximately .32 and .45. This is a consequence of the size of the initial integration step and also of the number of coefficients used.

Pyrolysis Retardation

Although the primary interest of this investigation is not pyrolysis, examination of Figure 10 reveals that, for a constant heat flux with one exothermic reaction considered, deviation from the inert

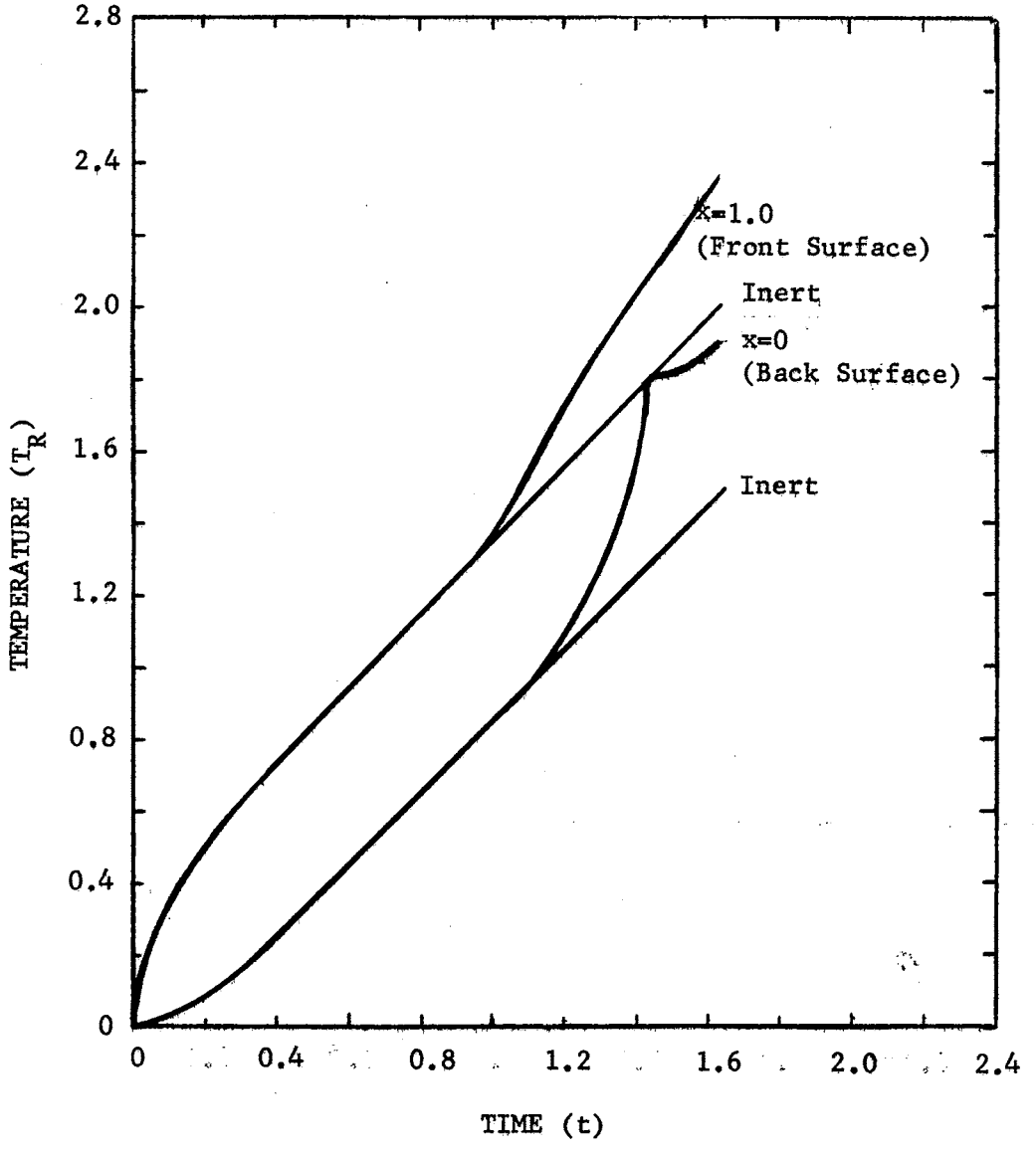

Figure 10. Effect of Heat of Reaction: Temperature History of Front and Back Surfaces - Constant Heat Flux, One Exothermic Reaction, Case 0, Rittmann (21)

solution occurs at a time of approximately $\bar{t}_W = .1$. The temperatures at this point for the front and back surfaces are $\overline{T} = 1.3$ and $\overline{T} = .9$, respectively. The seven coefficient computation utilized in Figures 7 and 8 obtained complete vaporization of the saturated liquid within a time a $\bar{t}_W = 1.094$. The maximum temperature attained by the front surface being $\overline{T} = .9312$ with the back surface restricted to $\overline{T} = .2438$ (i.e. The temperature of vaporization $\overline{T}_v$). Within the same time frame, (i.e. $0 \leq \bar{t}_W \leq 1.0$), comparison of the aformentioned figures discloses the temperature of the front surface in the saturated problem to be just slightly greater than that of the back surface of the pyrolysis example. Also, the back surface of the saturated problem is seen to be at a temperature much lower than the corresponding temperature of the pyrolysis problem. Thus, as expected, the dissipation of heat energy by vaporization of the liquid causes the temperatures within the initially saturated porous solid to be much lower than the temperatures of the initially dry heated solid thereby delaying pyrolysis of the solid material.

The solution of the vaporization problem presented here assumes thermal properties which yield values of the Fourier number and non-dimensional temperatures consistent with those used by Rittmann (21) in the calculation of various constant, radiative heat flux type pyrolysis problems. These values in no way attempt to model known substances. In Appendix H values of the non-dimensional parameters $\overline{A}$ and $\overline{K}$ are computed assuming water and fir are the substances used in a volumetric ratio of one to four. The values of $\overline{A}$ and $\overline{K}$ thus attained do not approach unity unless the ratio of liquid to solid is very small. Therefore, in future investigations the incorporation of these non-dimensional parameters

into the resultant energy equation must be resolved to extend this study to various combinations of known substances.

CHAPTER V

SUMMARY AND CONSLUSIONS

Summary

An analytic study of the heating of a porous material initially saturated with a liquid was undertaken. Examination of the complexity of the problem led to a division into two areas of analysis, the vaporization of the liquid and the pyrolysis of the porous material. This study concentrated on the phenomena of vaporization.

The vaporization of the liquid from a saturated porous solid was modeled by a semi-infinite, homogeneous and isotropic slab initially saturated with a homogeneous and isotropic liquid. The slab was considered exposed to a constant, radiative heat flux at the front surface and insulated against heat conduction at the back surface. With the onset of vaporization the slab was divided into two regions by the vaporization interface. Applying the conservation of energy principle to each region and across the interface produced three energy equations.

Non-dimensionalization of each equation gave rise to the ratios of thermal diffusivity and thermal conductivity. Considering these parameters unity the integral technique of reducing a partial differential equation to a system of ordinary differential equations was employed. Multiplication of each energy equation by a weighting function in the space variable and then integrating with respect to this space variable

enabled the combination of the three energy equations into one equation representing the entire slab.

The weighting and temperature approximation functions used in applying the integral method (i.e. $\cos n\pi\bar{x}$ and the Fourier cosine series, respectively) were so chosen as to give valid temperatures throughout the slab. These functions are also orthogonal which reduced computations immensely. The fact that the chosen functions do not represent the slope of the temperature validly for all $\bar{x}$ within the slab is not critical since the integrated equation contains no derivatives of temperature with respect to $\bar{x}$ and leads to the so-called weak solution of the original energy equation. It should be noted here that the temperatures obtained by this method can not be differentiated to yield local heat flux values.

The resulting N+1 ordinary differential equations along with an additional equation obtained from the condition of constant temperature at the vaporization interface were integrated by a multistep numerical integration routine employing Hamming's modified predictor-corrector technique. Computer solutions employing three, five and seven coefficients in the temperature approximation were generated. While not modeling any particular substances, the temperature profiles and interface velocities obtained appear to be physically realistic. The vaporization process is shown to prevent the temperature of the solid from attaining values which would cause significant pyrolysis.

Conclusions

The following conclusions and observations evolved from this study:

1. The complex analysis of the heating of a saturated porous material

can be divided into two areas of investigation, the vaporization of the liquid initially present, which was the object of this study and the pyrolysis of the dry solid material remaining after vaporization.

2. The discontinuity of the derivative of temperature with respect to time and the spacial coordinate at the interface represents the main difficulty in solving this problem. A transformation of coordinates is possible but results in singularities at the front and back surfaces. Thus in order to initialize the vaporization process a finite distance into the slab must be approximated. The division of the slab into regions, with the application of the integral method to reduce and combine the resulting energy equations into one, thereby eliminating the discontinuity from the problem, results in a weak solution of the problem. This approach appears to be the most practical.

3. Two non-dimensional parameters, the ratios of thermal diffusivity and thermal conductivity, appear in the analysis of the problem. The incorporation of these parameters in the resultant energy equation must be resolved in future studies if known liquids and solids are to be considered in various degrees of combination.

4. The effects of the escaping vapor, neglected in this study, might be included in future studies depending on the magnitude and type of heat flux applied at the exposed surface.

5. The vaporization problem solved in this study, while pertaining to no known substances, appears physically valid. By resolving the thermal diffusivity and thermal conductivity parameters, this study can be combined with previous pyrolysis studies to yield solutions of the heating of a saturated slab from the initial application of a heat flux to the surface ignition of the solid substance.

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APPENDIX A

EFFECTS OF VAPOR EFFLUX

The effects on the dry region caused by the escaping vapor involves consideration of flow through a porous media, free convection, and forced convection. Ignoring free convection the porosity of the solid and the velocity of the vapor must be known to correctly evaluate the hindrance or contribution of the vapor efflux to the heating of the slab. Since the porosity of the solid and the velocity of the vapor are not known, term V of equation (2.7) will be used. This term expresses the net rate of thermal energy convected per unit volume by the vapor as it escapes through the pores of the dry solid

$$\frac{\partial}{\partial x} \rho_v v_v \left[u_v + \frac{1}{\rho_v} P_v\right] = \frac{\partial}{\partial x} \rho_v v_v h_v \tag{A.1}$$

At the interface the mass-flow rate of vapor per unit area is equal to the mass flow rate of liquid per unit area. Thus assuming this mass flow rate is constant through the dry solid

$$\rho_v v_v = \rho_\ell v_\ell \tag{A.2}$$

Substituting (A.2) into (A.1) yields

$$\frac{\partial}{\partial x} \rho_\ell v_\ell h_v \tag{A.3}$$

Considering the velocity of the liquid equal to the interface velocity (A.3) is then

$$\frac{\partial}{\partial x} \rho_\ell \frac{d\ell}{dt} h_v$$

or, since the mass flow rate is assumed constant

$$\rho_\ell \frac{d\ell}{dt} \frac{\partial}{\partial x} h_v \tag{A.4}$$

Enthalpy is a function of temperature alone, at constant pressure, thus

$$\rho_\ell \frac{d\ell}{dt} \frac{\partial}{\partial x} \int (C_{P_v}\, dt) = \rho_\ell \frac{d\ell}{dt} C_{P_v} \frac{dT}{dx} \tag{A.5}$$

From the non-dimensionalization of variables

$$x = \bar{x}L$$

$$\ell = \bar{\ell}L$$

$$\frac{d\ell}{dt} = \frac{\alpha_W}{L} \frac{d\bar{\ell}}{d\bar{t}_W}$$

$$\frac{dT}{dx} = \frac{1}{L} \frac{q_o L}{K_w} [\bar{T}_o - \bar{T}_v]$$

where $\bar{T}_o$ is the non-dimensional temperature at the front surface. Substituting these values into (A.5) yields

$$\rho_\ell \frac{d\ell}{dt} C_{P_v} \frac{dT}{dx} = \rho_\ell C_{P_v} \frac{K_W}{C_W \rho_W L} \frac{d\bar{\ell}}{d\bar{t}_W} \frac{1}{L} [\bar{T}_o - \bar{T}_v] \frac{q_o L}{K_W} \tag{A.6}$$

