NUREG/CR-1375
SAND79-1694
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USER'S MANUAL FOR USINT

A Program for Calculating Heat and Mass Transfer in Concrete Subjected to High Heat Fluxes

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Date Published: May 1980

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operated by
Sandia Corporation
for the
U. S. Department of Energy

Prepared for
Division of Reactor Safety Research
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, D.C. 20555
Under Memorandum of Understanding DOE 40-550-75
NRC FIN Nos. A1054 and A1198

8008270224

ABSTRACT

This report is a user's manual for the intelligent application of PROGRAM USINT which is for calculation of heat and mass transfer in concrete subjected to high heating rates. The describing differential equations for energy, mass transfer of water and CO_2 are provided along with appropriate boundary and initial conditions. The concrete is considered to contain two basic regions: wet and dry. In the wet region, steam, CO_2 and liquid water may co-exist but in the dry region there is no liquid water. There is also the possibility of a third region in which there is only liquid water and no gases. Decomposition of the concrete is treated by utilizing first order chemical kinetic equations; three reactions are assumed that treat evaporable water, chemically bound water and CO_2. A modified Clausius-Clapeyron equation is used as the equation of state in the wet region.

The finite difference representations of the partial differential equations are provided including details regarding several models for Darcy's law for two phase flow. The energy equation and certain mass transfer equations are essentially parabolic for which reliable techniques are known; a general implicit procedure is employed that contains the Crank-Nicolson approximation. These procedures permit much larger time steps that the explicit procedure utilized by others. For each time step a very efficient analytical technique is provided for the solution of kinetic equations.

A test case is included that also provides a comparison of the program with some test data. The temperatures, pressures and water release are compared and show excellent agreement. The complete program is available on a microfiche card that is attached.

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NOMENCLATURE

c_p - specific heat

c_{p_1} - specific heat of water vapor

c_{p_2} - specific heat of CO_2

D_1 - Darcy constant defined by eq. (31b)

E - Arrhenius activation energy

$E_2(x)$ - exponential integral defined by eq. (56a)

G_i - related to orthogonal coordinates

h_{fg} - heat of vaporization of water

h_i - related to orthogonal coordinates

$\Delta h_{1'}$ - change in enthalpy due to forming vapor from the evaporable water per unit mass of evaporable water

$\Delta h_{1''}$ - change in enthalpy due to forming vapor from the chemically bound water per unit mass of chemically bound water

Δh_2 - change in enthalpy due to forming CO_2 gas per unit mass of CO

k - thermal conductivity

K - permeability

K_A - Arrhenius frequency factor; see eqs. (13)-(15).

$k_{r\ell}$ - constant in Darcy's law for liquid water;

k_{rm} - constant in Darcy's law; see eqs. (7) and (20f)

L - initial length of concrete

p - total pressure in the pores

p_1 - partial pressure of the water vapor

p_2 - partial pressure of the CO_2

q - surface heat flux

$\dot{Q}$ - heat source term

R - universal gas constant

R_1 - gas constant for water vapor

$\dot{s}_1$ - source of free water; see eq. (9)

$\dot{s}_2$ - source of CO_2

$\dot{s}_3$ - source term for liquid water; see eq. (201)

t - time

T - temperature

u - velocity

U - temperature

u_m - velocity of gas mixture

u_3 - velocity of liquid water

V_{voids} - volume of the voids

V_0 - total volume of the concrete

x - coordinate measured from the heated surface

$\alpha_{1'}$ - evaporable water mass fraction

$\alpha_{1''}$ - chemically bound mass fraction

α_2 - CO_2 mass fraction

β_k - parameter in permeability relation given by (8b)

ε - porosity, see eq. (2c)

$\theta = \frac{V_{vapor}}{V_{total}}$ - volume fraction of vapor; varies from 0 (only liquid) to ε(dry).

μ_m - viscosity of the mixture

μ_3 - viscosity of liquid water

ρ - density

ρ_0 - initial density of concrete

ρ_1 - density of water vapor

ρ_2 - density of CO_2 gas

ρ_3 - density of water

ρ_{2s} - density of CO_2 in its solid state bound in concrete

$\rho^o_{1'}$ - total mass of concrete that can be lost as evaporable water per unit volume of original concrete

$\rho^o_{1''}$ - total mass of concrete that can be lost as chemically bound water per unit volume of concrete

ρ^o_2 - total mass of concrete that can be lost as CO_2 gas per unit volume of concrete

σ - surface tension

User's Manual for USINT

1. INTRODUCTION

This report presents a model for heat and mass transfer in concrete, finite difference approximations of the equations of the model and discussion of a computer program (USINT) for solution of the finite difference equations. Comparisons of the temperature, pressure and water release predicted by the program and measured values are provided.

For the event of an hypothetical core disruptive accident (HCDA) in the current generation of fast reactors, the inherent retention capabilities of concrete and other construction materials must be understood. In an HCDA the high temperature liquid metal coolants and molten core materials are retained by a structure predominantly composed of concrete.

The major phenomena treated include 1) conductive energy transport, 2) chemical decomposition of concrete and 3) two phase-three component heat and mass transfer of the decomposition products: steam, liquid water and carbon dioxide. Another unique aspect of the model is the provision for the porosity to increase as the water and CO_2 are formed from the concrete.

In the numerical solution of several of the finite difference equations, an implicit approach is used. A parameter, η, is incorporated in the equations that permit the equations to vary from forward difference to backward difference approximations; if η is equal to 0.5, a Crank-Nicolson type approximation is used. The equations using these approximations have dependent variables of temperature and partial pressure of the water vapor. Kinetic equations for the decomposition of the concrete are solved exactly for one time step to another assuming that the temperature is known for one time step to the next and varies linearly with time. This method of exact solution greatly reduces the computation that would be required if the kinetic equations were solved using finite differences. The implicit approach in the equations for temperature and partial pressure also has the great advantage over the explicit approach (forward differences) in that much larger time steps can be taken without stability problems.

The numerical procedure has other features that should be mentioned. One of these is that iteration at each time step is not required. In each step a particular order of solution of the equations is used and as the quantities for the next time step become known, they are introduced as needed for the quantities yet to be found. For example, the energy equation is first in each iteration. It produces the temperatures at the next time which can be used in the decomposition equations and mass conservation equations. Another feature is that there are fixed nodes in the code even though there is a moving dry-wet interface. Such nodes are easier to consider because the derivation and programming of the equations is much easier than for moving nodes.

2. DESCRIPTION OF MODEL

Upon heating to sufficiently high temperatures the concrete decomposes with a resulting increase in porosity. At the lowest decomposition temperatures (about 350 K), evaporable water begins to be released. At the somewhat higher temperature of 600 K chemically constituted water begins to be significantly released. Above 900 K carbon dioxide gas is formed and released. The model to be described includes all three of these possible chemical reactions. Since the experiments to date usually have had concrete temperatures below 900 K, the emphasis in the computer program has been on the evaporable and chemically constituted water; though parts of the program consider CO_2, the program is not fully operational for CO_2.

In developing the mathematical description of the heat and mass transfer in terms of partial differential equations, equations of state and constitutive relations, the concrete is assumed to have two regions. The first is called a "wet" region in which water and steam coexist at the same pressure and temperature conditions. This occurs at the lower temperatures. The second main region is a "dry" region in which there is steam and CO_2 gas--no liquid water is present. If one wishes to include air initially in the pores of the concrete, then it could be simulated by having an initial concentration of CO_2 instead since the gas constants of air and CO_2 are not greatly different. Until, however, USINT is checked out for CO_2 this treatment of the air is not permitted by USINT but the equations to be given can be interpreted as including CO_2. A third region is for only water present. This region is usually quite small so that it is not treated by special treatment of the differential equations. Instead a simple constraint is used that is discussed below.

2.1 Assumptions

The major assumptions for the heat and mass transfer in concrete subjected to high heat fluxes are given below.

1. Concrete is idealized as being homogeneous and hence permits one-dimensional analysis provided the heating is uniform over the surface and the geometry can be considered to be a flat plate, long cylinder or other simple basic geometry in which a single space variable is sufficient. Concrete, in reality, is a complex, heterogeneous material in which the temperature and pressure distributions are three-dimensional even for simple basic geometries with uniform-in-space boundary conditions. Consequently, the dependent variables (temperature and pressure,

for example) are considered to be averages over space normal to the space (independent) variable utilized.

2. Concrete is assumed to be a porous medium with connected pores. The porosity, initially uniform in the body, is postulated to increase linearly with the volume loss of evaporable water, chemically constituted water and carbon dioxide.

3. Local thermodynamic equilibrium is considered to exist between the solid concrete and any vapor or liquid passing through the concrete.

4. The liquid that may be present is water and it may move.

5. The water may evaporate or condense. When both water and steam are present, a special equation of state is used to relate the pressure and temperature. The relation is a modified form of the Clausius-Clapeyron equation. This latter equation is not strictly valid because the pores are extremely small.

6. In addition to steam, CO_2 may be present in the gaseous phase.

7. Dalton's law is valid.

8. The perfect gas law is used for both the water vapor and CO_2.

9. Darcy's law can be used for the water vapor, CO_2 and liquid water. The water and the gases need not have the same velocity but the components of the steam-CO_2 mixture have the same velocity.

10. The process is assumed to involve two regions: dry and wet. In the dry region, only water vapor and CO_2 exist in the pores while in the wet region the pores may contain water vapor, liquid water and CO_2.

11. Mass transfer caused by one gas diffusing into another is neglected.

2.2 Model for Dry Region

The models are somewhat different in the dry and wet regions. In each region the basic equations include conservation of energy (one equation), conservation of mass (two equations, one for water of both phases and the other for CO_2) and three empirical kinetic models given by D. Powers (Ref. 1) for the decomposition events yielding volatile products. These three events are assigned to (a) loss of evaporable water, (b) loss of chemically bound water and (c) loss of carbon dioxide.

Energy Equation

The energy equation for the dry region includes net energy transport by conduction, rate of change in internal energy of the concrete, net energy transport by the moving fluid and a heat source term due to decomposition, condensation and/or evaporation. The energy equation is

$$\rho c_{p_s} \frac{\partial T}{\partial t} + \rho c_{p_g} u_m \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x}\right) + \dot{Q} \qquad (1)$$

where

$$\rho c_{p_s} = \rho_0 c_{p_c} (1-\varepsilon) + \varepsilon \rho c_{p_g} \qquad (2a)$$

$$\rho c_{p_g} = \rho_1 c_{p_1} + \rho_2 c_{p_2} \qquad (2b)$$

$$\varepsilon = \frac{V_{voids}}{V_0} = \text{porosity} \qquad (2c)$$

ρ_0 = initial density of concrete, kg/m^3

V_{voids} = volume of the voids, m^3

V_0 = total volume, m^3

c_p = specific heat, kJ/kg-K

k = thermal conductivity, W/m-K

T = temperature, K (In USINT, T is given the symbol U.)

x = distance measured from the heated surface, m

u_m = mixture velocity, m/s

The subscript 1 denotes water vapor and 2 denotes CO_2. The porosity ϵ is a function of time and position. The heat source term, $\dot{Q}$, is present mainly as result of the endothermic reactions involving the production of the CO_2 gas and the water vapor; it is given by

$$\dot{Q} = -\rho^o_{1'}\Delta h_{1'} \frac{\partial \alpha_{1'}}{\partial t} - \rho^o_{1''}\Delta h_{1''} \frac{\partial \alpha_{1''}}{\partial t} - \rho^o_2 \Delta h_2 \frac{\partial \alpha_2}{\partial t} + \frac{\partial (p\epsilon)}{\partial t} \qquad (3)$$

where

$\rho^o_{1'}$ = total mass of original concrete that can be lost as evaporable water per unit volume of original concrete, kg free water/m^3 concrete

$\rho^o_{1''}$ = total mass of concrete that can be lost as chemically bound water per unit volume of concrete, kg chemically bound water/m^3 concrete

ρ^o_2 = total mass of concrete that can be lost as CO_2 gas per unit volume of concrete, kg CO_2/m^3 concrete

$\Delta h_{1'}$ = change in enthalpy due to forming vapor from the evaporable water per unit mass of evaporable water, J/kg

$\Delta h_{1''}$ = change in enthalpy due to forming vapor from the chemically bound water per unit mass of chemically bound water, J/kg

Δh_2 = change in enthalpy due to forming CO_2 gas per unit mass of CO_2, J/kg

$\alpha_{1'}$ = evaporable water mass fraction; ratio of the mass of evaporable water converted to water to the mass of initially available evaporable water in the concrete, kg/m^3 converted evap. H_2O to kg/m^3 initial evap. H_2O.