Picking

$$\frac{q_o L}{K_W} = 300^\circ \text{ K}$$

and considering saturated water, saturated steam, and white fir as the porous solid yields

$$\rho_\ell = 60.053 \text{ lb}_m/\text{ft}^3$$

$$C_{P_v} = .4764 \text{ Btu/lb}_m\ ^\circ\text{F}$$

$$K_W = .1286 \text{ Btu ft/hr ft}^2\ ^\circ\text{F}$$

$$\rho_W C_W = 26.406 \text{ Btu/ft}^3\ ^\circ\text{F}$$

$$L = 1 \text{ cm} = .3937 \text{ ft}$$

Choosing the interface at a point midway into the slab for the seven coefficient computational run

$$\frac{d\bar{\ell}}{d\bar{t}_W} = .96949$$

$$\bar{T}_o - \bar{T}_v = .37407$$

Therefore,

$$[\bar{T}_o - \bar{T}_v] \frac{q_o L}{K_W} = [.37407]\ 300^o\ K$$

$$= 112.212\ K^o$$

$$= 1.8\ [112.212]\ R^o$$

$$= 201.98\ F^o$$

$$\frac{\rho_\ell C_{P_v} K_W}{\rho_W C_W L^2} = \frac{(60.053)(.4764)(.1286)}{(26.406)(.3937)^2} \frac{Btu}{hr\ ft^3\ ^oF} = .899 \frac{Btu}{hr\ ft^3\ ^oF}$$

Thus

$$\rho_\ell \frac{d\ell}{dt} C_{P_v} \frac{dT}{dx} = (.899)(.96949)(201.98) \frac{Btu}{hr\ ft^3} = 176.04 \frac{Btu}{hr\ ft^3}$$

On a unit volume basis the vapor is considered to occupy 20% of the volume, the convective term then yields

$$.2\ ft^3\ (176.04) \frac{Btu}{hr\ ft^3} = 35.21 \frac{Btu}{hr} \qquad (A.7)$$

The vapor negotiates a positive temperature gradient, therefore this thermal energy can be considered convected away from the solid. The heat flux at the front surface for this example is

$$q_o = \frac{(.1286)(1.8)(300)}{.3937} \frac{Btu}{hr\ ft^2} = 176.39 \frac{Btu}{hr\ ft^2}$$

On a unit volume basis multiplying by the area and dividing by the volume

$$\frac{A}{V}q_o = \frac{176.39}{L}\ \frac{Btu}{hr\ ft^3} = 448.032\ \frac{Btu}{hr\ ft^3}$$

Multiplying by the percent of volume occupied by the solid yields

$$Aq_o = .8\ ft^3\ (488.032)\ \frac{Btu}{hr\ ft^3} = 358.43\ \frac{Btu}{hr} \qquad (A.8)$$

The ratio of the thermal energy convected by the vapor to the heat flux available to the solid is on the order of

$$\frac{35.21}{358.43} = .0982$$

APPENDIX B

NON-DIMENSIONALIZATION OF EQUATIONS AND BOUNDARY CONDITIONS

Division of x and $\ell(t)$ by the characteristic length L yields

$$\bar{x} = \frac{x}{L}$$

$$\bar{\ell}(t) = \frac{\ell(t)}{L}$$

The non-dimensional temperature $\overline{T}$ and time $\bar{t}$ are chosen as

$$\overline{T} = \frac{T}{T_z}$$

$$\bar{t} = \frac{t}{t_z}$$

where

$$T = T_A - T_R$$

Substituting these terms into equation (2.6)

$$\rho_W C_W \frac{T_z}{t_z} \frac{\partial \overline{T}(\bar{x}, \bar{t}_W)}{\partial \bar{t}_W} = K_W \frac{T}{L^2} \frac{\partial^2 \overline{T}(\bar{x}, \bar{t}_W)}{\partial \bar{x}^2} \quad [11]$$

rearranging

$$\frac{\partial \overline{T}(\bar{x}, \bar{t}_W)}{\partial \bar{t}_W} = \left(\frac{K_W}{\rho_W C_W}\right)\left(\frac{t^2}{L^2}\right) \frac{\partial^2 \overline{T}(\bar{x}, \bar{t}_W)}{\partial \bar{x}^2}$$

---

[11] The subscripts W and D refer to the wetted and dry regions, respectively.

The thermal diffusivity is defined as

$$\frac{K_W}{C_W \rho_W} = \alpha_W$$

Now t_z can be defined as

$$t_z = \frac{L^2}{\alpha_W}$$

Here t_z is not a time constant as such but is a "significant time" or time scale of the problem. By rearranging, t_z can be shown to represent the product of the thermal capacitance and the internal thermal resistance (17).

$$t_z = \frac{L^2}{\alpha_W} = \frac{\rho_W C_W L^2}{K_W} = \rho_W C_W L A \frac{L}{A K_W} = \rho_W V C_W \left(\frac{L}{K_W A}\right)$$

Therefore $\bar{t}_W$ becomes the Fourier number

$$\bar{t}_W = \frac{t\alpha_W}{L^2}$$

Equation (2.6) is then

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} = \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^2} \qquad \text{(B.1)}$$

In a similar manner, equation (2.8) can be non-dimensionalized, letting

$$\bar{\rho}_D(\bar{x},\bar{t}_D) = \frac{\rho_D(x,t)}{\rho_D(x,0)}$$

$$\left(\rho_D(x,0)\ \frac{T_z}{t_z}\right) \bar{\rho}_D(\bar{x},\bar{t}_D)\, C_D\ \frac{\partial \bar{T}(\bar{x},\bar{t}_D)}{\partial \bar{t}_D} + \left(\rho_D(x,0)\ \frac{T_z}{t_z}\right) C_D \bar{T}(\bar{x},\bar{t}_D) \frac{\partial \bar{\rho}_D(\bar{x},\bar{t}_D)}{\partial \bar{t}_D}$$

$$= \left(\frac{T_z}{L^2}\right) K_D\ \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_D)}{\partial \bar{x}^2}$$

rearranging

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_D)}{\partial \bar{t}_D} + \frac{\bar{T}(\bar{x},\bar{t}_D)}{\bar{\rho}_D(\bar{x},\bar{t}_D)} \frac{\partial \bar{\rho}_D(\bar{x},\bar{t}_D)}{\partial \bar{t}_D} = \left(\frac{K_D}{C_D \rho_D} \frac{t_z}{L^2}\right) \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_D)}{\partial \bar{x}^2}$$

Again defining thermal diffusivity

$$\frac{K_D}{C_D \rho_D} = \alpha_D$$

Choosing

$$t_z = \frac{L^2}{\alpha_D}$$

yields the Fourier number

$$\bar{t}_D = \frac{t\alpha_D}{L^2}$$

Equation (2.8) thus becomes

$$\frac{\partial \bar{T}(\bar{x},\bar{t}_D)}{\partial \bar{t}_D} + \frac{\bar{T}(\bar{x},\bar{t}_D)}{\bar{\rho}_D(\bar{x},\bar{t}_D)} \frac{\partial \rho_D(\bar{x},\bar{t}_D)}{\partial \bar{t}_D} = \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_D)}{\partial \bar{x}^2} \tag{B.2}$$

The energy equation at the liquid-vapor interface (2.9) can be written

$$\rho_\ell h_{fg} \left(\frac{L}{t_z}\right) \frac{d\bar{\ell}(\bar{t})}{d\bar{t}} = K_W \left(\frac{T_z}{L}\right) \frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} \bigg|_{\ell^-} - K_D \left(\frac{T_z}{L}\right) \frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} \bigg|_{\ell^+}$$

dividing by K_W and rearranging

$$\left(\frac{h_{fg} L^2 \rho_\ell}{t_z T_z K_W}\right) \frac{d\bar{\ell}(\bar{t})}{d\bar{t}} = \frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} \bigg|_{\ell^-} - \left(\frac{K_D}{K_W}\right) \frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} \bigg|_{\ell^+} \tag{B.3}$$

Considering the boundary condition at the front surface (x = L)

$$q_o = K_W \frac{\partial T(x,t)}{\partial x} \bigg|_{x=L} = K_W \left(\frac{T_z}{L}\right) \frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} \bigg|_{\bar{x}=1} = \text{constant}$$

or

$$\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}} \bigg|_{\bar{x}=1} = \left(\frac{q_o L}{K_W}\right) \frac{1}{T_z}$$

Choosing

$$T_z = \frac{q_o L}{K_W}$$

$$\left.\frac{\partial \bar{T}(\bar{x},\bar{t})}{\partial \bar{x}}\right|_{\bar{x}=1} = 1$$

and

$$\bar{T}(\bar{x},\bar{t}) = \frac{T}{q_o L/K_W} = \frac{T_A - T_R}{q_o L/K_W} \tag{B.4}$$

with

$$\bar{t}_W = \frac{L^2}{\alpha_W}$$

then equation (B.3) becomes

$$\left[\frac{h_{fg}\rho_\ell \alpha_W}{q_o L}\right] \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} = \left.\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\right|_{\ell^-} - \left(\frac{K_D}{K_W}\right) \left.\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\right|_{\ell^+}$$

defining $\bar{H}$ as a non-dimensional parameter,

$$\bar{H} = \frac{h_{fg}\rho_\ell \alpha_W}{q_o L}$$

yields

$$\bar{H} \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} = \left.\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\right|_{\ell^-} - \left(\frac{K_D}{K_W}\right) \left.\frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\right|_{\ell^+} \tag{B.5}$$

From the boundary condition at the interface (2.26) and the non-dimensional temperature (B.4)

$$\bar{T}(\bar{\ell},\bar{t}) = \bar{T}_v = \text{constant}$$

$$\bar{T}(\bar{\ell},\bar{t}_W) = \frac{T_A - T_R}{T_z} = \frac{T_v - T_R}{q_o L/K_W}$$

or

$$\bar{T}(\bar{\ell},\bar{t}_D) = \frac{T_A - T_R}{T_z} = \frac{T_v - T_R}{q_o L/K_D}$$

where

$$\frac{q_o L}{K_D}\,\overline{T}\,(\bar{\ell},\bar{t}_D) \;=\; \frac{q_o L}{K_W}\,(\bar{\ell},\bar{t}_W)$$

$$\overline{T}(\bar{\ell},\bar{t}_D) \;=\; \frac{K_D}{K_W}\,\overline{T}(\bar{\ell},\bar{t}_W)$$

Thus

$$\overline{T}(\bar{x},\bar{t}_D) \;=\; \frac{K_D}{K_W}\;\overline{T}(\bar{x},\bar{t}_W) \tag{B.6}$$

Two Fourier numbers are created by the non-dimensionalization of the energy equations. In order to combine the energy equations properly only one dimensional time can exist. The following relationship is therefore apparent:

$$t = t$$

from

$$\bar{t} \;=\; \frac{t\alpha}{L^2}$$

$$\bar{t}_D\,\frac{L^2}{\alpha_D} \;=\; \bar{t}_W\,\frac{L^2}{\alpha_W}$$

$$\bar{t}_D = \frac{\alpha_D}{\alpha_W}\,\bar{t}_W \tag{B.7}$$

Adopting $\overline{T}(\bar{x},\bar{t}_W)$ and $\bar{t}_W$ as standards, equations (B.1) and (B.5) remain unchanged but equation (B.2) is transformed to

$$\frac{\dfrac{K_D}{K_W}}{\dfrac{\alpha_W}{\alpha_D}}\,\frac{\partial\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{t}_W} + \frac{\dfrac{K_D}{K_W}}{\dfrac{\alpha_W}{\alpha_D}}\,\frac{\overline{T}(\bar{x},\bar{t}_W)}{\bar{\rho}_D(\bar{x},\bar{t}_W)}\,\frac{\partial\bar{\rho}_D(\bar{x},\bar{t}_W)}{\partial\bar{t}_W} = \frac{K_D}{K_W}\,\frac{\partial^2\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}^2}$$

$$\frac{\partial\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{t}_W} + \frac{\overline{T}(\bar{x},\bar{t}_W)}{\bar{\rho}_D(\bar{x},\bar{t}_W)}\,\frac{\partial\bar{\rho}_D(\bar{x},\bar{t}_W)}{\partial\bar{t}_W} = \frac{\alpha_D}{\alpha_W}\,\frac{\partial^2\overline{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}^2} \tag{B.8}$$

Defining parameters $\overline{A}$ and $\overline{K}$ as

$$\overline{A} = \frac{\alpha_D}{\alpha_W}$$

$$\overline{K} = \frac{K_D}{K_W}$$

equations (2.17) through (2.19) are obtained.

APPENDIX C

INTEGRATION OF EQUATION (3.1)

Each term of equation (3.1) can be integrated as shown

$$\underbrace{\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} d\bar{x}}_{\text{I}} = \underbrace{\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x}) \frac{\partial^a \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^a} d\bar{x}}_{\text{II}}$$

Applying Leibnitz's formula to term I

$$\frac{d}{d\bar{t}_W} \int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W)\, d\bar{x} = \underbrace{\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} d\bar{x}}_{\text{(Term I)}}$$

$$+ Q(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W) \frac{\partial \bar{\ell}(\bar{t}_W)}{\partial \bar{t}_W}$$

$$- Q(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W) \frac{\partial (0)}{\partial \bar{t}_W}$$

rearranging

$$\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} d\bar{x} = \frac{d}{d\bar{t}_W} \int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W)\, d\bar{x}$$

$$- Q(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W) \frac{\partial \bar{\ell}(\bar{t}_W)}{\partial \bar{t}_W} \qquad \text{(C.1)}$$

Integrating term II by parts

$$\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x}) \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^2}\, d\bar{x} = Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\Bigg|_0^{\bar{\ell}(\bar{t}_W)} - \int_0^{\bar{\ell}(\bar{t}_W)} Q'(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\, d\bar{x}$$

Integrating once again by parts yields

$$\int_0^{\bar{\ell}(\bar{t}_W)} Q(\bar{x}) \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^2}\, d\bar{x} = Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}}\Bigg|_0^{\bar{\ell}(\bar{t}_W)} - Q'(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W)\Big|_0^{\bar{\ell}(\bar{t}_W)} + \int_0^{\bar{\ell}(\bar{t}_W)} Q''(\bar{x})\, \bar{T}(\bar{x},\bar{t}_W)\, d\bar{x} \qquad \text{(C.2)}$$

Substituting (C.1) and (C.2) into equation (3.1) yields equation (3.2).

APPENDIX D

INTEGRATION OF EQUATION (3.3)

Each term of equation (3.3) can be integrated as shown

$$\underset{\text{I}}{\int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} d\bar{x}} = \bar{A} \underset{\text{II}}{\int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x}) \frac{\partial^2 \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{x}^2} d\bar{x}}$$

Applying Leibnitz's formula to term I

$$\frac{d}{d\bar{t}_W} \int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x})\ \bar{T}(\bar{x},\bar{t}_W)\ d\bar{x} = \underset{\text{Term I}}{\int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} d\bar{x}} + Q(\bar{x})\ \bar{T}(\bar{x},\bar{t}_W) \frac{\partial 1}{\partial \bar{t}_W} - Q(\bar{x})\ \bar{T}(\bar{x},\bar{t}_W) \frac{\partial \bar{\ell}(\bar{t}_W)}{\partial \bar{t}_W}$$

(0)

rearranging

$$\int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x}) \frac{\partial \bar{T}(\bar{x},\bar{t}_W)}{\partial \bar{t}_W} d\bar{x} = \frac{d}{d\bar{t}_W} \int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x})\ \bar{T}(\bar{x},\bar{t}_W)\ d\bar{x} + Q(\bar{x})\ \bar{T}(\bar{x},\bar{t}_W) \frac{\partial \bar{\ell}(\bar{t}_W)}{\partial \bar{t}_W} \qquad \text{(D.1)}$$

Integrating term II by parts

$$\bar{A}\int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x})\,\frac{\partial^2\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}^2}\,d\bar{x} = \bar{A}\,Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Bigg|_{\bar{\ell}(\bar{t}_W)}^{1} - \bar{A}\int_{\bar{\ell}(\bar{t}_W)}^{1} Q'(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\,d\bar{x}$$

Integrating once again by parts yields

$$\bar{A}\int_{\bar{\ell}(\bar{t}_W)}^{1} Q(\bar{x})\,\frac{\partial^2\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}^2}\,d\bar{x} = \bar{A}\,Q(\bar{x})\,\frac{\partial\bar{T}(\bar{x},\bar{t}_W)}{\partial\bar{x}}\Bigg|_{\bar{\ell}(\bar{t}_W)}^{1} - \bar{A}\,Q'(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\Big|_{\bar{\ell}(\bar{t}_W)}^{1} + \bar{A}\int_{\bar{\ell}(\bar{t}_W)}^{1} Q''(\bar{x})\,\bar{T}(\bar{x},\bar{t}_W)\,d\bar{x}$$

Substituting (D.1) and (D.2) into equation (3.3) yields equation (3.4).

APPENDIX E

DERIVATION OF EQUATIONS (3.10) AND (3.11)

Substituting equations (3.8) and (3.9) into equation (3.7) yields

$$\frac{d}{d\bar{t}_W}\int_0^1 \cos(m\pi\bar{x}) \sum_{n=0}^{N} A_n(\bar{t}_W)\cos(n\pi\bar{x})\,d\bar{x} =$$

$$\text{I}$$

$$\cos(m\pi\bar{x})\Big|_{\bar{x}=\bar{\ell}} \bar{H}\frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} + \cos(m\pi)$$

$$\text{II} \qquad\qquad \text{III}$$

$$-(m\pi)\sin(m\pi\bar{x}) \sum_{n=0}^{N} A_n(\bar{t}_W)\cos(n\pi\bar{x})\Big|_{\bar{x}=0}$$

$$\text{IV}$$

$$+(m\pi)\sin(m\pi\bar{x}) \sum_{n=0}^{N} A_n(\bar{t}_W)\cos(n\pi\bar{x})\Big|_{\bar{x}=1}$$

$$\text{V}$$

$$-\int_0^1 (m\pi)^2 \cos(m\pi\bar{x}) \sum_{n=0}^{N} A_n(\bar{t}_W)\cos(n\pi\bar{x})\,d\bar{x} \qquad \text{(E.1)}$$

$$\text{VI}$$

For $\bar{x} = 0$

$$\sin(m\pi\bar{x}) = \sin(0) = 0.$$

For $\bar{x} = 1$, $\sin(m\pi\bar{x})$ reduces to $\sin(m\pi)$ which is zero for $m = 0,1,2,\ldots,M$, therefore terms IV and V are zero. Since the cosine is

an orthogonal function to itself on the interval [0,1], terms I and VI exist for m = n only and are zero for all m ≠ n. Equation (E.1) reduces to

$$\int_0^1 \cos^2 (n\pi \bar{x}) \frac{dA_n(\bar{t}_W)}{d\bar{t}_W} d\bar{x} = \cos (n\pi \bar{\ell}) \bar{H} \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}} + \cos (n\pi) - \int_0^1 (n\pi)^2 \cos^2 (n\pi \bar{x}) A_n(\bar{t}_W) d\bar{x}$$

rearranging

$$\frac{dA_n(\bar{t}_W)}{d\bar{t}_W} \int_0^1 \cos^2 (n\pi \bar{x}) d\bar{x} = \cos (n\pi \bar{\ell}) \bar{H} \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} + \cos (n\pi) - (n\pi)^2 A_n(\bar{t}_W) \int_0^1 \cos^2 (n\pi \bar{x}) d\bar{x} \quad (E.2)$$

for n ≠ 0

$$\int_0^1 \cos^2(n\pi \bar{x}) = \left[\tfrac{1}{2}\bar{x} + \frac{1}{4\pi n} \sin (2n\pi\bar{x}) \right]_0^1$$

$$= \tfrac{1}{2}\bar{x} \Big|_0^1 = \tfrac{1}{2}$$

Equation (E.2) consequently becomes

$$\frac{dA_n(\bar{t}_W)}{d\bar{t}_W} = 2 \cos (n\pi\bar{\ell}) \bar{H} \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} + 2 \cos (n\pi) - (n\pi)^2 A_n(\bar{t}_W)$$

for n = 0

$$\int_0^1 \cos^2 (0) \pi\bar{x} \, d\bar{x} = \int_0^1 d\bar{x} = 1$$

Therefore

$$\frac{dA_o(\bar{t}_W)}{d\bar{t}_W} = \overline{H} \frac{d\bar{\ell}(\bar{t}_W)}{d\bar{t}_W} + 1$$

APPENDIX F

DERIVATION OF EQUATION (3.13)

Expanding the (N+1) equations represented by equations (3.10) and (3.11)

$$(0) \quad \dot{A}_o + 0 + \ldots - \bar{H}\,\dot{\bar{t}} = 1 \text{ [13]}$$

$$(1) \quad 0 + \dot{A}_1 + \ldots - 2\bar{H}\,\dot{\bar{t}} \cos(\pi \bar{t}) = 2\cos\pi - \pi^2 A_1$$

$$(2) \quad 0 + 0 + A_2 + \ldots - 2\bar{H}\,\dot{\bar{t}} \cos(2\pi \bar{t}) = 2\cos(2\pi) - (2\pi)^2 A_2$$

$$\vdots$$

$$(N) \quad 0 + 0 + \ldots + \dot{A}_N - 2\bar{H}\,\dot{\bar{t}} \cos(N\pi \bar{t}) = 2\cos(N\pi) - (N\pi)^2 A_N$$

Expanding equation (3.12) also

$$\dot{A}_o + \dot{A}_1 \cos(\pi \bar{t}) + \dot{A}_2 \cos(2\pi \bar{t}) + \ldots + \dot{A}_N \cos(N\pi \bar{t})$$

$$- \dot{\bar{t}} \sum_{j=1}^{N} (j\pi) A_j \sin(j\pi \bar{t}) = 0$$

Multiplying each (n) equation by $\cos(n\pi \bar{t})$ and subtracting in turn each (n) equation from equation (3.12) produces

---

[13] The dot used here indicates differentiation with respect to time (e.g. $\dot{A}_o = dA_o(\bar{t}_w)/d\bar{t}_w$).

$$\dot{\ell}\left\{\bar{H}\left[1 + 2\sum_{j=1}^{N}\cos^2(j\pi\bar{\ell})\right] - \sum_{j=1}^{N}(j\pi)A_j \sin(j\pi\bar{\ell})\right\} =$$

$$-\left\{1 + 2\sum_{j=1}^{N}\left[\cos(j\pi)\cos(j\pi\bar{\ell})\right]\right\} + \sum_{j=1}^{N}(j\pi)^2 A_j \cos(j\pi\bar{\ell})$$

Solving for $\dot{\ell}$ yields equation (3.13)

$$\dot{\ell} = -\frac{\left\{1 + 2\sum_{j=1}^{N}\left[\cos(j\pi)\cos(j\pi\bar{\ell})\right]\right\} - \sum_{j=1}^{N}(j\pi)^2 A_j \cos(j\pi\bar{\ell})}{\bar{H}\left\{1 + 2\sum_{j=1}^{N}\cos^2(j\pi\bar{\ell})\right\} - \sum_{j=1}^{N}(j\pi)A_j \sin(j\pi\bar{\ell})}$$

APPENDIX G

INTEGRATION OF EQUATION (3.14)

Rearranging equation (3.14)

$$\frac{d}{d\bar{t}_W} A_n(\bar{t}_W) + (n\pi)^2 A_n(\bar{t}_W) = 2 \cos (n\pi)$$

This is a first order ordinary differential equation of which the integration factor is

$$\mu = \exp (n\pi)^2 \bar{t}_W$$

Thus

$$\frac{d}{d\bar{t}_W} \left(A_n \exp(n\pi)^2 \bar{t}_W \right) = \left(2 \cos (n\pi) \right) \exp (n\pi)^2 \bar{t}_W$$

or integrating

$$A_n(\bar{t}_W) \exp (n\pi)^2 \bar{t}_W = \frac{2 \cos (n\pi)}{(n\pi)^2} \exp (n\pi)^2 \bar{t}_W + c$$

Multiplying by

$$\exp \left[-(n\pi)^2 \bar{t}_W \right]$$

$$A_n(\bar{t}_W) = \frac{2(-1)^n}{(n\pi)^2} + c \exp \left[- (n\pi)^2 \bar{t}_W \right] \qquad (G.1)$$

for $\bar{t}_W = 0$

$$A_n(\bar{t}_W) = 0 \qquad (n > 0)$$

Therefore from (G.1)

$$0 = \frac{2(-1)^n}{(n\pi)^2} + c \exp \left[-(n\pi)^2 (0) \right]$$

or

$$c = -\frac{2(-1)^n}{(n\pi)^2}$$

and finally

$$A_n(\bar{t}_W) = \frac{2(-1)^n}{(n\pi)^2}\left\{\exp\left[-(n\pi)^2 t_W\right] - 1\right\}$$

APPENDIX H

EVALUATION OF PARAMETERS $\bar{A}$ AND $\bar{K}$

To obtain some idea of the relevance of these non-dimensional parameters, water and white fir are considered in a volumetric ratio of one to four.