$\alpha_{1''}$ = chemically bound mass fraction; ratio of the mass of chemically bound water converted to water to the mass of initially available chemically bound water in the concrete

α_2 = CO_2 mass fraction; ratio of the mass of CO_2 in concrete converted to CO_2 gas to the initial mass of CO_2 in the concrete

p = total pressure in the pores, N/m^2

Continuity Equations

Conservation of mass equations are needed for both the water vapor and CO_2. The water vapor mass conservation equation for the dry region is

$$\frac{\partial(\rho_1 \varepsilon)}{\partial t} + \frac{\partial(\rho_1 u_m)}{\partial x} = \dot{s}_1 \qquad (4)$$

The density ρ_1 of the water vapor in a small void is the mass of the water vapor in this void divided by the volume of this void. This density is related to its partial pressure p_1 and temperature T by the perfect gas law,

$$p_1 = \rho_1 R_1 T \qquad (5)$$

where R_1 is the gas constant for water vapor. The total pressure p for both water vapor and CO_2 gas being present is the sum of their partial pressures,

$$p = p_1 + p_2 \tag{6}$$

which is a statement of Dalton's law for this case.

The velocity of the mixture of the water vapor and CO_2, u_m, is found using Darcy's law in the form

$$u_m = -\frac{k_{rm}}{\mu_m} K \frac{\partial p}{\partial x} = -\frac{k_{rm}}{\mu_m} K \frac{\partial (p_1 + p_2)}{\partial x} \tag{7}$$

where

μ_m = viscosity of the mixture, kg/m-s

p = total pressure, N/m^2

K = permeability, m^2

k_{rm} = 1 for no liquid present

Many relations have been proposed for the permeability K in terms of the porosity ε. One of these is on page 141 of Scheidegger [2],

$$K = \frac{\varepsilon^3}{5S_o^2(1-\varepsilon)^2} \tag{8a}$$

which is called the Kozeny-Carman equation and where S_0 is Carman's "specific" surface exposed to the fluid. This expression is used in USINT in the form

$$K = \frac{\varepsilon^3 \beta_k}{(1-\varepsilon)^2} \tag{8b}$$

where β_k is a constant to be found from tests by utilizing parameter estimation.

The source of the free water, $\dot{s}_1$, is the evaporable water and chemically bound water in the concrete; it is given by

$$\dot{s}_1 = \rho^o_{1'} \frac{\partial \alpha_{1'}}{\partial t} + \rho^o_{1''} \frac{\partial \alpha_{1''}}{\partial t} \tag{9}$$

There are several ways that the water vapor continuity equation, (4), can be written. A form is chosen for which the partial pressures appear explicitly. Introducing (5), (6), (7), and (9) into (4) yields the water vapor continuity equation for the dry region,

$$\frac{\partial}{\partial t} \left(\frac{p_1 \varepsilon}{R_1 T}\right) = \frac{\partial}{\partial x} \left[\frac{p_1 k_{rm} K}{R_1 T \mu_m} \frac{\partial (p_1 + p_2)}{\partial x}\right] + \rho^o_{1'} \frac{\partial \alpha_{1'}}{\partial t} + \rho^o_{1''} \frac{\partial \alpha_{1''}}{\partial t} \tag{10}$$

The primary dependent variable in (10) is p_1. If CO_2 is not considered, then p_2 is dropped in (10).

The continuity equation for CO_2 for the dry region is

$$\frac{\partial (\rho_2 \varepsilon)}{\partial t} + \frac{\partial (\rho_2 u_m)}{\partial x} = \dot{s}_2 \tag{11}$$

which can be given in a similar manner as (10) by

$$\frac{\partial}{\partial t} \left(\frac{p_2 \varepsilon}{R_2 T}\right) = \frac{\partial}{\partial x} \left[\frac{p_2 k_{rm} K}{R_2 T \mu_m} \frac{\partial (p_1 + p_2)}{\partial x}\right] + \rho^o_2 \frac{\partial \alpha_2}{\partial t} \tag{12}$$

Both (10) and (12) involve a first derivative of pressure with respect to time and a second derivative of pressure with respect to x. Hence, an initial condition and two boundary conditions are needed for each pressure. The equations display mainly a "parabolic" or diffusive character rather than predominantly an "hyperbolic" or wave behavior. They can be solved numerically in a similar way as the energy equation (1), which is also predominantly diffusive in character for the range of property values of interest. Both continuity equations and the energy equation are nonlinear so that a numerical method of solution is necessary.

Kinetic Equations

The kinetic equations describing the decomposition of the concrete have been given by Powers [1]. They are first order, Arrhenius rate equations,

$$\frac{\partial \alpha_{1'}}{\partial t} = K_{A1'}(1-\alpha_{1'})\exp(-E_{1'}/RT) \qquad (13)$$

$$\frac{\partial \alpha_{1''}}{\partial t} = K_{A1''}(1-\alpha_{1''})\exp(-E_{1''}/RT) \qquad (14)$$

$$\frac{\partial \alpha_{2}}{\partial t} = K_{A2}(1-\alpha_{2})\exp(-E_{2}/RT) \qquad (15)$$

where the subscripts 1', 1" and 2 refer respectively to evaporable water, chemically bound water and CO_2. As before, T is temperature in degrees kelvin. The α's refer to the fraction of reactant decomposed and start at zero and increase to a maximum of unity. K_A is an Arrhenius frequency factor with units of s^{-1}; E is the Arrhenius activation energy (J/kg); R is the universal gas constant (J/kg-K); and t is time in seconds. The ratio E/R has been given by Powers [1] to be 5557, 20560 and 19362K for evaporable water, chemically bound water and CO_2, respectively, for calcareous concrete used in Sandia's light water reactor safety program. The corresponding values of K_A are 21497, 3.2864E10 and 3.296E5 s^{-1}.

The above constants are incorporated into the program but can be changed as better data become available. Since the values were obtained for concrete powders, at one atmosphere and at relatively low, constant rates of temperature rise, the values may not be accurate for solid concrete structures, up to eight atmospheres of internal pressure and for arbitrary and variable rates of temperature rise.

Porosity Equation

A relation between the porosity and certain dependent variables is also needed and is given in subroutine PORE. An assumption made by several investigators is that ε is constant. It is more reasonable to assume that it increases as the concrete decomposes. In USINT a linear relation between ε and $\alpha_{1'}$, $\alpha_{1''}$ and α_2 is utilized. It is

$$\varepsilon = \varepsilon_0 + \frac{\rho^o_{1'}}{\rho_3} \alpha_{1'} + \frac{\rho^o_{1''}}{\rho_3} \alpha_{1''} + \frac{\rho^o_2}{\rho_{2s}} \alpha_2 \qquad (16)$$

where ε_0 is the porosity of the virgin concrete, ρ_3 is the density of water and ρ_{2s} is the density of the CO_2 in its solid state when chemically bound in the concrete. A relation such as (16) for the porosity predicts that ε can increase quite appreciably. For example, for magnetite concrete the initial porosity might be 0.047 but increases to 0.232 as a result of the evaporable and chemically bound water being formed. The CO_2 decomposition would result in ε increasing substantially more. Thonguthai and Bazant [3] have given an expression similar to (16) but even larger increases in ε are permitted by an additional multiplicative factor on the right hand side of (16).

Dependent Variables

There are six dependent variables for the dry region: T, p_1, p_2, $\alpha_{1'}$, $\alpha_{1''}$, and α_2. The porosity ε could also be considered a dependent variable but it can be eliminated by using (16). Also note that

$$\frac{\partial \varepsilon}{\partial t} = \frac{\rho_{1'}}{\rho_3} \frac{\partial \alpha_{1'}}{\partial t} + \frac{\rho_{1''}}{\rho_3} \frac{\partial \alpha_{1''}}{\partial t} + \frac{\rho^o_2}{\rho_{2s}} \frac{\partial \alpha_2}{\partial t} \qquad (17)$$

which can be used in (10) and (12).

A recommended set of equations for the dry region is the energy equation (1) which needs (2), (3) and (7); the continuity equations, (10) and (12); the kinetic equations (13), (14) and (15); and the porosity equation (16).

2.3 Model for Wet Region

In the wet region, water, steam and CO_2 are considered to be in the pores.

Energy Equation

The energy equation for the wet region is

$$\rho c_{p_s} \frac{\partial T}{\partial t} + (\rho c_{p_g} u_m + \rho_3 c_{p_3} u_3) \frac{\partial T}{\partial x} = \frac{\partial}{\partial x} \left(k \frac{\partial T}{\partial x}\right) + \dot{Q} \qquad (19)$$

where

$$\rho c_{p_s} = \rho_0 c_{p_c} (1-\varepsilon) + \rho c_{p_g} \theta + \rho_3 c_{p_3} (\varepsilon-\theta) \qquad (20a)$$

$$\theta = \frac{V_{vapor}}{V_{total}} = \text{volume fraction of vapor (including } CO_2 \text{ gas)} \qquad (20b)$$

$$\rho c_{p_g} = \rho_1 c_{p_1} + \rho_2 c_{p_2} \qquad (20c)$$

$$u_m = - \frac{k_{rm}}{\mu_m} K \frac{\partial p}{\partial x} = - \frac{k_{rm}}{\mu_m} K \frac{\partial (p_1 + p_2)}{\partial x} \qquad (20d)$$

$$u_3 = - \frac{k_{r\ell}}{\mu_3} K \frac{\partial p}{\partial x} = - \frac{k_{r\ell}}{\mu_3} K \frac{\partial (p_1 + p_2)}{\partial x} \qquad (20e)$$

μ_3 = viscosity of water

$$k_{rm} = 1.1 \frac{\theta}{\varepsilon} - .1 \quad \text{for } \frac{.1}{1.1} < \frac{\theta}{\varepsilon} \leq 1$$

$$= 0 \quad \text{for } 0 < \frac{\theta}{\varepsilon} < \frac{.1}{1.1} \qquad (20f)$$

$$k_{r\ell} = \left(1 - \frac{\theta}{\varepsilon}\right)^3 \qquad (20g)$$

$$\dot{Q} = -\rho^{o}_{1'}\Delta h_{1'}\frac{\partial\alpha_{1'}}{\partial t} - \rho^{o}_{1''}\Delta h_{1''}\frac{\partial\alpha_{1''}}{\partial t} - \rho^{o}_{2}\Delta h_{2}\frac{\partial\alpha_{2}}{\partial t}$$

$$- h_{fg}\dot{s}_3 + \frac{\partial}{\partial t}(p\theta) \qquad (20h)$$

$$\dot{s}_3 = -\frac{\partial}{\partial t}\Big[\rho_3(\varepsilon-\theta)\Big] - \frac{\partial(\rho_3 u_3)}{\partial x} \qquad (20i)$$

Expressions (20f) and (20g) are given by Scheidegger (Ref. 2, p.255).

The quantity θ defined by (20b) is the fraction of a element of the total volume of the concrete that is occupied by vapor. If θ is equal to the porosity ε, the voids are only filled with vapor--that is, no liquid water is present. This is the case for the dry region. The other extreme θ value is zero. In this case the voids are completely filled with liquid water.