The mean specific heats of water and white fir in the temperature range of 32-212° F are approximately

$$C_{H_2O} = 1.004 \text{ Btu/lb}_m \ ^oF$$

$$C_{fir} = .65 \text{ Btu/lb}_m \ ^oF$$

The average densities of these substances within the same temperature range are approximately

$$\rho_{H_2O} = 61.582 \text{ lb}_m/ft^3$$

$$\rho_{fir} = 27.0 \text{ lb}_m/ft^3$$

Assuming constant thermal conductivities of

$$K_{H_2O} = .367 \text{ Btu ft/hr ft}^2 \ ^oF$$

$$K_{fir} = .069 \text{ Btu ft/hr ft}^2 \ ^oF$$

On a unit volumetric basis

$$K_W = .8(K_{fir}) + .2(K_{H_2O})$$

$$K_W = .1286 \text{ Btu ft/hr ft}^2 \ ^oF$$

Therefore,

$$\overline{K} = \frac{K_D}{K_W} = \frac{K_{fir}}{K_W} = .537$$

From Table II

$$\overline{A} = \frac{\alpha_D}{\alpha_W} = \frac{K_D}{K_W} \cdot \frac{\rho_W C_W}{\rho_D C_D} = \overline{K} \cdot \frac{\rho_W C_W}{\rho_D C_D}$$

where

$$\rho_W C_W = .8(\rho_{FIR} C_{fir}) + .2(\rho_{H_2O} C_{H_2O})$$

$$= (14.04 + 12.366) \text{ Btu/ft}^3 \text{ }^\circ\text{F}$$

$$= 26.406 \text{ Btu/ft}^3 \text{ }^\circ\text{F}$$

and

$$\rho_D C_D = \rho_{fir} C_{fir} = 17.55 \text{ Btu/ft}^3 \text{ }^\circ\text{F}$$

Therefore,

$$\overline{A} = (.537) \frac{26.406}{17.55} = .808$$

APPENDIX I

COMPUTER LISTING OF ALL PROGRAMS

80/80 LIST

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      0000000001111111112222222222333333333344444444455555555556666666667777777778
      1234567890123456789012345678901234567890123456789012345678901234567890123456789
CARD
0001  C*******************************************************************************MAIN0010
0002  C***                            MAIN SECTION                                  ***MAIN0020
0003  C***                         (INITIALIZATION)                                 ***MAIN0030
0004  C*******************************************************************************MAIN0040
0005        EXTERNAL DERFUN,DEROUT                                                    MAIN0050
0006        DOUBLE PRECISION ETA1(10),ETA2(10),H,DLDT,G,TV,T,ONE,ZERO,CH20,           MAIN0060
0007       *                 TEND,TMIN,TPRT,PI,EL,DELI                               MAIN0070
0008        COMMON/COM1/ETA1,ETA2,H,DLDT,G,TV,T,ONE,ZERO,CH20,TEND,TMIN,TPRT,         MAIN0080
0009       *            PI,EL,DELI,                                                  MAIN0090
0010       *           N,MCOUNT,NCOUNT,NPRNT,NSTEP,ISTEP,ISTART,                     MAIN0100
0011       *           NM1,NP1,NP2                                                   MAIN0110
0012        DOUBLE PRECISION TX,Y(36),DERY(36),A(24),                                 MAIN0120
0013  C                                                                               MAIN0130
0014  C                 THE ABOVE SPECIFICATION CARDS ARE COMMON                      MAIN0140
0015  C                 TO - 'MAIN' , 'DEROUT' , & 'DERFUN'                           MAIN0150
0016  C                 THE FOLLOWING SPECIFICATIONS ARE PARTICULAR                   MAIN0160
0017  C                          TO  'MAIN'                                           MAIN0170
0018  C                                                                               MAIN0180
0019       *               AUX(16,36),PRMT(5),ASUM,RSUM,PINSQ,                      MAIN0190
0020       *               HFG,ROW,CP,QQ,THERMK,TR,TB,ELL,                          MAIN0200
0021       *               DEL,DLMN,ERMX,DCOS,DSIN                                  MAIN0210
0022  1000  FORMAT(I3)                                                              MAIN0220
0023  1001  FORMAT(D16.8)                                                           MAIN0230
0024  2005  FORMAT('1*************************************************************MAIN0240
0025       *************************************************************************MAIN0250
0026       *****')                                                                  MAIN0260
0027  2006  FORMAT(' *************************************************************MAIN0270
0028       *************************************************************************MAIN0280
0029       *****')                                                                  MAIN0290
0030  2010  FORMAT(' *************************************************************MAIN0300
0031       *** DATA *****************************************************************MAIN0310
0032       *****')                                                                  MAIN0320
0033  2020  FORMAT(' HFG =',E13.6,'   ROW =',E13.6,'    CP =',E13.6,              MAIN0330
0034       *       /' TR  =',E13.6,'   TB  =',E13.6,'   G   =',E13.6,              MAIN0340
0035       *        '   QQ  =',E13.6,'   EL  =',E13.6,'THERMK =',E13.6             MAIN0350
0036       *        '   H   =',E13.6,'   TV  =',E13.6)                             MAIN0360
0037  2040  FORMAT(' TEND=',E13.6,'   DEL =',E13.6,'   DELI=',E13.6,               MAIN0370
0038       *        '   ERMX=',E13.6,'   DLMN=',E13.6,'   TMIN=',E13.6)           MAIN0380
0039  2050  FORMAT(' ',4('ETA1(',I2,')=',E11.5,' '))                               MAIN0390
0040  2051  FORMAT(' ',4('ETA2(',I2,')=',E11.5,' '))                               MAIN0400
0041  2070  FORMAT(' N = ',I3,5X,'NE = ',I3,5X,'MCOUNT = ',I3,5X,'NPRNT = ',       MAIN0410
0042       *       I3,5X,'NSTEP = ',I3,5X,'ISTART = ',I3)                          MAIN0420
0043  2222  FORMAT(7I5)                                                             MAIN0430
0044  4000  FORMAT(11H S.S. FOR A)                                                  MAIN0440
0045  4444  FORMAT(4E20.6)                                                          MAIN0450
0046  9000  FORMAT('  ERROR = 11  ****  DEL = ',E15.8)                             MAIN0460
0047  9001  FORMAT('  ERROR = 12  ****  DEL = ',E15.8)                             MAIN0470
0048  9002  FORMAT('  ERROR = 13  ****  DEL = ',E15.8,5X,'DLMX = ',E15.8,          MAIN0480
0049       *      5X,'DLMN = ',E15.8)                                              MAIN0490
0050  9010  FORMAT (' ***** ENTIRE TIME INTERVAL EXECUTED   TEND = ',              MAIN0500
0051       *       D16.6,'***** IHLF = ',I4,'**** PRMT(5) = ',D16.6,'****')        MAIN0510
0052  9020  FORMAT('0***** NPRNT IS BEYOND CAPABILITY OF PLOTIT *****')           MAIN0520
0053  9030  FORMAT('0   *** ISTART =',I3)                                          MAIN0530
0054  9701  FORMAT('0',6('A',I2,' =',D14.6,2X))                                    MAIN0540
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80/80 LIST