Mass Transfer Equations

The conservation equation for water vapor and liquid can be derived to be

$$\frac{\partial(\rho_1\theta)}{\partial t} + \frac{\partial(\rho_1 u_m)}{\partial x} + \left[\frac{\partial}{\partial t}\rho_3(\varepsilon-\theta) + \frac{\partial(\rho_3 u_3)}{\partial x}\right] = \dot{s}_1 \qquad (21)$$

where $\dot{s}_1$ is given by (9). Notice that the term inside the brackets of (21) is equal to the negative of $\dot{s}_3$, which is defined by (20i). Using $\dot{s}_3$ in (21), and putting $\dot{s}_3$ on the right hand side indicates that the bracketed term can be considered to be a source term for a water vapor continuity equation; the $\dot{s}_3$ term would represent a source of liquid water.

If Darcy's law is introduced in (21), the water vapor and liquid continuity equation becomes

$$\frac{\partial}{\partial t}\left[\rho_1\theta + \rho_3(\varepsilon-\theta)\right] = \frac{\partial}{\partial x}\left[K\left(\frac{\rho_1 k_{rm}}{\mu_m} + \frac{\rho_3 k_{r\ell}}{\mu_3}\right)\frac{\partial p}{\partial x}\right] + \rho^o_{1'}\frac{\partial \alpha_{1'}}{\partial t} + \rho^o_{1''}\frac{\partial \alpha_{1''}}{\partial t} \tag{22}$$

An equation of state is needed in the wet region to relate the pressure and temperature of the water vapor. A number of investigators have used the Clausius-Clapeyron equation for this purpose. One of these is Dayan [4] although he did not explicitly state how it was utilized. For a liquid being in equilibrium with its vapor, Ref. [5] gives

$$\frac{dp}{dT} = \frac{ph_{fg}}{RT^2} = \frac{ph_{fg}}{T} \tag{23}$$

where the perfect gas law is used and the volume of the liquid is neglected compared to the volume of the vapor. The p in (23) is the partial pressure p_1 of the water vapor and R is the water vapor gas constant. If h_{fg} is independent of the temperature T, (23) can be integrated from $p_1 = p_0$ to p_{1s} and $T = T_0$ to T to get

$$p_{1s} = p_0 \exp\left[-\frac{h_{fg}}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right] \tag{24a}$$

The $\exp(h_{fg}/RT_0)$ term could also be included in the constant before the exponential. If that is done, one can fit the recommended values given by Irvine and Hartnett [6] to within 2% between one and six atmospheres by the equation

$$p_{1s} = 4.76E10\ \exp(-4872/T) \tag{24b}$$

where p_{1s} is in N/m^2 and T is in kelvin.

Unfortunately (24b) is not completely satisfactory as an equation of state inside the concrete even though Dayan [4] and others have been able to fit the measured pressures fairly well using this model. Postma, McCormack and Schur [7] have also matched their data with a model but their model includes more complex relations than the Clausius-Clapeyron equation. Postma et al relate the amount of sorbed water held in the concrete at any position and time to the local temperature and relative humidity (p_1/p_s, where p_s is the saturation pressure for a given temperature and is given by p_{1s} of (24b).) In their view there are three water phases that are in local thermodynamic equilibrium: vapor water, liquid water and solid water. (In the present model the same view is taken although the same terms are not used.) By vapor water is meant ordinary steam that fills a portion of the pores. Liquid water is ordinary unbound water also in a portion of the pores; in <u>their</u> view liquid water can exist only for relative humidities of unity. Solid water is water sorbed by the cement paste and they state that it includes gel water, capillary water and chemically bound water. (In the present paper "evaporable" and chemically bound water are considered.) In effect, the Postma et al [7] relationships involving the sorbed (solid) water and a modified perfect gas relationship provide their equation of state; at least 6 empirical constants are involved.

Another approach similar to that taken by Postma et al [7] is that due to Bazant and Thonguthai [3]. They give sorption isotherms (Fig. 2a in [3]) which are the free water to cement ratio versus relative humidity for fixed temperatures. They also use empirical relations, some of which were found using parameter estimation. The sorption isotherms have three regions: relative humidities 0 to .96, .96 to 1.04 and finally larger than 1.04. Notice that Bazant and Thonguthai [3] specifically include relative humidities greater than unity.

As pointed out by Bazant and Thonguthai [3] and also Whitaker [8], the liquid water being in extremely small capillaries has the effect of greatly increasing the pressure over that given by the Clausius-Clapeyron relation unless the vapor-liquid interface is flat. When surface tension effects are important, one must take into account the effect of curvature and surface tension on the vapor pressure-temperature relation. In the capillary condensation region Defay et al [8, p. 237] suggest that the vapor isotherms can be represented by the Kelvin equation in the form

$$p_{1s} = p_0 \exp(-2\sigma / r\rho_3 RT) \qquad (25)$$

Here r is the radius of the capillary meniscus and σ is the water surface tension. Whitaker [8] combines the Kelvin equation and the Clausius-Clapeyron equation to get

$$p_{1s} = p_0 \exp\left\{-\left[\frac{2\sigma}{r\rho_3 RT} + \frac{h_{fg}}{R}\left(\frac{1}{T} - \frac{1}{T_0}\right)\right]\right\} \qquad (26)$$

which has exactly the same explicit dependence on temperature T as does the Clausius-Clapeyron equation.

Rather than utilize the relatively complex relations for the equation of state given in [3] and [7], which are different and involve a number of empirical constants, it was decided to modify the Clausius-Clapeyron equation. In the future as more consistent information becomes available a better equation of state can be introduced into computer program USINT.

For the lower temperatures an equation of the Clausius-Clapeyron form is chosen that gives approximately one atmosphere partial pressure at room temperature. The expression is

$$p_{1s} = 2.654E7\ e^{-1594/T} \qquad (27)$$

from the lowest temperatures to 437.6 K above which (24b) is utilized. At 286 K, (27) gives a partial pressure of about one atmosphere.

The steam density in the wet region is found by using the perfect gas law with the pressure replaced by either (27) for T < 437.6 K and (24b) above 437.6 K. More explicitly

$$\rho_1 = C_1/(R_1 T\, e^{C_2/T}) \quad \text{for} \quad T < 437.6 \text{ K} \tag{28a}$$

$$\rho_1 = C_3/(R_1 T\, e^{C_4/T}) \quad \text{for} \quad T > 437.6 \text{ K} \tag{28b}$$

where C_1 = 2.654E7, C_2 = 1594, C_3 = 4.76E10 and C_4 = 4872.

Consider (22) again. The dependent variable is θ. The steam density is simply a function of temperature as indicated by (28). The water density ρ_3 is also a function of temperature and is

$$\rho_3 = 1000/\left[1 + ((T-273.15)/475)^2\right] \tag{29}$$

which gives water density values accurate to 2% to about 600 K. Even considerably below that temperature, our calculations (and measurements of others) indicate liquid water would not be present. The pressure p on the right side of (22) is $p_1 + p_2$ but p_1 is given by p_{1s}, (24b) or (27). Furthermore, ε and T can also be considered known in (22). Hence the dependent variable is θ as stated above; θ appears explicitly on the left of (22) and implicitly on the right through k_{rm} and $k_{r\ell}$ which are given by (20f) and (20g). Unlike the other partial differential equations, (22) does not involve a second derivative in space of the dependent variable.

A continuity equation is also required for the CO_2 gas in the wet region. One form for it is

$$\frac{\partial(\rho_2\theta)}{\partial t} + \frac{\partial(\rho_2 u_m)}{\partial x} = \rho_2^o \frac{\partial \alpha_2}{\partial t} \tag{30}$$

which can also be written as

$$\frac{\partial}{\partial t}\left(\frac{p_2\theta}{R_2T}\right) = \frac{\partial}{\partial x}\left[\frac{p_2}{R_2T}D_1\left(\frac{\partial p_1}{\partial x} + \frac{\partial p_2}{\partial x}\right)\right] + \rho_2^o\frac{\partial\alpha_2}{\partial t} \tag{31a}$$

where

$$D_1 = \frac{k_{rm}K}{\mu_m} \tag{31b}$$

and p_1 is the known function of T as given by (24b) and (27). Here the dependent variable is p_2 and (31a) appears to be in the form of a nonlinear parabolic (or diffusion) equation.

Dependent Variables

For the wet region the dependent variables are T, θ, p_2, $\alpha_{1'}$, $\alpha_{1''}$ and α_2. There is a coupling between all the equations but each equation can be identified with a particular dependent variable. The temperature T is found from the energy equation, (19). The kinetic equations, (13), (14) and (15), are the same as for the dry region and are associated with $\alpha_{1'}$, $\alpha_{1''}$ and α_2, respectively. The pressure of the CO_2 gas, p_2, is identified with (31) and θ with (22).

2.4 Interface Considerations

At the interface between the dry and wet regions the solution for the two regions must be matched. There must be continuity of T, p_1, p_2 and θ in the x-direction. In addition there must be conservation of energy and mass.

Some of the equations pose little difficulty since they are solved in a finite difference procedure in exactly the same manner on either side of the interface. The kinetic equations (13), (14) and (15) have this characteristic. The energy equations (1) and (19) are quite similar for both regions. For this reason the energy equation approximated by finite difference equations is solved for both regions simultaneously. The p_2 equations for both regions are also nearly the same.

The continuity equations for the water, however, must be treated in quite different ways in the two regions. In the dry region, (10) has p_1 as the dependent variable and the equation is similar in structure to the energy and p_2 equations, that is, a first derivative on time and a second derivative in space are present. In the wet region θ is the dependent variable. At the interface, $\theta = \varepsilon$ and there must be conservation of mass of the water.

3. FINITE DIFFERENCE EQUATIONS

In this section a set of finite difference equations is given that closely approximates those in USINT. Since the program at present does not have the CO_2 option checked-out, the CO_2 terms are not considered for all the equations. The program was written to permit various one-dimensional systems rather than just the cartesian coordinate x. For this reason the x derivatives have been written as

$$\frac{\partial}{\partial x}\left(A\,\frac{\partial U}{\partial x}\right) \rightarrow G_1\,\frac{\partial}{\partial x_i}\left(G_2 A\,\frac{\partial U}{\partial x_i}\right) \tag{32a}$$

$$\frac{\partial U}{\partial x} \rightarrow G_3\,\frac{\partial U}{\partial x_i} \tag{32b}$$

where x_i is a generalized orthogonal coordinate and

$$G_1 = \frac{1}{h_1 h_2 h_3} \tag{33a}$$

$$G_2 = \frac{h_j h_k}{h_i}\ ,\ i,j,k \text{ cyclic} \tag{33b}$$

$$G_3 = \frac{1}{h_i} \tag{33c}$$

For cartesian coordinates the h_i's are all unity. For cylindrical coordinates the h_i's are

$$h_1 = 1, \quad h_2 = r, \quad h_3 = 1 \quad (r,\theta,z) \tag{34}$$

and for spherical polar coordinates,

$$h_1 = 1, \quad h_2 = r, \quad h_3 = r \sin \theta \quad (r,\theta,\phi) \tag{35}$$

Another change in the program from the notation given above is that U represents temperature instead of T which denotes time in USINT.

In all the partial differential equations of the parabolic type (that is, all except θ and α) a Crank-Nicolson type approximation is utilized. Parameters called ETA and ZETA are introduced that permit a forward difference approximation by setting ETA and ZETA equal to zero, Crank-Nicolson by setting equal to 0.5 and backward difference (fully implicit) approximation by setting ETA and ZETA equal to unity.

The basic subroutines that are used for the dry and wet regions simultaneously existing (the most commonly occurring case) are the following:

1. H1DP - for temperature, denoted U(I)
2. DECOMP - for fraction of reactants decomposed; for evaporable water A1(I), for chemically bound water A2(I), and for CO_2 gas A3(I)
3. PORE - for calculating the porosity in the concrete, denoted EP(I)
4. P1WET - for calculating the steam pressure in the wet region, denoted P1(I). (This subroutine contains the modified Clausius-Clapeyron equations.)
5. P1DH2O - for calculating the steam pressure in the dry region, denoted P1(I)

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6. THWH2O - for calculating θ in the wet region, denoted THETA(I)

For a given time step the basic equations are solved in the order indicated by these subroutines: U, $\alpha_{1'}$, $\alpha_{1''}$, α_2, ε, p_1 and θ. No iteration at each time step is used. Note, however, that U values at times t_n and t_{n+1} ("present" and "future" times) can be used for all the other variables, ε can be calculated using the α's at times t_n and t_{n+1}, and so on. The temperatures U_i^{n+1} (for locations x_i and times t_{n+1}) must be calculated, however, using quantities known only at time t_n.

Energy Equation

The energy equation for both the wet and dry regions (which are coded in subroutine H1DP) can be written in the form

$$\rho c_{ps} \frac{\partial U}{\partial t} = G_1 \frac{\partial}{\partial x}\left(G_2 k \frac{\partial U}{\partial x}\right) - \left(\rho c_{p_g} u_m + \rho_3 c_{p_3} u_3\right) G_3 \frac{\partial U}{\partial x} + \dot{Q} \qquad (36)$$

A finite difference form of this equation for node x_i and time t_n is

$$\frac{(\rho c_{p_s})_i^n}{\Delta t}\left(U_i^{n+1} - U_i^n\right) = \frac{G_{1i}(G_2 k)_{i+1/2}^n}{(\Delta x)^2}\Big[\eta\left(U_{i+1}^{n+1} - U_i^{n+1}\right)$$

$$+ (1-\eta)\left(U_{i+1}^n - U_i^n\right)\Big] - \frac{G_{1i}(G_2 k)_{i-1/2}^n}{(\Delta x)^2}\Big[\eta\left(U_i^{n+1} - U_{i-1}^{n+1}\right)$$

$$+ (1-\eta)\left(U_i^n - U_{i-1}^n\right)\Big] - \frac{G_{3i}}{2\Delta x}\left(\rho c_{p_g} u_m + \rho_3 c_{p_3} u_3\right)_i^{n+\eta} \cdot$$

$$\Big[\eta\left(U_{i+1}^{n+1} - U_{i-1}^{n+1}\right) + (1-\eta)\left(U_{i+1}^n - U_{i-1}^n\right)\Big] + \dot{Q}_i^{n+\eta} \qquad (37)$$

The symbol η in (37) is denoted ETA in the program and is a Crank-Nicolson parameter mentioned above.

Define for convenience the following where a FORTRAN-like notation is used:

$$C11_i^n = \frac{(\rho c_{p_s})_i^n}{\Delta t} \qquad (38)$$

$$C12_i^n = G11_i k_{i+1/2}^n \qquad (39a)$$

where

$$G11_i = \frac{G_{1i} G_{2,i+1/2}}{(\Delta x)^2} \qquad (39b)$$

$$C13_i^n = G12_i k_{i-1/2}^n \qquad (40a)$$

where

$$G12_i = \frac{G_{1i} G_{2,i-1/2}}{(\Delta x)^2} \qquad (40b)$$

$$C14_i^n = G13_i (\rho c_{p_g} u_m + \rho_3 c_{p_3} u_3)_i^{\eta+n} \qquad (41a)$$

where

$$G13_i = \frac{G_{3i}}{2\Delta x} \qquad (41b)$$

$$t_{n+1} = t_n + \Delta t \qquad (42a)$$

$$x_{i+1} = x_i + \Delta x \qquad (42b)$$

Using the above definitions (38-41) in (37) and collecting terms permits writing

$$-A_i^n U_{i+1}^{n+1} + B_i^n U_i^{n+1} - C_i^n U_{i-1}^{n+1} = D_i^n \qquad (43)$$

where

$$A_i^n = \eta(C12_i^n - C14_i^n) \qquad (44a)$$

$$B_i^n = C11_i^n + \eta(C12_i^n + C13_i^n) \qquad (44b)$$

$$C_i^n = \eta(C13_i^n + C14_i^n) \qquad (44c)$$

$$D_i^n = C11_i^n U_i^n + (1-\eta)\Big[C12_i^n(U_{i+1}^n - U_i^n) + C13_i^n(U_{i-1}^n - U_i^n)$$

$$+ C14_i^n(U_{i-1}^n - U_{i+1}^n)\Big] + \dot{Q}_i^{n+\eta} \qquad (44d)$$

Let the one-dimensional segment of concrete have the length of

$$L = (IM-1)\Delta x \qquad (45)$$

where IM is the number of nodes which is one more than the number of Δx's. Then (43) can be used to generate finite difference equations for nodes $i=2,\ldots,IM-1$.

At present there are two boundary conditions permitted at $x=0$, a constant prescribed heat flux and a time-temperature history of arbitrary time dependence that is entered through a table of temperatures with a corresponding time table. Another prescribed temperature history can be specified at $x=L$. A prescribed surface temperature is easily incorporated into the program. Suppose that the surface at $x=0$ is to have a specified temperature at time t_{n+1} of T^{n+1}. Then (43) would be replaced by

$$U_1^{n+1} = T^{n+1} \qquad (46)$$

or in other symbols, i=1, $A_i = B_i = 0$, $B_i=1$ and $D_i^n = T^{n+1}$.

The tridiagonal set of equations formed from (43) and appropriate boundary condition equations comprises a set of algebraic equations that can be solved very efficiently. The algorithm used is the one given on page 200 of Richtmyer and Morton [9].

Heat Flux Boundary Condition

The heat flux boundary condition used in USINT is

$$q = -k \left.\frac{\partial U}{\partial x}\right|_{x=0} \tag{47}$$

where q is the surface heat flux and is given by QFLUX in the program. In the present form of the program q may only be a constant value but it is not difficult to program a time variable condition. The boundary condition given by (47) does not include any terms for ablation or movement of gases through the surface. The energy carried by gases through the surface may not be large, however.

The first node is located at x=0 and the second one is at x=Δx but the finite volume associated with the first node is from x=0 to Δx/2. Assume now that the various terms in the partial differential equation given by (36) is to be evaluated at x=Δx/4. Hence

$$k \left.\frac{\partial U}{\partial x}\right|_{\Delta x/4} \approx \frac{1}{2}\left[k \left.\frac{\partial U}{\partial x}\right|_{x=0} + k \left.\frac{\partial U}{\partial x}\right|_{\Delta x/2}\right] \approx \frac{1}{2}\left[-q + k_{3/2}\,\frac{U_2-U_1}{\Delta x}\right] \tag{48a}$$

$$C \left.\frac{\partial U}{\partial x}\right|_{\Delta x/4} \approx \frac{1}{2}\left[C \left.\frac{\partial U}{\partial x}\right|_{x=0} + C \left.\frac{\partial U}{\partial x}\right|_{\Delta x/4}\right] \approx \frac{1}{2}\left[-\frac{C_1 q}{k_1} + C_{3/2}\,\frac{U_2-U_1}{\Delta x}\right] \tag{48b}$$

$$\frac{\partial}{\partial x}\left(G_1 k \frac{\partial U}{\partial x}\right)\Big|_{\Delta x/4} \approx \frac{G_1 k \left.\frac{\partial U}{\partial x}\right|_{\Delta x/2} - G_1 k \left.\frac{\partial U}{\partial x}\right|_0}{\Delta x/2}$$

$$\approx \frac{2}{\Delta x}\left[G_{1,3/2} k_{3/2} \frac{U_2 - U_1}{\Delta x} + G_{1,1} q\right] \qquad (48c)$$

The time derivative is approximated using

$$\frac{\partial U}{\partial t} \approx \lambda \frac{U_1^{n+1} - U_1^n}{\Delta t} + (1-\lambda)\frac{U_2^{n+1} - U_2}{\Delta t} \qquad (48d)$$

The best choice of λ is usually 0.75. (The input symbol for λ is LAMBA and it is declared real.)

Introducing the above relations in (36) and rearranging in the form

$$B_1 U_1^{n+1} - A_1 U_2^{n+1} = D_1 \qquad (50a)$$

one finds the B_1, C_1, and D_1 coefficients to be

$$B_1 = C14 + C10 - C17 \qquad (50b)$$

$$A_1 = C10 - C15 - C17 \qquad (50c)$$

$$D_1 = C14\, U_1^n + C15\, U_2^n + \eta q^{n+1}\left[\frac{2G_{1,3/2}G_{2,1}}{\Delta x} + \frac{C_{11}}{2k_1^n}\right]$$

$$+ (1-\eta)\left\{\frac{2G_{1,3/2}}{\Delta x}\left[G_{2,3/2} k_{3/2}^n \frac{U_2^n - U_1^n}{\Delta x} + G_{2,1} q^n\right] - \frac{C13C16}{2}\right.$$

$$\left. + \frac{q^n C11}{2k_1^n}\right\} + \dot{Q}_1^{n+1} \qquad (50d)$$

where

$$C10 = \frac{2\eta G_{1,3/2} G_{2,3/2} k_{3/2}^n}{(\Delta x)^2}$$

$$C11 = \left[(\rho c_{p_g} u_m + \rho_3 c_{p_3} u_3)G_3\right]_1^n$$

$$C12 = \left[(\rho c_{p_g} u_m + \rho_3 c_{p_3} u_3)G_3\right]_1^n$$

$$C13 = \frac{1}{2}(C11 + C12)$$

$$C14 = \left[\frac{\lambda \rho c_p}{\Delta t}\right]_1^n$$

$$C15 = \left[\frac{(1-\lambda) \rho c_p}{t}\right]_2^n$$

$$C16 = \frac{U_2^n - U_1^n}{\Delta x}$$

$$C17 = \frac{\eta C13}{2\Delta x}$$

The one subscript refers to node 1 (at the heated surface, x=0); the two subscript refers to node 2; and the 3/2 subscript refers to midway between nodes 1 and 2.

Kinetic Equations

The kinetic equations for evaporable water, chemically bound water and CO_2 are solved in subroutine DECOMP.

A typical kinetic equation can be written as

$$\frac{\partial\alpha}{\partial t} = K_A(1-\alpha)\exp(-E/RU) \qquad (51)$$

It is assumed from one time step to another that the temperature U varies linearly with time. The temperature at time t_n is U^n and at time t_{n+1} is U^{n+1}. For convenience, define the rate of change of temperature with time at a particular location as β,

$$\beta = \frac{U^{n+1} - U^n}{\Delta t} \qquad (52)$$

If U varies linearly with time over some interval, then α can be considered to be a function of U,

$$\alpha(t) = \alpha\Big(U(t)\Big) \qquad (53a)$$

where the space dependence of α is omitted. Differentiating α with respect to t, permits (53a) to be written as

$$\frac{\partial\alpha}{\partial t} = \frac{\partial\alpha}{\partial U}\,\frac{\partial U}{\partial t} = \beta\frac{\partial\alpha}{\partial U} \qquad (53b)$$

Using (53b) in (51) then gives

$$\beta\frac{\partial\alpha}{\partial U} = K_A(1-\alpha)\exp(-E/RU) \qquad (54)$$

Separating the variables in (54) and integrating gives

$$\int_{\alpha^n}^{\alpha^{n+1}} \frac{d\alpha}{1-\alpha} = \frac{K_A}{\beta}\int_{U^n}^{U^{n+1}} e^{-E/RU}du \qquad (55a)$$

which has the solution

$$\alpha^{n+1} = 1 - (1-\alpha^{n})\exp\left\{- \frac{K_A}{\beta}\left[U^{n+1}E_2(\frac{E}{RU^{n+1}}) - U^{n}E_2(\frac{E}{RU^{n}})\right]\right\} \qquad (55b)$$

The function $E_2(\cdot)$ is an exponential integral and is defined by

$$E_2(x) = \int_1^{\infty} t^{-2}e^{-xt}dt \qquad (56a)$$

which for large values of the argument x can be closely approximated by

$$E_2(x) \simeq \frac{e^{-x}}{x + \frac{2}{1 + \frac{1}{x+2.6}}} \qquad (56b)$$

In realistic cases for concrete and using measured values of E/R, the argument of $E_2(\cdot)$ should be about 10 and larger. For x=5, the error is less than .1% and for x > 10, the error is at most in the 6th significant figure.