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     00000000011111111112222222222333333333344444444445555555556666666666777777777 8
     12345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
0055  9702  FORMAT('0 MAIN '/6(' (',I2,') = ',D12.6))                                MAIN0550
0056  9703  FORMAT('0',6('AP',I2,' =',D14.6,1X))                                     MAIN0560
0057  9704  FORMAT('0',6('T',I2,' =',D14.6,2X))                                      MAIN0570
0058  9705  FORMAT('0',6('TP',I2,' =',D14.6,1X))                                     MAIN0580
0059  9706  FORMAT('0   DLDT =',D16.6)                                               MAIN0590
0060  9708  FORMAT('1 MAIN LEVEL 100')                                               MAIN0600
0061        DATA NDFUN,MDFUN/0,0/                                                    MAIN0610
0062        IF(NDFUN.EQ.0) WRITE(6,9708)                                             MAIN0620
0063        NDFUN = 1                                                                MAIN0630
0064        READ(5,1000) N,MCOUNT,NPRNT,NSTEP,ISTART                                 MAIN0640
0065        READ(5,1001) HFG,ROW,   CP,QO,EL,ELL,THERMK,TO,TB,TEND,DEL,DELI,         MAIN0650
0066       *             ERMX,DLMN,TMIN                                            MAIN0660
0067        READ(5,1001) (ETA1(I),I=1,4),(ETA2(I),I=1,4)                             MAIN0670
0068        NE  = N + 2                                                              MAIN0680
0069        NP1=N+1                                                                  MAIN0690
0070        NP2=N+2                                                                  MAIN0700
0071        NM1 = N - 1                                                              MAIN0710
0072        ZERO = 0.00D+00                                                          MAIN0720
0073        ONE = 1.00D+00                                                           MAIN0730
0074        TX = (QO*ELL)/THERMK                                                     MAIN0740
0075  C                 THE HEAT FLUX PARAMETER 'G' IS INCLUDED                    MAIN0750
0076  C                 FOR FUTURE REFERENCE. THIS STUDY                           MAIN0760
0077  C                 REQUIRES A 'G' OF UNITY.                                   MAIN0770
0078        G = TX/TR                                                              MAIN0780
0079        H =(HFG*ROW) / (TX*CP)                                                 MAIN0790
0080        TV  = ((TB/TO) - ONE) /G                                               MAIN0800
0081        PI  = 3.141592653600                                                   MAIN0810
0082        DLDT = ZERO                                                            MAIN0820
0083        PRMT(5) = ZERO                                                         MAIN0830
0084        NCOUNT = 0                                                             MAIN0840
0085        ISTEP = 0                                                              MAIN0850
0086     2  WRITE(6,2006)                                                          MAIN0860
0087        WRITE(6,2010)                                                          MAIN0870
0088        WRITE(6,2006)                                                          MAIN0880
0089        WRITE(6,2020) HFG,ROW,CP,QO,EL,THERMK,TR,TB,G,H,TV                     MAIN0890
0090        WRITE(6,2070) N,NE,MCOUNT,NPRNT,NSTEP,ISTART                           MAIN0900
0091        WRITE(6,2040) TEND,DEL,DELI,ERMX,DLMN,TMIN                             MAIN0910
0092        WRITE(6,2050) (I,ETA1(I),I=1,4)                                        MAIN0920
0093        WRITE(6,2051) (I,ETA2(I),I=1,4)                                        MAIN0930
0094        WRITE(6,2006)                                                          MAIN0940
0095        IF(MCOUNT.EQ.0)GO TO 8                                                 MAIN0950
0096        WRITE(7,2222) N,NE,MCOUNT,NPRNT,NSTEP,ISTART,IPT                       MAIN0960
0097        WRITE(7,4444) HFG,ROW,CP,QO,EL,THERMK,TR,TB,ELS,G,H,TV,TEND,           MAIN0970
0098       *              DEL,ERMX,DLMN,TMIN,DELI                                 MAIN0980
0099  C*************************************************************************MAIN0990
0100  C***          CALCULATION OF INITIAL                                    ***MAIN1000
0101  C***                    TEMPERATURE COEFFICIENTS                        ***MAIN1010
0102  C*************************************************************************MAIN1020
0103     8  IF(MDFUN.NE.0) GO TO 268                                            MAIN1030
0104        MDFUN = 1                                                           MAIN1040
0105        T = ZERO                                                            MAIN1050
0106        DO 9 I=1,NP1                                                        MAIN1060
0107        A(I) = ZERO                                                         MAIN1070
0108     9  CONTINUE                                                            MAIN1080
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CARD
0109   10  DO 11 J=1,NP1                                                        MAIN1090
0110       Y(J) = A(J)                                                         MAIN1100
0111   11  CONTINUE                                                           MAIN1110
0112       Y(NP2) = EL                                                         MAIN1120
0113       DERY(NP2) = DLDT                                                    MAIN1130
0114       TX = T                                                              MAIN1140
0115       CALL DEROUT(TX,Y,DERY,IHLF,NE,PRMT)                                 MAIN1150
0116       IF(PRMT(5).NE.0.0D0) GO TO 20                                       MAIN1160
0117       T = T + DELI                                                        MAIN1170
0118       A(1) = G * T                                                        MAIN1180
0119       DO 12 K=2,NP1                                                       MAIN1190
0120       NN = K-1                                                            MAIN1200
0121       PINSQ = (PI*NN)**2                                                  MAIN1210
0122       A(K) =(((2.0D0*((-ONE)**NN)*G)/PINSQ)*(ONE-(ONE/DEXP(PINSQ*T))))   MAIN1220
0123   12  CONTINUE                                                           MAIN1230
0124       GO TO 10                                                            MAIN1240
0125   C*************************************************************************MAIN1250
0126   C***                        START OF INTEGRATION                      ***MAIN1260
0127   C*************************************************************************MAIN1270
0128   20  CONTINUE                                                           MAIN1280
0129       ISTART = 2                                                          MAIN1290
0130       NCOUNT = 11                                                         MAIN1300
0131       DO 21 I=1,NP1                                                       MAIN1310
0132       Y(I) = A(I)                                                         MAIN1320
0133       DERY(I) = ONE/NP2                                                   MAIN1330
0134   21  CONTINUE                                                           MAIN1340
0135       DERY(NP2) = ONE/NP2                                                 MAIN1350
0136       Y(NP2) = EL                                                         MAIN1360
0137       PRMT(1) = T                                                         MAIN1370
0138       PRMT(2) = TEND                                                      MAIN1380
0139       PRMT(3) = DEL                                                       MAIN1390
0140       PRMT(4) = ERMX                                                      MAIN1400
0141       PRMT(5) = ZERO                                                      MAIN1410
0142       TPRT = ZERO                                                         MAIN1420
0143       GO TO 2                                                             MAIN1430
0144    268  CALL DHPCG(PRMT,Y,DERY,NE,IHLF,DERFUN,DEROUT,AUX)                 MAIN1440
0145   C*************************************************************************MAIN1450
0146   C***                        RETURN FROM 'DHPCG'                       ***MAIN1460
0147   C***          IHLF ='  '                                                ***MAIN1470
0148   C***                 11 - MORE THAN 10 BISECTIONS OF THE INITIAL       ***MAIN1480
0149   C***                      INTERVAL ARE NECESSARY FOR SATISFACTORY      ***MAIN1490
0150   C***                      ACCURACY.                                    ***MAIN1500
0151   C***                 12 - INITIAL INCREMENT OF THE INDEPENDENT         ***MAIN1510
0152   C***                      VARIABLE (DEL) = 0.                          ***MAIN1520
0153   C***                 13 - SIGN OF (DEL) NOT EQUAL TO THE SIGN OF       ***MAIN1530
0154   C***                      UPPER BOUND MINUS LOWER BOUND (DLMX-DLMN)    ***MAIN1540
0155   C***                                                                   ***MAIN1550
0156   C***          OTHERWISE -- THE ENTIRE INTEGRATION INTERVAL MUST HAVE   ***MAIN1560
0157   C***          WORKED THROUGH.                                          ***MAIN1570
0158   C*************************************************************************MAIN1580
0159    269  IF(IHLF.NE.11) GO TO 27                                           MAIN1590
0160       WRITE(6,9000) DEL                                                   MAIN1600
0161       WRITE(6,9702) (I,Y(I),I=1,NE),(I,DERY(I),I=1,NE)                    MAIN1610
0162       STOP                                                                MAIN1620
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CARD
0163    27  IF(IHLF.NE.12) GO TO 271                                                MAIN1630
0164        WRITE(6,9001) DEL                                                       MAIN1640
0165        STOP                                                                    MAIN1650
0166    271 IF(IHLF.NE.13) GO TO 28                                                 MAIN1660
0167        WRITE(6,9002) DEL,DLMX,DLMN                                             MAIN1670
0168        STOP                                                                    MAIN1680
0169    28  WRITE(6,9010) TEND,IHLF,PRMT(5)                                         MAIN1690
0170        STOP                                                                    MAIN1700
0171        END                                                                     MAIN1710
0172
0173
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CARD
0001  C                                                                          DHCG  10
0002  C     ....................................................................DHCG  20
0003  C                                                                          DHCG  30
0004  C        SUBROUTINE DHPCG                                                  DHCG  40
0005  C                                                                          DHCG  50
0006  C        PURPOSE                                                           DHCG  60
0007  C           TO SOLVE A SYSTEM OF FIRST ORDER ORDINARY GENERAL              DHCG  70
0008  C           DIFFERENTIAL EQUATIONS WITH GIVEN INITIAL VALUES.              DHCG  80
0009  C                                                                          DHCG  90
0010  C        USAGE                                                             DHCG 100
0011  C           CALL DHPCG (PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)                DHCG 110
0012  C           PARAMETERS FCT AND OUTP REQUIRE AN EXTERNAL STATEMENT.         DHCG 120
0013  C                                                                          DHCG 130
0014  C        DESCRIPTION OF PARAMETERS                                         DHCG 140
0015  C           PRMT   - DOUBLE PRECISION INPUT AND OUTPUT VECTOR WITH         DHCG 150
0016  C                    DIMENSION GREATER THAN OR EQUAL TO 5, WHICH           DHCG 160
0017  C                    SPECIFIES THE PARAMETERS OF THE INTERVAL AND OF       DHCG 170
0018  C                    ACCURACY AND WHICH SERVES FOR COMMUNICATION BETWEENDHCG 180
0019  C                    OUTPUT SUBROUTINE (FURNISHED BY THE USER) AND         DHCG 190
0020  C                    SUBROUTINE DHPCG. EXCEPT PRMT(5) THE COMPONENTS       DHCG 200
0021  C                    ARE NOT DESTROYED BY SUBROUTINE DHPCG AND THEY ARE    DHCG 210
0022  C           PRMT(1)- LOWER BOUND OF THE INTERVAL (INPUT),                  DHCG 220
0023  C           PRMT(2)- UPPER BOUND OF THE INTERVAL (INPUT),                  DHCG 230
0024  C           PRMT(3)- INITIAL INCREMENT OF THE INDEPENDENT VARIABLE         DHCG 240
0025  C                    (INPUT),                                              DHCG 250
0026  C           PRMT(4)- UPPER ERROR BOUND (INPUT). IF ABSOLUTE ERROR IS       DHCG 260
0027  C                    GREATER THAN PRMT(4), INCREMENT GETS HALVED.          DHCG 270
0028  C                    IF INCREMENT IS LESS THAN PRMT(3) AND ABSOLUTE        DHCG 280
0029  C                    ERROR LESS THAN PRMT(4)/50, INCREMENT GETS DOUBLED.DHCG 290
0030  C                    THE USER MAY CHANGE PRMT(4) BY MEANS OF HIS           DHCG 300
0031  C                    OUTPUT SUBROUTINE.                                    DHCG 310
0032  C           PRMT(5)- NO INPUT PARAMETER. SUBROUTINE DHPCG INITIALIZES      DHCG 320
0033  C                    PRMT(5)=0. IF THE USER WANTS TO TERMINATE             DHCG 330
0034  C                    SUBROUTINE DHPCG AT ANY OUTPUT POINT, HE HAS TO       DHCG 340
0035  C                    CHANGE PRMT(5) TO NON-ZERO BY MEANS OF SUBROUTINE     DHCG 350
0036  C                    OUTP. FURTHER COMPONENTS OF VECTOR PRMT ARE           DHCG 360
0037  C                    FEASIBLE IF ITS DIMENSION IS DEFINED GREATER          DHCG 370
0038  C                    THAN 5. HOWEVER SUBROUTINE DHPCG DOES NOT REQUIRE     DHCG 380
0039  C                    AND CHANGE THEM. NEVERTHELESS THEY MAY BE USEFUL      DHCG 390
0040  C                    FOR HANDING RESULT VALUES TO THE MAIN PROGRAM          DHCG 400
0041  C                    (CALLING DHPCG) WHICH ARE OBTAINED BY SPECIAL         DHCG 410
0042  C                    MANIPULATIONS WITH OUTPUT DATA IN SUBROUTINE OUTP.     DHCG 420
0043  C           Y      - DOUBLE PRECISION INPUT VECTOR OF INITIAL VALUES       DHCG 430
0044  C                    (DESTROYED).   LATER Y IS THE RESULTING VECTOR OF     DHCG 440
0045  C                    DEPENDENT VARIABLES COMPUTED AT INTERMEDIATE          DHCG 450
0046  C                    POINTS X.                                             DHCG 460
0047  C           DERY   - DOUBLE PRECISION INPUT VECTOR OF ERROR WEIGHTS        DHCG 470
0048  C                    (DESTROYED). THE SUM OF ITS COMPONENTS MUST BE        DHCG 480
0049  C                    EQUAL TO 1.   LATER DERY IS THE VECTOR OF             DHCG 490
0050  C                    DERIVATIVES, WHICH BELONG TO FUNCTION VALUES Y AT     DHCG 500
0051  C                    INTERMEDIATE POINTS X.                                DHCG 510
0052  C           NDIM   - AN INPUT VALUE, WHICH SPECIFIES THE NUMBER OF         DHCG 520
0053  C                    EQUATIONS IN THE SYSTEM.                              DHCG 530