If due to a problem with stability the calculated temperatures become much too large, then another approximation can be used; it is

$$\alpha^{n+1} = 1 - (1-\alpha^{n})\exp\left[- K_A\Delta t\exp(-E/RU^{n})\right] \qquad (56c)$$

which is used in DECOMP if

$$\frac{E}{RU^{n}} < 0.01 \qquad (56d)$$

This modification helps to prevent DECOMP from becoming a cause of the program becoming unstable.

MASS TRANSFER EQUATION FOR DRY REGION

The finite difference approximations of the mass transfer equation for the water vapor in the dry region is coded in subroutine P1H2O. The partial differential equation to be approximated can be obtained from (10). The finite difference equation in P1H2O does not include CO_2 so that p_2 is dropped in (10). In addition, T is replaced by U, $k_{rm}K/\mu_m$ is replaced by D_1 and generalized orthogonal coordinates are used. The resulting equation is

$$\frac{\partial}{\partial t}\left(\frac{p_1\varepsilon}{U}\right) = G_1\frac{\partial}{\partial x}\left(\frac{G_2D_1}{U}p_1\frac{\partial p_1}{\partial x}\right) + R_1\dot{s}_1 \qquad (57a)$$

or

$$\frac{\partial}{\partial t}\left(\frac{p_1\varepsilon}{U}\right) = G_1\frac{\partial p_1}{\partial x}\frac{\partial}{\partial x}\left(\frac{G_2D_1}{U}p_1\right) + \frac{G_1G_2D_1}{U}p_1\frac{\partial^2 p_1}{\partial x^2} + R_1\dot{s}_1 \qquad (57b)$$

Because $\varepsilon=\theta$ in the dry region, the finite difference approximation in P1H2O starts with

$$\begin{aligned}
\left(\frac{\theta}{U}p_1\right)_i^{n+1} - \left(\frac{\theta}{U}p_1\right)_i^{n} = \frac{G_1\Delta t}{4(\Delta x)^2}\Bigg|\eta\Bigg[&\left(\frac{G_2D_1}{U}p_1\right)_{i+1}^{n} \\
-\left(\frac{G_2D_1}{U}p_1\right)_{i-1}^{n}\Bigg]&\left(p_{1,i+1}^{n+1} - p_{1,i-1}^{n+1}\right) + (1-\eta)\Bigg[\left(\frac{G_2D_1}{U}p_1\right)_{i+1}^{n+1} \\
-\left(\frac{G_2D_1}{U}p_1\right)_{i-1}^{n+1}\Bigg]&\cdot\left(p_{1,i+1}^{n} - p_{1,i-1}^{n}\right)\Bigg| \\
+\frac{\eta\Delta t}{(\Delta x)^2}&\left(\frac{G_1G_2D_1}{U}p_1\right)_i^n\left(p_{1,i+1}^{n+1} - 2p_{1,i}^{n+1} + p_{1,i-1}^{n+1}\right)
\end{aligned}$$

$$+ \frac{(1-\eta)\Delta t}{(\Delta x)^2} \left(\frac{G_1 G_2 D_1}{U} p_1\right)_i^{n+1} \left(p_{1,i+1}^n - 2p_{1,i}^n + p_{1,i-1}^n\right)$$

$$+ R_1 \Delta t \, \dot{s}_{1,i}^{n+1} \qquad (58)$$

Notice that the nonlinear terms are handled in such a manner that $\eta=0$ does not yield an explicit procedure. This approximation is more accurate than the more common Crank-Nicolson procedure in which all the terms with the $(1-\eta)$ coefficient are evaluated at time t_n.

Define in a FORTRAN-like form the following:

$$CT11 = \Delta t/\left(4(\Delta x)^2\right) \qquad (59a)$$

$$CT20 = \Delta t/(\Delta x)^2 \qquad (59b)$$

$$G1I = G_{1i} \qquad (59c)$$

$$G2I = G_{2i} \qquad (59d)$$

$$H10_i = \frac{G_{1i}\Delta t}{4(\Delta x)^2} = G1I*CT11 \qquad (60a)$$

$$H11_i = \frac{G_{1i}G_{2i}\Delta t}{(\Delta x)^2} = G1I*G2I*CT20 \qquad (60b)$$

$$C10_i^n = H10_i^n\left[\left(\frac{G_2 D_1}{U} p_1\right)_{i+1}^n - \left(\frac{G_2 D_1}{U} p_1\right)_{i-1}^n\right] \qquad (60c)$$

$$C11_i^n = H10_i(1-\eta)\left(p_{1,i+1}^n - p_{1,i-1}^n\right) \qquad (60d)$$

$$C12_i^n = H11_i \eta (\frac{D_1 p_1}{U})_i^n \tag{60e}$$

$$C13_i^n = H11_i (1-\eta)(p_{1,i+1}^n - 2p_{1,i}^n + p_{1,i-1}^n) \tag{60f}$$

Using the above definitions in (58) yields

$$\begin{aligned}(\frac{\theta}{U}\, p_1)_i^{n+1} &= (\frac{\theta}{U}\, p_1)_i^n + C10_i^n\,(p_{1,i+1}^{n+1} - p_{1,i-1}^{n+1}) \\ &+ C11_i^n \left[(\frac{G_2 D_1}{U}\, p_1)_{i+1}^{n+1} - (\frac{G_2 D_1}{U}\, p_1)_{i-1}^{n+1}\right] \\ &+ C12_i^n\,(p_{1,i+1}^{n+1} - 2p_{1i}^{n+1} + p_{1,i-1}^{n+1}) + C13_i^n (\frac{D_1 p_1}{U})_i^{n+1} + R_1 \Delta t \dot{s}_{1i}^{n+\eta}\end{aligned} \tag{61}$$

which can be simplified and written as

$$-A_i^n p_{1,i+1}^{n+1} + B_i^n p_{1i}^{n+1} - C_i^n p_{1,i-1}^{n+1} = D_i^n \tag{62}$$

where

$$A_i^n = C10_i^n + C11_i^n\,(\frac{G_2 D_1}{U})_{i+1}^{n+1} + C12_i^n \tag{63a}$$

$$B_i^n = (\frac{\theta}{U})_i^{n+1} + 2C12_i^n - C13(\frac{D_1}{U})_i^{n+1} \tag{63b}$$

$$C_i^n = C12_i^n - C10_i^n - C11_i^n(\frac{G_2 D_1}{U})_{i-1}^{n+1} \tag{63c}$$

$$D_i^n = (\frac{\theta}{U}\, p_1)_i^n + R_1 \Delta t\, \dot{s}_{1i}^{n+\eta} \tag{63d}$$

In the coefficients A, B and C certain terms are to be evaluated at time t_{n+1}. This is done whenever possible; it can be done, for example, for U and also for $\dot{s}_{1i}^{n+\eta}$ which is

$$\dot{s}_{1i}^{n+\eta} = \eta\, \dot{s}_{1i}^{n+1} + (1-\eta)\dot{s}_{1i}^{n} \tag{64}$$

where $\dot{s}_1$ is defined by (9). This is because in a given time step U and the α's have been calculated prior to p, for the dry region. On the other hand, D_1 is a function of ε(a function of the α's) and θ. Here θ cannot be used at t_{n+1} because it has not been evaluated.

A boundary condition for p_1 at x=0 is a prescribed value, denoted P1B in the input.

MASS TRANSFER EQUATION FOR WET REGION

The wet region finite difference approximations for the mass transfer of steam and liquid water are given in subroutine THWH2O. The dependent variable of interest is θ. The pressure in this region is first calculated using subroutine P1WET which uses the modified Clausius-Calpeyron equations, (24b) and (27). Using this latter subroutine the pressure is found as a function of U_i^{n+1}.

The mass transfer equation for both water vapor and liquid water can be written as

$$\frac{\partial}{\partial t}\left[\rho_1\theta + \rho_3(\varepsilon-\theta)\right] = G_1 \frac{\partial}{\partial x}\left[G_2(\rho_1 D_1 + \rho_3 D_3)\frac{\partial p_1}{\partial x}\right] + \dot{s}_1 \tag{65}$$

A difference approximation of this equation is

$$\frac{1}{\Delta t}\left\{\left[(\rho_1 - \rho_3)\theta + \rho_3\varepsilon\right]_i^{n+1} - \left[(\rho_1 - \rho_3)\theta + \rho_3\varepsilon\right]_i^{n}\right\}$$

$$
\begin{aligned}
&= \frac{G_{1i}G_{2,i+1/2}}{2\Delta x^2}\left[(\rho_1 D_1 + \rho_3 D_3)_i^{n+\eta} + (\rho_1 D_1 + \rho_3 D_3)_{i+1}^{n+\eta}\right] \\
&\cdot \left[\eta(p_{1,i+1}^{n+1} - p_{1i}^{n+1}) + (1-\eta)(p_{1,i+1}^{n} - p_{1i}^{n})\right] \\
&+ \frac{G_{1i}G_{2,i-1/2}}{2\Delta x^2}\left[(\rho_1 D_1 + \rho_3 D_3)_i^{n+\eta} + (\rho_1 D_1 + \rho_3 D_3)_{i-1}^{n+\eta}\right] \\
&\cdot \left[\eta(p_{1,i-1}^{n+1} - p_{1i}^{n+1}) + (1-\eta)(p_{1,i-1}^{n} - p_{1i}^{n})\right] + \dot{s}_{1i}^{n+\eta} \qquad (66)
\end{aligned}
$$

The unknown in this equation is θ_i^{n+1} which appears explicitly in the left and implicitly in D_1^{n+1} and D_3^{n+1}. The implicit dependence in solving for θ is neglected. Though tedious, it is not difficult to solve (66) for θ_i^{n+1}.

INTERFACE CONDITIONS FOR THE MASS TRANSFER EQUATIONS

Since the mass transfer equations for the wet and dry regions must be solved in different ways, an interface condition is needed. Though at some time it might be desirable to develop a moving interface condition, USINT uses the more simple and straightforward method of fixed nodes, even for the interface. This then causes the location of the interface to jump from one node to the next one further in the body. The condition used to indicate when the interface has moved is that θ in the wet region becomes equal to ϵ. In the calculations thus far this node is always the one adjacent to the interface. Actually the θ values in the wet region invariably drop quite appreciably near the near interface, reach a minimum at some location and finally increase deeper inside the body. This is illustrated in later figures.

For the wet region, θ is calculated; the interface condition for θ is simply $\theta=\epsilon$. For the dry region the interface condition is that the interface pressure p_1 is equal to the value of pressure given by the modified Clausius-Clapeyron equation of state for the temperature at the present interface node just before the interface last moved. This causes the pressure p_1 to be constant at the interface until the interface moves. In reality the calculations indicate that the pressure p_1 tends to drop with distance from the interface in the dry region. In other words the pressure p_1 tends to be at or near its maximum at the interface and this interface moves deeper into the body as it is heated. Hence, for a fixed location just inside the dry region the pressure should tend to decrease slowly with time (after the interface has passed by). The approximation used in the program (subroutine P1DH2O) uses the constant p_1 condition (until the interface moves) at the interface node. Actually the true interface would have moved deeper into the body at that time and as a consequence the correct pressure might have decreased at that location. This interface condition is considerably better and more stable than some other conditions that were investigated.

One of these latter conditions involved calculating the interface node pressure p_1 using the temperature existing at the node in the modified Clausius-Clapeyron equations of state. This caused the interface node pressure (for a given node) to continually increase in time when the surface of the concrete is heated. Since the Clausius-Clapeyron relations are highly dependent on temperature, the interface node pressure could then increase very considerably while the interface was assumed to be at that node. But as mentioned above, the true interface would have moved deeper into the body resulting in a possible drop, rather than increase, in the pressure at that location. Hence, this approach is not satisfactory.

Another approximation for the interface treats θ as mentioned above but the pressure boundary condition for p_1 of the dry region is that calculated from the temperature one node <u>inside</u> the wet region. This allows the pressure to vary with time at the interface but again tends to increase the pressure with time at a given interface node. It works fairly well, but the constant p_1 condition at the interface mentioned above appears to be better.

PORES COMPLETELY FILLED WITH LIQUID (θ=0)

In addition to the dry and wet regions another region is possible. This is the case of the pores being completely filled with water. Sometimes this region is very narrow or not even exists in the calculations. For this reason the program simply restricts θ to being not less than zero since θ=0 corresponds to the pores being completely filled with water. The vapor pressure is still found using a modified Clausius-Clapeyron equation of state. This treatment of the θ=0 region is a part of the program that could be improved upon in the future.

4. INPUT PARAMETERS

The present version of USINT has most input quantities separate from the programming and is intended for batch processing. Hence it is convenient to discuss the input in a card to card basis. For each input card, 80 spaces are divided into 8 blocks of 10 spaces. In each block a single number appears so that at most each card contains eight numbers.

The subroutine INPUTS is used for the input into the program. It also prints out with headers the input in the same form that it was entered. The numbers that are printed out are the same as the input except for the situation in which the measured temperature histories are in degrees Fahrenheit and kelvin is desired. In this exception (associated with the index IFTOK being 1) the input is in ^{o}F but the values used later in the program and those printed out are in K. Another feature of INPUTS is that it contains a dictionary of input and other quantities used in USINT.

A consistent set of units, such as SI, should be used in the input.

Card 1, (format: 4F10.0, 2I10, F10.0, I10)

CASE - case number (not used in program)
DATE - date (not used in program)
ETA - Crank-Nicolson parameter η
LAMBA - heat flux boundary condition parameter λ. See (48d).
NPRNT - printing index, =1 to print each time step, =2 to print every other time step, etc.
NOPT - index to solve simple heat conduction model, =0 to skip all subroutines except H1DP (hence simple conduction model), =1 for heat and mass transfer model
ZETA - Crank-Nicolson parameter in THWH2O (θ calculations)
ISTATE - equation of state index used in P1WET, =0 for Clausius-Clapeyron equation of state, ≠0 for modified equation of state

Card 2, (format: F10.0, 7I10)

DX - Δx width, m
IM - Total number of nodes, length of body is $(IM-1)\Delta x$

IDEBUG - =0 for omitting NAMELIST DEBUG in subroutine THWH2O, =1 for calling NAMELIST DEBUG

ICOEFF - =0 for omitting NAMELIST COEFF in subroutine H1DP, =1 for calling NAMELIST COEFF

IHEAT - =0 for omitting NAMELIST HEAT in subroutine H1DP, =1 for calling NAMELIST HEAT

IDARCY - =0 for omitting NAMELIST DARCY in subroutine CARCO, =1 for calling NAMELIST DARCY

IP1DH - =0 for omitting NAMELIST P1DH in subroutine P1DH2O; =1,2,3,··· for calling NAMELIST 1,2,3,··· times

IVDAR - =0,1 for omitting NAMELIST VDAR in subroutine VDARCY, =2 for printing NAMELIST VDAR

Card 3, (format: F10.0, 3I10, 4F10.0)

DT - time step, s

NTS - total number of time steps

IDARCO - =Maximum number of times that subroutine DARCO is to be called; usually IDARCO>NTS Fixes Darcy coefficients at the value at the time index equal to IDARCO.

MDARCO - =0 for HEDL form of Darcy coefficients
=1 for HEDL form of Darcy coefficients with void fraction corrections
=2 for GE form of Darcy coefficients
=3 for form of Darcy coefficients described above in this report, has corrections for void fraction and porosity

UMIN1 - lowest temperature for which decomposition for evaporable water is calculated, K

UMIN2 - lowest temperature for which decomposition for chemically bound water is calculated, K

UMIN3 - lowest temperature for which decomposition for CO_2 is calculated, K

D10C - Darcy factor for MDARCO =2 or 3 (See discussion on pages 39-41.)

The index MDARCO is used to designate several different forms of the Darcy coefficients, as indicated above. Each of these models is given in subroutine DARCO. The units for the Darcy coefficient D_i are m^3-s/kg for SI units. The vapor and liquid water velocities are given by

$$u_m = -D_1 \frac{\partial p}{\partial x} , \quad u_3 = -D_3 \frac{\partial p}{\partial x} \tag{67}$$

where D_1 and D_3 are given by

$$D_1 = \frac{K}{\mu_m} , \quad D_3 = \frac{K}{\mu_3} \tag{68}$$

where K is called the permeability and μ is the viscosity.

For DARCO equal to zero, the HEDL [7] expressions are given for K for magnetite. They are functions of temperature only (not porosity and/or θ). These functions are for temperatures below 230°F,

$$K = 3.16E\text{-}27 \exp(0.038376T) \tag{69a}$$

and above 230°F,

$$K = 2.54E\text{-}21 \exp(0.01867T) \tag{69b}$$

where T is in degrees Rankine and K is in ft^2. At 230°F (690°R) the K value given by both these equations is about $10^{-15} ft^2$ which is about the value shown [7] on Figures 9 and 11 which are for magnetite and limestone concrete. At 1200°F, however, (69b) gives the value of 7.3E-8ft^2 which is almost 8 orders of magnitude larger. Though the above mentioned figures in [7] show a strong temperature dependence, it is not that large. For example, Fig. 9 which is said to be for magnetite concrete [7] has a K value of about 2E-12 ft^2. This value is about 3 orders of magnitude larger than the 230°F value; though the temperature dependence is large it is not nearly as severe as predicted by (69b). Because of this extremely large temperature dependence given by (69b) and also because it does not fit the data given by Fig. 9 for magnetite concrete another expression is used instead of (69b) in DARCO; it is

$$K = 4.2510E - 18 \exp(0.007869T) \qquad (69c)$$

where again T is in °R. This equation was found by fitting the exponential at 230°F (690°R) to the values of 1E-15 and 2E-12 ft^2 mentioned above. Hence, the MDARCO = 0 option though called the HEDL values utilizes (69a,c), one of which was not given explicitly by HEDL. Conversion factors are used in DARCO to change the temperature in °R to K and the units from ft^2 to m^2.

Also the viscosities of steam and liquid water are given by curve fits. The expressions are

$$\mu_m = 2.5E\text{-}7\left(\frac{T_R}{660}\right)^{1.24} \qquad (70a)$$

$$\mu_3 = 1.42E\text{-}5\left(\frac{T_F}{100}\right)^{-1.15} \qquad (70b)$$

where μ is in lb_f-s/ft^2, T_R is in °R and T_F is in °F. Proper conversion factors are again used for SI units.

The values calculated for the Darcy coefficients ($D=K/\mu$) at 383K(230°F) using (69a,c) and (70a,b) are

D_1 = 7.9E-12 m^4/N-s

D_3 = 3.8E-13 m^4/N-s

and at 589K (600°F),

D_1 = 9.3E-11 m^4/N-s

D_3 = 2.3E-11 m^4/N-s

If MDARCO = 1, the "HEDL" values discussed above are multiplied by the θ corrections given by (20f,g).

For MDARCO = 2 the General Electric [4] form of the Darcy coefficients is utilized in the program. GE also used (67) and (68) with D_1 and D_3 given by

$$D_1 = K_c\theta/(\varepsilon\mu_m)$$

$$D_3 = K_c/\mu_3 \tag{71}$$

and hence, the vapor Darcy coefficient has a void fraction dependence. (It seems that GE like HEDL keep ε constant throughout the calculations.) The quantity K_c is simply the permeability of dry concrete. A K_c/μ value chosen by GE [4] for water vapor is 5E-11 m^4/N-s and the corresponding K_c/μ for water is 5E-15 m^4/N-s. In other words the Darcy coefficient for the liquid water is one 10^4th of the water vapor. In another GE report [10] the permeability/viscosity (gas)is given the value 2.4E-11 m^2/N-s and the permeability/viscosity (wet) is given the same value; these values are associated with magnetite concrete. At 383K the liquid water to water vapor ratio for viscosity is about 21 while at 589K it has dropped to about 4. Hence, a ratio of 10^4 is much too high while a ratio of 1 is too low. The MDARCO = 2 ratio is taken to be 10^4 because this value is explicitly given by GE. The magnitude of the coefficient is arbitrary, however, and is specified by the last number, D1OC, on card 3 and a factor of 10^{-10} to make the coefficient about 1. More explicitly for MDARCO = 2 the Darcy coefficients are given by

$$D_1 = \text{D1OC} \cdot 10^{-10}\theta/\varepsilon \tag{72a}$$

$$D_3 = \text{D10C} \cdot 10^{-14} \tag{72b}$$

The MDARCO = 3 option is the one discussed in Section 2 of this report. A θ <u>and</u> ε dependence is included and a temperature effect enters through the temperature dependence of the viscosities. The same viscosity-temperature relations, (70a,b), proposed by HEDL are used. The expressions for D_1 and D_3 are

$$D_1 = \frac{(\varepsilon/\varepsilon_0)^3 \text{D10C}}{(1-\varepsilon)^2 \mu_m} \left(1.1\,\frac{\theta}{\varepsilon} - 0.1\right) 10^{-20} \tag{73a}$$

$$\text{for } 1 - \frac{1}{1.1} < \frac{\theta}{\varepsilon} < 1$$

$$D_1 = 0 \quad \text{for} \quad 0 < \frac{\theta}{\varepsilon} < 1 - \frac{1}{1.1} \tag{73b}$$

$$D_3 = \frac{(\varepsilon/\varepsilon_0)^3 \text{D10C}}{(1-\varepsilon)^2 \mu_3} \left(1 - \frac{\theta}{\varepsilon}\right)^3 10^{-20} \tag{74}$$

Notice that in this case of MDARCO = 3 a factor of 10^{-20} is associated with the multiplicative factor D10C; it is related to β_k of (8b) and the initial porosity ε_0 by

$$\text{D10C} = \beta_k \varepsilon_0^3 \text{E20}$$

Card 4, (format: 6F10.0, I10, F10.0)

UP - initial temperature, K
EP0 - initial porosity
THETA0 - initial theta (must be between zero and EP0)
P10 - initial partial pressure p_1 of water vapor, N/m^2
P20 - initial partial pressure p_2 of CO_2, N/m^2 (not used presently)
VOLATM - volume of atmosphere in subroutine PATM, m^3 (Used only for NFLAG=0)

NFLAG - index in subroutine PATM
=0 for calculation of pressure in volume VOLATM assumed at the heated surface
=1 to set partial pressures at the surface equal to zero.

=2 to set surface p_1 equal to P1B and surface $p_2 = 0$.

P1B - surface pressure at x=0 for NFLAG = 2 (see just above), N/m^2

Card 5, (format: 7F10.0, I10)

QFLUX - applied heat flux at x=0, W/m^2. Used if index KBOUND=0

KBOUND - boundary condition index.
= -1 for prescribed temperature condition
=0 to specify heat flux boundary condition

NTMBCA - number of times for table of prescribed temperature history at x=0 ($1 \leq$ NTMBCA ≤ 150)

NTMBCB - number of times for table of prescribed temperature history at x=L ($1 \leq$ NTMBCB ≤ 150)

IFTOK - index to indicate units of input temperature histories at x=0 and L (and internally if given)
=0 for input temperatures at x=0 and L in kelvin
=1 for input temperatures at x=0 and L in degrees Fahrenheit. These values are converted to kelvin and the kelvin values are printed.

NKTEMP - number of thermal conductivities in input table ($1 \leq$ NKTEMP ≤ 20)

NCTEMP - not used

IKCAL - =0 for omitting NAMELIST KCAL in subroutine KCALC
=1,2,3,··· for calling NAMELIST KCAL 1,2,3,··· times

Card 6, (format: 8F10.0)

Note: this "card" and the following four may not be only one "card" each

TIMA(i), I=1, NTMBCA - times associated with prescribed surface temperature history at $x=0$(s)

Card 7, (format: 8F10.0)

TBCA(I), I=1, NTMBCA - prescribed temperatures for $x=0$ associated with TIMA(I) (May be in K or °F; see IFTOK on card 5.)