0054  C           IHLF   - AN OUTPUT VALUE, WHICH SPECIFIES THE NUMBER OF        DHCG 540
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CARD
0055  C                       BISECTIONS OF THE INITIAL INCREMENT. IF IHLF GETS  DHCG 550
0056  C                       GREATER THAN 10, SUBROUTINE DHPCG RETURNS WITH     DHCG 560
0057  C                       ERROR MESSAGE IHLF=11 INTO MAIN PROGRAM.           DHCG 570
0058  C                       ERROR MESSAGE IHLF=12 OR IHLF=13 APPEARS IN CASE   DHCG 580
0059  C                       PRMT(3)=0 OR IN CASE SIGN(PRMT(3)).NE.SIGN(PRMT(2)-DHCG 590
0060  C                       PRMT(1)) RESPECTIVELY.                             DHCG 600
0061  C              FCT    - THE NAME OF AN EXTERNAL SUBROUTINE USED. IT        DHCG 610
0062  C                       COMPUTES THE RIGHT HAND SIDES DERY OF THE SYSTEM   DHCG 620
0063  C                       TO GIVEN VALUES OF X AND Y. ITS PARAMETER LIST     DHCG 630
0064  C                       MUST BE X,Y,DERY. THE SUBROUTINE SHOULD NOT        DHCG 640
0065  C                       DESTROY X AND Y.                                   DHCG 650
0066  C              OUTP   - THE NAME OF AN EXTERNAL OUTPUT SUBROUTINE USED.   DHCG 660
0067  C                       ITS PARAMETER LIST MUST BE X,Y,DERY,IHLF,NDIM,PRMT.DHCG 670
0068  C                       NONE OF THESE PARAMETERS (EXCEPT, IF NECESSARY,    DHCG 680
0069  C                       PRMT(4),PRMT(5),...) SHOULD BE CHANGED BY          DHCG 690
0070  C                       SUBROUTINE OUTP. IF PRMT(5) IS CHANGED TO NON-ZERO,DHCG 700
0071  C                       SUBROUTINE DHPCG IS TERMINATED.                    DHCG 710
0072  C              AUX    - DOUBLE PRECISION AUXILIARY STORAGE ARRAY WITH 16   DHCG 720
0073  C                       ROWS AND NDIM COLUMNS.                             DHCG 730
0074  C                                                                          DHCG 740
0075  C          REMARKS                                                         DHCG 750
0076  C             THE PROCEDURE TERMINATES AND RETURNS TO CALLING PROGRAM, IF  DHCG 760
0077  C             (1) MORE THAN 10 BISECTIONS OF THE INITIAL INCREMENT ARE     DHCG 770
0078  C                 NECESSARY TO GET SATISFACTORY ACCURACY (ERROR MESSAGE    DHCG 780
0079  C                 IHLF=11),                                                DHCG 790
0080  C             (2) INITIAL INCREMENT IS EQUAL TO 0 OR HAS WRONG SIGN        DHCG 800
0081  C                 (ERROR MESSAGES IHLF=12 OR IHLF=13),                     DHCG 810
0082  C             (3) THE WHOLE INTEGRATION INTERVAL IS WORKED THROUGH,        DHCG 820
0083  C             (4) SUBROUTINE OUTP HAS CHANGED PRMT(5) TO NON-ZERO.         DHCG 830
0084  C                                                                          DHCG 840
0085  C          SUBROUTINES AND FUNCTION SUBPROGRAMS REQUIRED                   DHCG 850
0086  C             THE EXTERNAL SUBROUTINES FCT(X,Y,DERY) AND                   DHCG 860
0087  C             OUTP(X,Y,DERY,IHLF,NDIM,PRMT) MUST BE FURNISHED BY THE USER.DHCG 870
0088  C                                                                          DHCG 880
0089  C          METHOD                                                          DHCG 890
0090  C             EVALUATION IS DONE BY MEANS OF HAMMING'S MODIFIED PREDICTOR-DHCG 900
0091  C             CORRECTOR METHOD. IT IS A FOURTH ORDER METHOD, USING 4       DHCG 910
0092  C             PRECEEDING POINTS FOR COMPUTATION OF A NEW VECTOR Y OF THE   DHCG 920
0093  C             DEPENDENT VARIABLES.                                         DHCG 930
0094  C             FOURTH ORDER RUNGE-KUTTA METHOD SUGGESTED BY RALSTON IS      DHCG 940
0095  C             USED FOR ADJUSTMENT OF THE INITIAL INCREMENT AND FOR          DHCG 950
0096  C             COMPUTATION OF STARTING VALUES.                              DHCG 960
0097  C             SUBROUTINE DHPCG AUTOMATICALLY ADJUSTS THE INCREMENT DURING  DHCG 970
0098  C             THE WHOLE COMPUTATION BY HALVING OR DOUBLING.                DHCG 980
0099  C             TO GET FULL FLEXIBILITY IN OUTPUT, AN OUTPUT SUBROUTINE      DHCG 990
0100  C             MUST BE CODED BY THE USER.                                   DHCG1000
0101  C             FOR REFERENCE, SEE                                           DHCG1010
0102  C             (1)  RALSTON/WILF, MATHEMATICAL METHODS FOR DIGITAL          DHCG1020
0103  C                  COMPUTERS, WILEY, NEW YORK/LONDON, 1960, PP.95-109.     DHCG1030
0104  C             (2)  RALSTON, RUNGE-KUTTA METHODS WITH MINIMUM ERROR BOUNDS,DHCG1040
0105  C                  MTAC, VOL.16, ISS.80 (1962), PP.431-437.                DHCG1050
0106  C                                                                          DHCG1060
0107  C      ..................................................................DHCG1070
0108  C                                                                          DHCG1080
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CARD
0109          SUBROUTINE DHPCG(PRMT,Y,DERY,NDIM,IHLF,FCT,OUTP,AUX)                DHCG1090
0110  C                                                                            DHCG1100
0111  C                                                                            DHCG1110
0112          DIMENSION PRMT(1),Y(1),DERY(1),AUX(16,1)                             DHCG1120
0113          DOUBLE PRECISION Y,DERY,AUX,PRMT,X,H,Z,DELT,DABS                     DHCG1130
0114          N=1                                                                  DHCG1140
0115          IHLF=0                                                               DHCG1150
0116          X=PRMT(1)                                                            DHCG1160
0117          H=PRMT(3)                                                            DHCG1170
0118          PRMT(5)=0.D0                                                         DHCG1180
0119          DO 1 I=1,NDIM                                                        DHCG1190
0120          AUX(16,I)=0.D0                                                       DHCG1200
0121          AUX(15,I)=DERY(I)                                                    DHCG1210
0122        1 AUX(1,I)=Y(I)                                                        DHCG1220
0123          IF(H*(PRMT(2)-X))3,2,4                                               DHCG1230
0124  C                                                                            DHCG1240
0125  C       ERROR RETURNS                                                        DHCG1250
0126        2 IHLF=12                                                            DHCG1260
0127          GOTO 4                                                               DHCG1270
0128        3 IHLF=13                                                            DHCG1280
0129  C                                                                            DHCG1290
0130  C       COMPUTATION OF DERY FOR STARTING VALUES                              DHCG1300
0131        4 CALL FCT(X,Y,DERY)                                                   DHCG1310
0132  C                                                                            DHCG1320
0133  C       RECORDING OF STARTING VALUES                                         DHCG1330
0134          CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                   DHCG1340
0135          IF(PRMT(5))6,5,6                                                     DHCG1350
0136        5 IF(IHLF)7,7,6                                                        DHCG1360
0137        6 RETURN                                                             DHCG1370
0138        7 DO 8 I=1,NDIM                                                      DHCG1380
0139        8 AUX(8,I)=DERY(I)                                                   DHCG1390
0140  C                                                                            DHCG1400
0141  C       COMPUTATION OF AUX(2,I)                                              DHCG1410
0142          ISW=1                                                                DHCG1420
0143          GOTO 100                                                             DHCG1430
0144  C                                                                            DHCG1440
0145        9 X=X+H                                                              DHCG1450
0146          DO 10 I=1,NDIM                                                       DHCG1460
0147       10 AUX(2,I)=Y(I)                                                      DHCG1470
0148  C                                                                            DHCG1480
0149  C       INCREMENT H IS TESTED BY MEANS OF BISECTION                          DHCG1490
0150       11 IHLF=IHLF+1                                                        DHCG1500
0151          X=X-H                                                                DHCG1510
0152          DO 12 I=1,NDIM                                                       DHCG1520
0153       12 AUX(4,I)=AUX(2,I)                                                  DHCG1530
0154          H=.5D0*H                                                             DHCG1540
0155          N=1                                                                  DHCG1550
0156          ISW=2                                                                DHCG1560
0157          GOTO 100                                                             DHCG1570
0158  C                                                                            DHCG1580
0159       13 X=X+H                                                              DHCG1590
0160          CALL FCT(X,Y,DERY)                                                   DHCG1600
0161          N=2                                                                  DHCG1610
0162          DO 14 I=1,NDIM                                                       DHCG1620
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CARD
0163        AUX(2,I)=Y(I)                                                      DHCG1630
0164     14 AUX(9,I)=DERY(I)                                                   DHCG1640
0165        ISW=3                                                              DHCG1650
0166        GOTO 100                                                           DHCG1660
0167  C                                                                        DHCG1670
0168  C     COMPUTATION OF TEST VALUE DELT                                     DHCG1680
0169     15 DELT=0.D0                                                          DHCG1690
0170        DO 16 I=1,NDIM                                                     DHCG1700
0171     16 DELT=DELT+AUX(15,I)*DABS(Y(I)-AUX(4,I))                            DHCG1710
0172        DELT=.0666666666666667D0*DELT                                      DHCG1720
0173        IF(DELT-PRMT(4))19,19,17                                           DHCG1730
0174     17 IF(IHLF-10)11,18,18                                                DHCG1740
0175  C                                                                        DHCG1750
0176  C     NO SATISFACTORY ACCURACY AFTER 10 BISECTIONS. ERROR MESSAGE.       DHCG1760
0177     18 IHLF=11                                                            DHCG1770
0178        X=X+H                                                              DHCG1780
0179        GOTO 4                                                             DHCG1790
0180  C                                                                        DHCG1800
0181  C     THERE IS SATISFACTORY ACCURACY AFTER LESS THAN 11 BISECTIONS.       DHCG1810
0182     19 X=X+H                                                              DHCG1820
0183        CALL FCT(X,Y,DERY)                                                 DHCG1830
0184        DO 20 I=1,NDIM                                                     DHCG1840
0185        AUX(3,I)=Y(I)                                                      DHCG1850
0186     20 AUX(10,I)=DERY(I)                                                  DHCG1860
0187        N=3                                                                DHCG1870
0188        ISW=4                                                              DHCG1880
0189        GOTO 100                                                           DHCG1890
0190  C                                                                        DHCG1900
0191     21 N=1                                                                DHCG1910
0192        X=X+H                                                              DHCG1920
0193        CALL FCT(X,Y,DERY)                                                 DHCG1930
0194        X=PRMT(1)                                                          DHCG1940
0195        DO 22 I=1,NDIM                                                     DHCG1950
0196        AUX(11,I)=DERY(I)                                                  DHCG1960
0197     220Y(I)=AUX(1,I)+H*(.375D0*AUX(8,I)+.7916666666666667D0*AUX(9,I)      DHCG1970
0198       1-.2083333333333333D0*AUX(10,I)+.04166666666666667D0*DERY(I))       DHCG1980
0199     23 X=X+H                                                              DHCG1990
0200        N=N+1                                                              DHCG2000
0201        CALL FCT(X,Y,DERY)                                                 DHCG2010
0202        CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                 DHCG2020
0203        IF(PRMT(5))6,24,6                                                  DHCG2030
0204     24 IF(N-4)25,200,200                                                  DHCG2040
0205     25 DO 26 I=1,NDIM                                                     DHCG2050
0206        AUX(N,I)=Y(I)                                                      DHCG2060
0207     26 AUX(N+7,I)=DERY(I)                                                 DHCG2070
0208        IF(N-3)27,29,200                                                   DHCG2080
0209  C                                                                        DHCG2090
0210     27 DO 28 I=1,NDIM                                                     DHCG2100
0211        DELT=AUX(9,I)+AUX(9,I)                                             DHCG2110
0212        DELT=DELT+DELT                                                     DHCG2120
0213     28 Y(I)=AUX(1,I)+.3333333333333333D0*H*(AUX(8,I)+DELT+AUX(10,I))      DHCG2130
0214        GOTO 23                                                            DHCG2140
0215  C                                                                        DHCG2150
0216     29 DO 30 I=1,NDIM                                                     DHCG2160
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CARD
0217         DELT=AUX(9,I)+AUX(10,I)                                                DHCG2170
0218         DELT=DELT+DELT+DELT                                                    DHCG2180
0219      30 Y(I)=AUX(1,I)+.375D0*H*(AUX(8,I)+DELT+AUX(11,I))                       DHCG2190
0220         GOTO 23                                                                DHCG2200
0221   C                                                                            DHCG2210
0222   C     THE FOLLOWING PART OF SUBROUTINE DHPCG COMPUTES BY MEANS OF            DHCG2220
0223   C     RUNGE-KUTTA METHOD STARTING VALUES FOR THE NOT SELF-STARTING           DHCG2230
0224   C     PREDICTOR-CORRECTOR METHOD.                                            DHCG2240
0225     100 DO 101 I=1,NDIM                                                        DHCG2250
0226         Z=H*AUX(N+7,I)                                                         DHCG2260
0227         AUX(5,I)=Z                                                             DHCG2270
0228     101 Y(I)=AUX(N,I)+.4D0*Z                                                   DHCG2280
0229   C     Z IS AN AUXILIARY STORAGE LOCATION                                     DHCG2290
0230   C                                                                            DHCG2300
0231         Z=X+.4D0*H                                                             DHCG2310
0232         CALL FCT(Z,Y,DERY)                                                     DHCG2320
0233         DO 102 I=1,NDIM                                                        DHCG2330
0234         Z=H*DERY(I)                                                            DHCG2340
0235         AUX(6,I)=Z                                                             DHCG2350
0236     102 Y(I)=AUX(N,I)+.2969776092477536OD0*AUX(5,I)+.1587596449710358 3D0*ZDHCG2360
0237   C                                                                            DHCG2370
0238         Z=X+.4557372542187894 3D0*H                                            DHCG2380
0239         CALL FCT(Z,Y,DERY)                                                     DHCG2390
0240         DO 103 I=1,NDIM                                                        DHCG2400
0241         Z=H*DERY(I)                                                            DHCG2410
0242         AUX(7,I)=Z                                                             DHCG2420
0243     103 Y(I)=AUX(N,I)+.2181003882259204 7D0*AUX(5,I)-3.0509651486929308D0*     DHCG2430
0244        1AUX(6,I)+3.832864760467010 3D0*Z                                      DHCG2440
0245   C                                                                            DHCG2450
0246         Z=X+H                                                                  DHCG2460
0247         CALL FCT(Z,Y,DERY)                                                     DHCG2470
0248         DO 104 I=1,NDIM                                                        DHCG2480
0249     1040Y(I)=AUX(N,I)+.1747602822626903 7D0*AUX(5,I)-.5514806628787329 4D0*    DHCG2490
0250        1AUX(6,I)+1.2055355993965235D0*AUX(7,I)+.1711847812195190 3D0*         DHCG2500
0251        2H*DERY(I)                                                             DHCG2510
0252         GOTO(9,13,15,21),ISW                                                   DHCG2520
0253   C                                                                            DHCG2530
0254   C     POSSIBLE BREAK-POINT FOR LINKAGE                                       DHCG2540
0255   C                                                                            DHCG2550
0256   C     STARTING VALUES ARE COMPUTED.                                          DHCG2560
0257   C     NOW START HAMMINGS MODIFIED PREDICTOR-CORRECTOR METHOD.                DHCG2570
0258     200 ISTEP=3                                                                DHCG2580
0259     201 IF(N-8)204,202,204                                                     DHCG2590
0260   C                                                                            DHCG2600
0261   C     N=8 CAUSES THE ROWS OF AUX TO CHANGE THEIR STORAGE LOCATIONS           DHCG2610
0262     202 DO 203 N=2,7                                                           DHCG2620
0263         DO 203 I=1,NDIM                                                        DHCG2630
0264         AUX(N-1,I)=AUX(N,I)                                                    DHCG2640
0265     203 AUX(N+6,I)=AUX(N+7,I)                                                  DHCG2650
0266         N=7                                                                    DHCG2660
0267   C                                                                            DHCG2670
0268   C     N LESS THAN 8 CAUSES N+1 TO GET N                                      DHCG2680
0269     204 N=N+1                                                                  DHCG2690
0270   C                                                                            DHCG2700
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CARD
0271  C      COMPUTATION OF NEXT VECTOR Y                                          DHCG2710
0272         DO 205 I=1,NDIM                                                      DHCG2720
0273         AUX(N-1,I)=Y(I)                                                      DHCG2730
0274    205  AUX(N+6,I)=DERY(I)                                                   DHCG2740
0275         X=X+H                                                                DHCG2750
0276    206  ISTEP=ISTEP+1                                                        DHCG2760
0277         DO 207 I=1,NDIM                                                      DHCG2770
0278        0DELT=AUX(N-4,I)+1.3333333333333333D0*H*(AUX(N+6,I)+AUX(N+6,I)-       DHCG2780
0279        1AUX(N+5,I)+AUX(N+4,I)+AUX(N+4,I))                                    DHCG2790
0280         Y(I)=DELT-.9256198347107438D0*AUX(16,I)                              DHCG2800
0281    207  AUX(16,I)=DELT                                                       DHCG2810
0282  C      PREDICTOR IS NOW GENERATED IN ROW 16 OF AUX, MODIFIED PREDICTOR      DHCG2820
0283  C      IS GENERATED IN Y. DELT MEANS AN AUXILIARY STORAGE.                  DHCG2830
0284  C                                                                           DHCG2840
0285         CALL FCT(X,Y,DERY)                                                   DHCG2850
0286  C      DERIVATIVE OF MODIFIED PREDICTOR IS GENERATED IN DERY                DHCG2860
0287  C                                                                           DHCG2870
0288         DO 208 I=1,NDIM                                                      DHCG2880
0289        0DELT=.125D0*(9.D0*AUX(N-1,I)-AUX(N-3,I)+3.D0*H*(DERY(I)+AUX(N+6,I)DHCG2890
0290        1+AUX(N+6,I)-AUX(N+5,I)))                                            DHCG2900
0291         AUX(16,I)=AUX(16,I)-DELT                                             DHCG2910
0292    208  Y(I)=DELT+.07438016528925620D0*AUX(16,I)                             DHCG2920
0293  C                                                                           DHCG2930
0294  C      TEST WHETHER H MUST BE HALVED OR DOUBLED                             DHCG2940
0295         DELT=0.D0                                                            DHCG2950
0296         DO 209 I=1,NDIM                                                      DHCG2960
0297    209  DELT=DELT+AUX(15,I)*DABS(AUX(16,I))                                  DHCG2970
0298         IF(DELT-PRMT(4))210,222,222                                          DHCG2980
0299  C                                                                           DHCG2990
0300  C      H MUST NOT BE HALVED. THAT MEANS Y(I) ARE GOOD.                      DHCG3000
0301    210  CALL FCT(X,Y,DERY)                                                   DHCG3010
0302         CALL OUTP(X,Y,DERY,IHLF,NDIM,PRMT)                                   DHCG3020
0303         IF(PRMT(5))212,211,212                                               DHCG3030
0304    211  IF(IHLF-11)213,212,212                                               DHCG3040
0305    212  RETURN                                                               DHCG3050
0306    213  IF(H*(X-PRMT(2)))214,212,212                                        DHCG3060
0307    214  IF(DABS(X-PRMT(2))-.1D0*DABS(H))212,215,215                         DHCG3070
0308    215  IF(DELT-.02D0*PRMT(4))216,216,201                                   DHCG3080
0309  C                                                                           DHCG3090
0310  C                                                                           DHCG3100
0311  C      H COULD BE DOUBLED IF ALL NECESSARY PRECEEDING VALUES ARE            DHCG3110
0312  C      AVAILABLE                                                            DHCG3120
0313    216  IF(IHLF)201,201,217                                                  DHCG3130
0314    217  IF(N-7)201,218,218                                                   DHCG3140
0315    218  IF(ISTEP-4)201,219,219                                               DHCG3150
0316    219  IMOD=ISTEP/2                                                         DHCG3160
0317         IF(ISTEP-IMOD-IMOD)201,220,201                                       DHCG3170
0318    220  H=H+H                                                                DHCG3180
0319         IHLF=IHLF-1                                                          DHCG3190
0320         ISTEP=0                                                              DHCG3200
0321         DO 221 I=1,NDIM                                                      DHCG3210
0322         AUX(N-1,I)=AUX(N-2,I)                                                DHCG3220
0323         AUX(N-2,I)=AUX(N-4,I)                                                DHCG3230
0324         AUX(N-3,I)=AUX(N-6,I)                                                DHCG3240
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CARD
0325        AUX(N+6,I)=AUX(N+5,I)                                                  DHCG3250
0326        AUX(N+5,I)=AUX(N+3,I)                                                  DHCG3260
0327        AUX(N+4,I)=AUX(N+1,I)                                                  DHCG3270
0328        DELT=AUX(N+6,I)+AUX(N+5,I)                                             DHCG3280
0329        DELT=DELT+DELT+DELT                                                    DHCG3290
0330      2210AUX(16,I)=8.962962962962963D0*(Y(I)-AUX(N-3,I))                      DHCG3300
0331         1-3.36111111111111111D0*H*(DERY(I)+DELT+AUX(N+4,I))                   DHCG3310
0332        GOTO 201                                                               DHCG3320
0333  C                                                                            DHCG3330
0334  C                                                                            DHCG3340
0335  C     H MUST BE HALVED                                                       DHCG3350
0336      222 IHLF=IHLF+1                                                          DHCG3360
0337        IF(IHLF-10)223,223,210                                                 DHCG3370
0338      223 H=.5D0*H                                                             DHCG3380
0339        ISTEP=0                                                                DHCG3390
0340        DO 224 I=1,NDIM                                                        DHCG3400
0341       JY(I)=.390625D-2*(8.D1*AUX(N-1,I)+135.D0*AUX(N-2,I)+4.D1*AUX(N-3,I))DHCG3410
0342       1+AUX(N-4,I))-.1171875D0*(AUX(N+6,I)-6.D0*AUX(N+5,I)-AUX(N+4,I))*H DHCG3420
0343       0AUX(N-4,I)=.390625D-2*(12.D0*AUX(N-1,I)+135.D0*AUX(N-2,I)+          DHCG3430
0344       1108.D0*AUX(N-3,I)+AUX(N-4,I))-.0234375D0*(AUX(N+6,I)+               DHCG3440
0345       218.D0*AUX(N+5,I)-9.D0*AUX(N+4,I))*H                                   DHCG3450
0346        AUX(N-3,I)=AUX(N-2,I)                                                  DHCG3460
0347      224 AUX(N+4,I)=AUX(N+5,I)                                                DHCG3470
0348        X=X-H                                                                  DHCG3480
0349        DELT=X-(H+H)                                                           DHCG3490
0350        CALL FCT(DELT,Y,DERY)                                                  DHCG3500
0351        DO 225 I=1,NDIM                                                        DHCG3510
0352        AUX(N-2,I)=Y(I)                                                        DHCG3520
0353        AUX(N+5,I)=DERY(I)                                                     DHCG3530
0354      225 Y(I)=AUX(N-4,I)                                                      DHCG3540
0355        DELT=DELT-(H+H)                                                        DHCG3550
0356        CALL FCT(DELT,Y,DERY)                                                  DHCG3560
0357        DO 226 I=1,NDIM                                                        DHCG3570
0358        DELT=AUX(N+5,I)+AUX(N+4,I)                                             DHCG3580
0359        DELT=DELT+DELT+DELT                                                    DHCG3590
0360       0AUX(16,I)=8.962962962962963D0*(AUX(N-1,I)-Y(I))                      DHCG3600
0361       1-3.36111111111111111D0*H*(AUX(N+6,I)+DELT+DERY(I))                   DHCG3610
0362      226 AUX(N+3,I)=DERY(I)                                                   DHCG3620
0363        GOTO 206                                                               DHCG3630
0364        END                                                                    DHCG3640
0365
0366
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CARD
0001        SUBROUTINE DERFUN(TX,Y,DERY)                                          DFUN0010
0002   C*****************************************************************DFUN0020
0003   C***                      ROUTINE TO EVALUATE THE                      ***DFUN0030
0004   C***                      DERIVATIVE OF (NE)                           ***DFUN0040
0005   C***                      TEMPERATURE COEFFICIENTS                     ***DFUN0050
0006   C*****************************************************************DFUN0060
0007        DOUBLE PRECISION ETA1(10),ETA2(10),H,DLDT,G,TV,T,ONE,ZERO,CH2O,    DFUN0070
0008       *                 TEND,TMIN,TPRT,PI,EL,DELI                          DFUN0080
0009        COMMON/COM1/ETA1,ETA2,H,DLDT,G,TV,T,ONE,ZERO,CH2O,TEND,TMIN,TPRT,  DFUN0090
0010       *            PI,EL,DELI,                                            DFUN0100
0011       *            N,MCOUNT,NCOUNT,NPRNT,NSTEP,ISTEP,ISTART,              DFUN0110
0012       *            NM1,NP1,NP2                                            DFUN0120
0013        DOUBLE PRECISION TX,Y(36),DERY(36),A(24),                          DFUN0130
0014   C                                                                       DFUN0140
0015   C                 THE ABOVE SPECIFICATION CARDS ARE COMMON              DFUN0150
0016   C                 TO - 'MAIN' , 'DEROUT' , & 'DERFUN'                   DFUN0160
0017   C                 THE FOLLOWING SPECIFICATIONS ARE PARTICULAR           DFUN0170
0018   C                       TO  'DERFUN'                                    DFUN0180
0019   C                                                                       DFUN0190
0020       *               DA(24),DEXP,      ASUM,BSUM,CSUM,DSUM,ABSUM,       DFUN0200
0021       *               CDSUM,COSJPI,COSJPL,SINJPL,DCOS,DSIN               DFUN0210
0022   6000  FORMAT(' ',6(E12.6))                                               DFUN0220
0023   9708  FORMAT('0 DERFUN LEVEL 100')                                       DFUN0230
0024        DATA NDFUN/0/                                                      DFUN0240
0025        IF(NDFUN.EQ.0) WRITE(6,9708)                                       DFUN0250
0026        NDFUN = 1                                                          DFUN0260
0027        NE = N + 2                                                         DFUN0270
0028   C*****************************************************************DFUN0280
0029   C***                                                                 ***DFUN0285
0030   C*****************************************************************DFUN0290
0031     10  DO 11 J=1,NP1                                                     DFUN0300
0032         A(J) = Y(J)                                                      DFUN0310