Card 8, (format: 8F10.0)

TIMB(I), I=1, NTMBCB - times associated with prescribed temperature history at $x=L$ (s)

Card 9, (format: 8F10.0)

TBCB(I), I=1, NTMBCB - prescribed temperatures for $x=L$ associated with times TIMB(I)(May be in K or °F; see IFTOK on card 5.)

Card 10, (format: 2F10.0)

TKPROP(IK) - temperature for IKth entry of conductivity table (K)

CK(IK) - IKth thermal conductivity (W/m-K)

Card 11, (format: 4F10.0)

RHO1C - density of concrete due to evaporable water, (kg/m^3 of concrete)

RHO2C - density of concrete due to chemically constituted water (kg/m^3 of concrete)

RHO3C - density of concrete due to CO_2 (kg/m^3 of concrete)

RHO4C - density of concrete for all other constituents (kg/m^3 of concrete)

Card 12, (format: F10.0)

CP0 - specific heat of concrete (J/kg-K)

Card 13, (format: 5I10, 3F10.0)

NULOC - number of locations for experimental temperature histories ($0 \leq \text{NULOC} \leq 5$)

NUTIM - number of times for experimental temperature histories ($0 \leq \text{NUTIM} \leq 150$)

NPLOC - number of locations for experimental pressure histories ($0 \leq \text{NPLOC} \leq 4$)

NPTIM - number of times for experimental pressure histories ($0 \leq \text{NPTIM} \leq 150$)

NWRTIM - number of times for experimental water release ($0 \leq \text{NWRTIM} \leq 150$)

WEIGHT1 - estimated standard deviation for experimental temperatures (a weighting factor in sum of squares function)

WEIGHT2 - estimated standard deviation for pressures measured inside concrete

WEIGHT3 - estimated standard deviation for experimental water release

Program USINT can be used for estimating parameters by minimizing a sum of squares. The sum of squares is calculated using the equation,

$$
\begin{aligned}
S = & \sum_i \sum_j (Y_{T_{ij}} - U_{ij})^2 \frac{1}{\text{WEIGHT1**2}} \\
& + \sum_i \sum_j (Y_{p_{ij}} - p_{ij})^2 \frac{1}{\text{WEIGHT2**2}} \\
& + \sum_i (Y_{w_i} - W_i)^2 \frac{1}{\text{WEIGHT3**2}} \quad . \qquad (75)
\end{aligned}
$$

where

$Y_{T_{ij}}$ is the measured temperature at time t_i and location x_j,

U_{ij} is the calculated temperature at time t_i and x_j,

$Y_{p_{ij}}$ is the measured pressure at time t_i and location x_j,

p_{ij} is the calculated pressure at t_i and x_j,

Y_{W_i} is the measured water release at time t_i and

W_i is the calculated water release at time t_i.

In this summation the calculated temperature U_{ij} must correspond to the measured temperature YT_{ij} and same is true for the pressure and water release. It is not necessary, however, that the locations and times be the same for the temperatures, pressures, and water release. Notice that the tables given below permit different locations for temperature and water release and also permit different time entries for temperature, pressure and water release. Each temperature history has the same associated time values. This is also true for the pressures but the time table need not be the same as for the temperatures. Calculated values must occur at times at which measurements are [illegible] but there may be many times at which values are calculated [illegible] measured quantities are unknown. Usually the measured U, p and water release values are taken at convenient uniformly-spaced times. This is not true, however, for the locations of the sensors. For this reason a node need not be positioned at each sensor; instead linear interpolation in space is employed to obtain calculated temperatures and pressures when a sensor does not happen to be at a node.

If NULOC = 0, go to card 17.

Card 14, (format: 8F10.0)

TIMEU(I), I=1, NUTIM - time for measured temperatures, s

Card 15, (format: F10.0)

EULOC(J) - location of Jth temperature sensor, m

Card 16, (format: 8F10.0)

EU(I,J), I=1, NUTIM - measured temperatures at location EULOC(J) If IFTOK=0, these temperatures are in kelvin. If IFTOK=1, these temperatures are in °F and are converted to K by the program. Note that the boundary condition temperatures and the measured temperatures should have the same units, either °F or K.

Cards 15 and 16 are alternately read in until all the NULOC locations are considered.

If NPLOC = 0, go to card 20.

Card 17, (format: 8F10.0)

TIMEP(I), I=1, NPTIM - times for experimental pressures, s

Card 18, (format: F10.0)

EPLOC(J) - location of the Jth pressure sensor, m

Card 19, (format: 8F10.0)

EPR(I,J), J=1, NPTIM - pressures associated with measured pressures at location EPLOC(J), N/m^2

Cards 18 and 19 are alternately read in until all the NPLOC locations are considered.
If NWRTIM = 0, no further input is needed.

Card 20, (format: 8F10.0)

TIMEWR(I), I=1, NWRTIM - times for the measured water release, s

Card 21, (format: 8F10.0)

EINTWR(I), I=1, NWRTIM - measured values of the water release, kg/m^2

5. TEST CASE

In order to illustrate the use of program USINT a test case is provided. This case corresponds to the Test 1 data given in a HEDL report [7]. A magnetite concrete slab 12 inches thick was heated by an electrically heated steel plate on one side with a gap for venting of the steam. On the opposite face there were cooling coils. On both surfaces the water release was measured but for Test 1 the water release at the cooled surface was less than 5% of that at the heated surface.

Input data for the test case is given in Table 1. The input is quite extensive so that each input number cannot be discussed but a few are noted. Though the slab is one foot thick, measured temperature histories are impressed at the location of the first thermocouple (x=0) and the last one (x=0.938 ft=0.2859m). In the calculation IM=31 nodes are chosen. Hence, there are 30 Δx's so that Δx=DX=.2859/30=.00953m.

The time steps, DT, are each 60 seconds and there are 420 time steps so that the maximum time is 60(420)=25200s=7 hours. A short numerical study was performed to determine the time and space steps mentioned. For the same thermal properties and other parameters, DX and DT were varied and the overall sum of squares was noted; for this particular case it was found that these values of DX=.00953m and DT=60s gave acceptable accuracy. Reducing DX and DT did not significantly affect the accuracy but can affect the computer running time considerably.

These large time steps of 60s are possible due to the implicit calculational procedure. (In a similar calculation performed by GE with Δx=.00762m, slightly less than .00953m, the step times had to be as small as 0.037s as a result of the explicit calculational procedure. Explicit methods are much easier to program but may have severe time limitations.)

Measured temperature histories are prescribed at both x=0 and x=0.2859m. Experimental internal temperature histories are given at x=.0351m, .0872m, .1335m, .1777m and .2365m. These experimental temperatures are used in the sum of squares function along with pressures measured at .03505 and .1777 m and also the measured water release at x=0. The input times in each case are in seconds. The printed temperatures are in kelvin, the pressures are in N/m^2 and the water release in kg/m^2.

The different contributions to the density are 111.6, 73.4, 975, and 2579 kg/m^3 for evaporable water, chemically bound water, CO_2 and concrete, respectively. See RHO1C, etc. A constant concrete specific heat of 800 J/kg is used.

The thermal conductivity is specified as three linear segments from 0K to 1200K but the values below 290K and above 800K are not relevant for the calculations as the temperatures in the body are between 290 and 800K during the time interval of interest, i.e., to DT*NTS = 60*420 = 25200s.

Sample output produced by USINT for the input data given in Table 1 is displayed in Tables 2 and 3. The complete set of output for this case is recorded on an attached microfiche card. The initial conditions of temperature, pressure, $\alpha_{1'}$, θ and other quantities are provided in Table 2. Temperature is denoted U; QDOT is $\dot{Q}$ defined by (20h); A1 is $\alpha_{1'}$; S1DOT is for steam and is called $\dot{s}_1$ in (21); S2DOT is $\dot{s}_2$ given by the right side of (30) which is for CO_2; and S3DOT is for liquid water and is defined by (201). On the second page of Table 2, P1 is the pressure p_1 in N/m^2; EP stands for epsilon ϵ, the porosity; p is pressure; A2 is $\alpha_{1''}$; THETA is θ; and V1 is vapor velocity in m/s. For every time except zero the EP column contains the porosity values; the time=0 entries are the atmospheric pressure entered as P20.

At the end of Table 2 are five lines that are not initial quantities. Instead they contain output of measured and calculated values of pressure and water release at 1800s. Since the time step, DT, is 60s and the temperatures, pressures and so on are to be printed every 60 time steps (since NPRNT=60), the first time after zero that complete spatial information is to be printed is 60^2=3600s. The measured temperatures are given at 3600s intervals and the measured pressures and water release are given at 1800s steps. Consequently the bottom five lines of Table 2 are given before the first printed calculated spatial quantities which are at 3600s.

At 1800s and .03505 m the measured pressure is about 1 atm. or .101E6 N/m^2 and the corresponding calculated value is .191E6 N/m^2. The difference of these values is

PINT-EPR = -.903E5

which when divided by WEIGHT2=E5 and squared is equal to SUM=.815. The next pressure location is .1777 m and the pressure difference is -.141E5; dividing this latter value by WEIGHT2, squaring and adding to the previous sum yields the new sum of .835. Two of the terms of the sum of squares function defined by (75) are obtained in the manner just described. A third term is obtained from the water release data on the bottom line of Table 2.

The first time beyond zero of spatial output is listed in Table 3. These are given after 60 time steps of 60s each. The surface temperatures of 480.48 and 297.32K are prescribed values. See the TBCA and TBCB arrays in Table 1. The temperatures drop smoothly down from the maximum value at x=0 to about the initial value of 294K and then increase slightly near x=L. The QDOT behavior is much different from U in that QDOT is both positive and negative and varies over many orders of magnitude. The negative values can denote endothermic reactions in which heat is absorbed such as the production of water. Loss of energy for change of phase from water to steam can also cause QDOT to be negative; this is what is occurring at x=.0191m. The positive QDOT at x=.0286m indicates that net condensation or net production of water from steam is occurring.

The A1 column of Table 3 (which is for α_1,) has some zero and nonzero values. The zeros are a result of the production of evaporable water being restricted to being above 350K, the value of UMIN1 given in Table 1. There are three values of A1=1 and thus for these nodes all the possible evaporable water has been produced.

The last column of the first page of Table 3 lists S3DOT values with positive values denoting net production of liquid water. Notice that the greatest production is at x=.0477m which is also where S1DOT is the largest. This occurs at the location where A1 has the greatest change with time.

On the second page and second line of Table 3 there is a quantity IGPM which is equal to 2. This means that the interface between the wet and dry regions is at node 2. Notice that EP and THETA are equal only for the first two nodes and that the largest partial pressure ($p_1 = 5.4E5N/m^2$) occurs at the second node, the interface.

Plots of results given by USINT for the input data of Table 1 have been obtained. The results to be displayed, however, come from a calculation which uses finer time and space steps but the resulting values are nearly the same. The time step is 20s rather than 60s and there are 46 nodes (with an appropriate DX value) rather than 31.

To make the plotting simpler, USINT produces a file called TAPE20, that contains input experimental temperatures, pressures and water release values and the corresponding calculated values. This is done in the main program.

Figures 1-5 provide a comparison of the measured and calculated temperatures for five locations. The calculated values are illustrated by the continuous lines and the measured values with dots. The time scale goes out to 25200s or 7 hours. The agreement of the calculated temperatures with the experimental values is good. Since the heated surface has the temperature prescribed, the measured temperature histories near the surface usually would be expected to be calculated most accurately and those deepest in the body the least accurately. For the curves shown, however, all of the calculated temperature histories agree quite well with the measured values.

In Figures 6 and 7 the measured pressure histories at two locations are shown along with the calculated values. The results for x=.0351m which are shown by Fig. 6 gives reasonably good agreement but the Fig. 7 results for x=.1777 do not show good agreement. This lack of agreement in Fig. 7 can be attributed to several different factors. One of these is that the model in the program is not adequate and another is that the experimental conditions may be different from those expected. Many possibilities exist regarding discrepancy in the experimental conditions. One of these is that there may be cracking of the concrete in the vicinity of the pressure sensor and another is that the sensor may not be located at the given depth.