0033     11  CONTINUE                                                         DFUN0320
0034         EL   = Y(NP2)                                                    DFUN0330
0035   C*****************************************************************DFUN0340
0036   C***              CALCULATION OF TEMPERATURE DERIVATIVE              ***DFUN0350
0037   C*****************************************************************DFUN0360
0038     20  ASUM = ZERO                                                      DFUN0370
0039         BSUM = ZERO                                                      DFUN0380
0040         CSUM = ZERO                                                      DFUN0390
0041         DSUM = ZERO                                                      DFUN0400
0042         DO 21 J=1,N                                                      DFUN0410
0043         COSJPI = DCOS(J*PI)                                              DFUN0420
0044         COSJPL = DCOS(J*PI*EL)                                           DFUN0430
0045         SINJPL = DSIN(J*PI*EL)                                           DFUN0440
0046         ASUM   = ASUM + (COSJPI*COSJPL)                                  DFUN0450
0047         BSUM   = BSUM + (A(J+1)*((PI*J)**2)*COSJPL)                      DFUN0460
0048         CSUM   = CSUM + (COSJPL**2)                                      DFUN0470
0049         DSUM   = DSUM + (A(J+1)*(PI*J)*SINJPL)                           DFUN0480
0050     21  CONTINUE                                                         DFUN0490
0051         ABSUM = (G*((2.0D0*ASUM) +ONE))- BSUM                            DFUN0500
0052         CDSUM = (H*((2.0D0*CSUM)+ONE))- DSUM                             DFUN0510
0053         DLDT  = -(ABSUM/CDSUM)                                           DFUN0520
0054         DA(1)  = (H*DLDT)+G                                              DFUN0530
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CARD
0055        DO 22 J=1,N                                                          DFUN0540
0056        ASUM   = DCOS(J*PI*EL)*H*DLDT                                        DFUN0550
0057        BSUM   = ((-ONE)**J)*G                                               DFUN0560
0058        DA(J+1) = (2.0D0*(ASUM+BSUM))-(((PI*J)**2)*A(J+1))                   DFUN0570
0059     22 CONTINUE                                                             DFUN0580
0060     30 DO 31 J=1,NP1                                                        DFUN0590
0061        DERY(J) = DA(J)                                                      DFUN0600
0062     31 CONTINUE                                                             DFUN0610
0063        DERY(NP2) = DLDT                                                     DFUN0620
0064        RETURN                                                               DFUN0630
0065        END                                                                  DFUN0640
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     12345678901234567890123456789012345678901234567890123456789012345678901234567890
CARD
0001        SUBROUTINE DEROUT(TX,Y,DERY,IHLF,NE,PRMT)                          DOUT0010
0002   C*****************************************************************DOUT0020
0003   C***                          OUTPUT ROUTINE                       ***DOUT0030
0004   C*****************************************************************DOUT0040
0005        DOUBLE PRECISION ETA1(10),ETA2(10),H,DLDT,G,TV,T,ONE,ZERO,CH2O,    DOUT0050
0006       *                 TEND,TMIN,TPRT,PI,EL,DELI                        DOUT0060
0007        COMMON/COM1/ETA1,ETA2,H,DLDT,G,TV,T,ONE,ZERO,CH2O,TEND,TMIN,TPRT,  DOUT0070
0008       *            PI,EL,DELI,                                           DOUT0080
0009       *            N,MCOUNT,NCOUNT,NPRNT,NSTEP,ISTEP,ISTART,             DOUT0090
0010       *            NM1,NP1,NP2                                           DOUT0100
0011        DOUBLE PRECISION TX,Y(36),DERY(36),A(24),                          DOUT0110
0012   C                                                                       DOUT0120
0013   C                 THE ABOVE SPECIFICATION CARDS ARE COMMON              DOUT0130
0014   C                 TO - 'MAIN' , 'DEROUT' , & 'DERFUN'                   DOUT0140
0015   C                 THE FOLLOWING SPECIFICATIONS ARE PARTICULAR           DOUT0150
0016   C                       TO  'DEROUT'                                    DOUT0160
0017   C                                                                       DOUT0170
0018       *               AUX(16,36),PRMT(5),EL,ASUM,TCHK,DABS,               DOUT0180
0019       *               X(10),XX(10),TEMP(10),TTEMP(10),COSPNX,DCOS         DOUT0190
0020   1010  FORMAT(' * TEMPERATURE PROFILE *',98X,'*')                        DOUT0200
0021   1020  FORMAT(' *',9(I1,') X=',F4.2,3X),I2,') X=',F4.2,2X,'*')          DOUT0210
0022   1111  FORMAT(' *',10E12.4,'*')                                         DOUT0220
0023   2010  FORMAT(' * COEFFICIENTS *',105X,'*')                             DOUT0230
0024   2020  FORMAT((' *',5(I1,') A(',I1,') =',E12.5,3X)),'*')                DOUT0240
0025   2777  FORMAT('+',121X,'*')                                             DOUT0250
0026   2888  FORMAT(' *',120X,'*')                                            DOUT0260
0027   2999  FORMAT('0'/'0*************************************************',DOUT0270
0028       *   '**  STEP  ',I4,'  ***********************************',      DOUT0280
0029       *       '************ *******')                                     DOUT0290
0030   3000  FORMAT(' * TIME =  ',E11.5,22X,'INTERFACE RATE = ',E11.5,16X,    DOUT0300
0031       *       ' INTERFACE POSITION = ',E11.5,' *')                        DOUT0310
0032   5000  FORMAT('0 *** DESIRED # OF PRINTS ACCOMPLISHED  NSTEP= ',I3)     DOUT0320
0033   5002  FORMAT(' *****************************************************',DOUT0330
0034       *        '*****************************************************',DOUT0340
0035       *       '*************')                                           DOUT0350
0036   6000  FORMAT('0 *** VAPORIZATION LIMIT REACHED ***')                   DOUT0360
0037   6666  FORMAT(3(E15.8,5X)/I2,8X,E15.8)                                 DOUT0370
0038   9708  FORMAT('0 DEROUT LEVEL 100')                                     DOUT0380
0039        DATA INTSP,NDFUN,TCHK/0,0,0.10D-02/                               DOUT0390
0040        IF(NDFUN.EQ.0) WRITE(6,9708)                                      DOUT0400
0041        NDFUN = 1                                                         DOUT0410
0042        T = TX                                                            DOUT0420
0043        DELT = T-TPRT                                                     DOUT0430
0044        NCOUNT = NCOUNT + 1                                               DOUT0440
0045        INTSP = INTSP + 1.                                                DOUT0450
0046        IF(ISTART.GE.2) GO TO 4                                           DOUT0460
0047   C*****************************************************************DOUT0470
0048   C***                     ITERATIVE CYCLE TO CALCULATE                ***DOUT0480
0049   C***                     THE INERT SOLUTION UP TO                    ***DOUT0490
0050   C***                     THE TEMPERATURE OF VAPORIZATION             ***DOUT0500
0051   C***                     AT THE FRONT SURFACE                        ***DOUT0510
0052   C*****************************************************************DOUT0520
0053        ASUM = ZERO                                                       DOUT0530
0054        X(10) = 0.10D+01                                                  DOUT0540
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CARD
0055       DO 3 I=1,NP1                                                          DOUT0550
0056       II = I-1                                                              DOUT0560
0057       COSPNX = DCOS(PI*II*X(10))                                            DOUT0570
0058       ASUM = ASUM + (Y(I)*COSPNX)                                           DOUT0580
0059     3 CONTINUE                                                              DOUT0590
0060       TEMP(10) = ASUM                                                       DOUT0600
0061       IF(TEMP(10).LT.TV) GO TO 4                                            DOUT0610
0062       IF(TEMP(10).EQ.TV)  GO TO 6                                           DOUT0620
0063       IF(TEMP(10).GT.TV.AND.DABS(TV-TEMP(10)).LE.0.10D-05) GO TO 6          DOUT0630
0064       T = T - DELI                                                          DOUT0640
0065       DELI = DELI/0.10D+02                                                  DOUT0650
0066       RETURN                                                                DOUT0660
0067  C*************************************************************************DOUT0670
0068     6 PRMT(5) = 1.0D0                                                       DOUT0680
0069       GO TO 5                                                               DOUT0690
0070     4 IF(NCOUNT.GE.NPRNT.OR.DELT.GE.TMIN) GO TO 5                           DOUT0700
0071       RETURN                                                                DOUT0710
0072     5 TPRT = T                                                              DOUT0720
0073       NCOUNT = 0                                                            DOUT0730
0074       IF(EL.GE.0.99D0) NCOUNT = 11                                          DOUT0740
0075    10 DO 11 J=1,NP1                                                         DOUT0750
0076       A(J) = Y(J)                                                           DOUT0760
0077    11 CONTINUE                                                             DOUT0770
0078       EL = Y(NP2)                                                           DOUT0780
0079       DLDT = DERY(NP2)                                                      DOUT0790
0080  C*************************************************************************DOUT0800
0081  C*************************** CALCULATION OF **************************DOUT0810
0082  C*************************** TEMPERATURE (X) *************************DOUT0820
0083  C*************************************************************************DOUT0830
0084    20 DO 21 J=1,10                                                         DOUT0840
0085       ASUM = ZERO                                                           DOUT0850
0086       X(J) = J/10.0                                                         DOUT0860
0087       DO 22 I=1,NP1                                                         DOUT0870
0088       II = I-1                                                              DOUT0880
0089       COSPNX = DCOS(PI*II*X(J))                                             DOUT0890
0090       ASUM = ASUM + (A(I)*COSPNX)                                           DOUT0900
0091    22 CONTINUE                                                             DOUT0910
0092       TEMP(J) = ASUM                                                        DOUT0920
0093    21 CONTINUE                                                             DOUT0930
0094    30 DO 31 J=1,8                                                          DOUT0940
0095       ASUM = ZERO                                                           DOUT0950
0096       XX(J) = ETA1(J)*EL                                                    DOUT0960
0097       IF(J.GT.4) XX(J) = (ETA2(J-4)*(ONE-EL)) + EL                          DOUT0970
0098       DO 32 I=1,NP1                                                         DOUT0980
0099       II = I-1                                                              DOUT0990
0100       COSPNX = DCOS(PI*II*XX(J))                                            DOUT1000
0101       ASUM = ASUM + (A(I)*COSPNX)                                           DOUT1010
0102    32 CONTINUE                                                             DOUT1020
0103       TTEMP(J) = ASUM                                                       DOUT1030
0104    31 CONTINUE                                                             DOUT1040
0105       XX(9) = ZERO                                                          DOUT1050
0106       XX(10) = ZERO                                                         DOUT1060
0107       IF(MCOUNT.EQ.0) GO TO 33                                              DOUT1070
0108       WRITE(7,6666) T,DLDT,EL,(I,A(I),I=1,NP1)                              DOUT1080
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CARD
0109  33     WRITE(6,2999) INTSP                                                    DOUT1090
0110         WRITE(6,3000) T,DLDT,EL                                                DOUT1100
0111         WRITE(6,5002)                                                          DOUT1110
0112         WRITE(6,2010)                                                          DOUT1120
0113         WRITE(6,2020) (I,I,A(I),I=1,NP1)                                       DOUT1130
0114         WRITE(6,2777)                                                          DOUT1140
0115         WRITE(6,5002)                                                          DOUT1150
0116         WRITE(6,1010)                                                          DOUT1160
0117         WRITE(6,1020) (I,X(I),I=1,10)                                          DOUT1170
0118         WRITE(6,2888)                                                          DOUT1180
0119         WRITE(6,1111) (TEMP(I),I=1,10)                                         DOUT1190
0120         WRITE(6,5002)                                                          DOUT1200
0121         WRITE(6,1020) (I,XX(I),I=1,8)                                          DOUT1210
0122         WRITE(6,2777)                                                          DOUT1220
0123         WRITE(6,2888)                                                          DOUT1230
0124         WRITE(6,1111) (TTEMP(I),I=1,8)                                         DOUT1240
0125         WRITE(6,2777)                                                          DOUT1250
0126         WRITE(6,5002)                                                          DOUT1260
0127         IF(NSTEP.EQ.0) GO TO 34                                                DOUT1270
0128         ISTEP = ISTEP + 1                                                      DOUT1280
0129         IF(ISTEP.GE.NSTEP) GO TO 40                                            DOUT1290
0130   34    IF(T.GE.TEND) GO TO 40                                                 DOUT1300
0131         IF(EL.LE.0.10D-01) GO TO 50                                            DOUT1310
0132         RETURN                                                                 DOUT1320
0133   40    WRITE(6,5000) NSTEP                                                    DOUT1330
0134         STOP                                                                   DOUT1340
0135   50    WRITE(6,6000)                                                          DOUT1350
0136         STOP                                                                   DOUT1360
0137         END                                                                    DOUT1370
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VITA

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Candidate for the Degree of

Master of Science

Thesis: VAPORIZATION INTERFACE PROPAGATION THROUGH A ONE-DIMENSIONAL POROUS SLAB

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