Other aspects of the difficulty with the pressure measurements are suggested in Ref. 7. HEDL ran two tests reported in Ref. 7 only one of which is analyzed herein. In Test 2 (called WRD-2 by HEDL) the temperatures rose to considerably higher values than in Test 1 but the maximum pore pressure measured was less than two atmospheres while in Test 1 the pressures reached 8 atmospheres. HEDL [7] stated that "the very low pressures measured in WRD-2 may be anomalous, and tend to cast doubt upon the validity of the method used. In particular, abnormally low pressures would be measured in the case of cracking or poor bonding of the pressure taps to the concrete." Further improvements in methods of pressure measurement inside concrete are clearly needed.

The integrated water release in kg/m^3 for both measured and calculated values is shown in Fig. 8. In general the agreement is quite good between the two with the maximum difference occurring at 25200s and being about 15%.

Concluding Comments on the Analysis of Data

In the above test case agreement was obtained between the measured values and calculated values by varying three parameters: the low and temperature thermal conductivities and the Darcy factor D10C. The procedure in determining these parameters was to vary the parameters in a more or less systematic way and to observe the value of the sum of squares, called SUM in the output. This is an inefficient procedure and much better methods are available [11] for estimating parameters simultaneously and automatically. One difficulty, however, is that the calculations for the parameters require many complete solutions of the temperature, pressure, etc., histories and thus the computer time for solution may be in excess of what is practical on a time-sharing system. For the data given in Table 1 about 14s of CDC6600 time is used for each case. A computer program to automatically search for the minimum sum of squares might take 50 complete solutions or about 700s which is excessive for normal CDC6600 time-sharing usage. It could readily be handled on the CDC7600 which would require considerable less time to perform the same calculations.

There is another problem in addition to computer capacity, however. As USINT is presently written, the interface jumps from one node to an adjacent one. This "jumping" can cause difficulties in automatic seeking of the minimum sum of squares because the sum may have several local minima.

Advantages of the present relatively inefficient method of estimating parameters include that it is very flexible since any particular combination of parameters may be found. Moreover it is capable of finding the global minimum even though local minima exist, although this depends on the skill of the one doing the search.

TABLE 1

SAMPLE INPUT DATA FOR USINT

```
     CASE      DATE       ETA     LAMBA     NPRNT      NOPT      ZETA    ISTATE
  35.0000    7.0300     .5000     .5000        60         1    .40000        10
       DX        IW    IDEBUG    ICOEFF     IHEAT    IDARCY     IPIDH     IVDAR
  .009530        31         0         0         0         0         0         0
       DT       NTS    IDARCO    WDARCO     UWIN1     UWIN2     UWIN3      DIOC
  60.0000       420     45000         3   350.000   400.000   650.000   115.000
       UO    THETAO       EPO       PIO       P2O    VOLATW     WFLAG       PIB
   292.90     .0450     .0470  114880.0  101325.0      1.00         2         0
    QFLUX          KBOUND    NTWBCA    NTWBCB     IFTOK    NKTEMP    NCTEMP IKCAL
  0.                   -1        36        36         0         4         1     0
      TIWA(I),I=1,NTWBCA
     0.00   3600.00   7200.00  10800.00  14400.00  18000.00  21600.00  25200.00
 28800.00  32400.00  36000.00  39600.00  43200.00  46800.00  50400.00  54000.00
 57600.00  61200.00  64800.00  68400.00  72000.00  75600.00  79200.00  82800.00
 86400.00  90000.00  93600.00  97200.00 100800.00 104400.00 108000.00 111600.00
115200.00 118800.00 122400.00 126000.00
      TBCA(I),I=1,NTWBCA
   292.87    480.48    573.21    635.48    681.54    715.82    745.93    768.98
   789.15    804.93    817.98    829.59    838.32    845.98    852.59    858.54
   863.32    867.54    871.71    875.71    878.87    881.71    885.26    887.37
   891.04    692.48    894.21    895.32    895.93    897.15    898.54    898.71
   898.76    898.59    898.48    897.04
      TIWB(I),I=1,NTWBCB
     0.00   3600.00   7200.00  10900.00  14400.00  18000.00  21600.00  25200.00
 28800.00  32400.00  36000.00  39600.00  43200.00  46800.00  50400.00  54000.00
 57600.00  61200.00  64800.00  68400.00  72000.00  75600.00  79200.00  82800.00
 86400.00  90000.00  93600.00  97200.00 100800.00 104400.00 108000.00 111600.00
115200.00 118800.00 122400.00 126000.00
      TBCB(I),I=1,NTWBCB
   293.09    297.32    297.98    299.32    301.37    302.71    307.21    311.76
   316.43    320.76    324.26    327.09    330.82    334.43    336.15    337.59
   339.04    339.93    340.87    341.21    341.87    342.37    343.26    340.98
   340.87    342.87    344.04    344.93    345.87    346.43    346.48    347.37
   347.71    347.71    347.48    347.48
   TKPROP  THERM.COND.
    0.000     2.800
  373.000     2.800
  800.000      .100
 1200.000      .200
INITIAL CONCRETE DENSITY=RHO1C+RHO2C+RHO3C+RHO4C+ VAPOR CONTRIBUTION
    RHO1C     RHO2C     RHO3C     RHO4C
   111.60     73.40    975.00   2579.00
CPO=CONCRETE SP. HT.
   800.00
    NULOC     NUTIW     NPLOC     NPTIW    NWRTIW   WEIGHT1   WEIGHT2   WEIGHT3
        5        35         2        16        16      10.0  100000.0    1.0000
```

TABLE I (CONTINUED)

```
      TIMEU(I),I=1,NUTIM
    0.00    3600.00    7200.00   10800.00   14400.00   18000.00   21600.00   25200.00
28800.00   32400.00   36000.00   39600.00   43200.00   46800.00   50400.00   54000.00
57600.00   61200.00   64800.00   68400.00   72000.00   75600.00   79200.00   82800.00
86400.00   90000.00   93600.00   97200.00  100800.00  104400.00  108000.00  111600.00
115200.00 118800.00 122400.00 126000.00
 EXPERIMENTAL TEMPERATURES AT X=      .035100
   293.43      384.82      437.59      484.43      526.93      563.26      591.54      616.65
   636.82      654.43      673.54      688.76      700.71      710.37      718.93      726.59
   733.15      739.09      744.15      748.93      753.43      757.87      761.59      763.82
   766.09      769.54      771.87      773.76      776.09      777.71      779.26      780.26
   780.98      781.71      781.87      781.76
 EXPERIMENTAL TEMPERATURES AT X=      .087200
   293.43      321.71      365.98      398.93      422.98      441.26      461.21      481.26
   498.82      516.65      534.48      550.26      564.54      576.21      585.71      593.32
   599.93      605.48      610.65      615.32      619.21      623.48      627.48      630.59
   633.54      636.09      638.98      641.48      644.37      646.48      648.59      650.43
   651.93      653.26      654.04      654.37
 EXPERIMENTAL TEMPERATURES AT X=      .133500
   293.59      314.26      325.82      353.43      374.43      391.87      406.32      417.32
   426.21      428.98      436.93      452.15      466.15      477.43      486.98      495.37
   502.54      508.87      514.43      519.87      524.54      529.21      531.98      535.26
   538.76      541.93      544.43      546.82      549.48      551.82      553.93      555.71
   557.32      558.09      558.59      560.09
 EXPERIMENTAL TEMPERATURES AT X=      .177700
   293.37      298.32      303.26      317.87      336.32      353.87      368.43      380.87
   388.82      396.32      404.26      410.21      415.21      420.21      424.59      428.87
   432.54      436.21      439.48      443.04      446.32      449.65      451.32      453.76
   456.82      460.09      462.87      465.71      468.21      470.65      472.54      475.09
   476.71      478.04      479.37      479.87
 EXPERIMENTAL TEMPERATURES AT X=      .236500
   293.09      298.26      303.43      308.82      313.76      321.76      330.87      339.71
   347.37      353.93      360.21      364.26      367.54      371.26      373.87      376.54
   378.87      381.09      382.93      384.54      386.43      388.15      390.65      391.04
   392.82      393.48      395.21      396.37      397.54      398.48      398.82      399.98
   400.32      400.37      400.32      400.21
      TIMEP(I),I=1,NPTIM
    0.00    1800.00    3600.00    5400.00    7200.00    9000.00   10800.00   12600.00
14400.00   16200.00   18000.00   19800.00   21600.00   23400.00   25200.00   27000.00
 EXPERIMENTAL PRESSURES AT X=      .035050
101000.00 101000.00 411000.00 443000.00 655000.00 820000.00 784000.00 738000.00
668000.00 612000.00 566000.00 532000.00 504000.00 482000.00 462000.00 444000.00
 EXPERIMENTAL PRESSURES AT X=      .177700
101000.00 101000.00 101000.00 101000.00 336000.00 508000.00 571000.00 616000.00
632000.00 625000.00 615000.00 604000.00 593000.00 581000.00 568000.00 553000.00
      TIMEWR(I),I=1,NWRTIM
    0.00    1800.00    3600.00    5400.00    7200.00    9000.00   10800.00   12600.00
14400.00   16200.00   18000.00   19800.00   21600.00   23400.00   25200.00   27000.00
 EINTWR(I),I=1,NRWTIM
    0.00        .09       1.13       2.75       4.14       5.57       6.95       8.33
    9.73      11.03      12.23      13.45      14.52      15.58      16.59      17.62
```

TABLE 2

SAMPLE OUTPUT FOR USINT. TIME EQUALS ZERO

```
 FIELD QUANTITIES AT N =    0   AND T = 0.          SEC = 0.          MIN
  X(I)       U         QDOT          AI        S1DOT(STM)  S2DOT(CO2)  S3DOT(LIQ)
0.0000  2.9290E+02  0.          0.          0.          0.          0.
 .0095  2.9290E+02  0.          0.          0.          0.          0.
 .0191  2.9290E+02  0.          0.          0.          0.          0.
 .0286  2.9290E+02  0.          0.          0.          0.          0.
 .0381  2.9290E+02  0.          0.          0.          0.          0.
 .0477  2.9290E+02  0.          0.          0.          0.          0.
 .0572  2.9290E+02  0.          0.          0.          0.          0.
 .0667  2.9290E+02  0.          0.          0.          0.          0.
 .0762  2.9290E+02  0.          0.          0.          0.          0.
 .0858  2.9290E+02  0.          0.          0.          0.          0.
 .0953  2.9290E+02  0.          0.          0.          0.          0.
 .1048  2.9290E+02  0.          0.          0.          0.          0.
 .1144  2.9290E+02  0.          0.          0.          0.          0.
 .1239  2.9290E+02  0.          0.          0.          0.          0.
 .1334  2.9290E+02  0.          0.          0.          0.          0.
 .1430  2.9290E+02  0.          0.          0.          0.          0.
 .1525  2.9290E+02  0.          0.          0.          0.          0.
 .1620  2.9290E+02  0.          0.          0.          0.          0.
 .1715  2.9290E+02  0.          0.          0.          0.          0.
 .1811  2.9290E+02  0.          0.          0.          0.          0.
 .1906  2.9290E+02  0.          0.          0.          0.          0.
 .2001  2.9290E+02  0.          0.          0.          0.          0.
 .2097  2.9290E+02  0.          0.          0.          0.          0.
 .2192  2.9290E+02  0.          0.          0.          0.          0.
 .2287  2.9290E+02  0.          0.          0.          0.          0.
 .2383  2.9290E+02  0.          0.          0.          0.          0.
 .2478  2.9290E+02  0.          0.          0.          0.          0.
 .2573  2.9290E+02  0.          0.          0.          0.          0.
 .2668  2.9290E+02  0.          0.          0.          0.          0.
 .2764  2.9290E+02  0.          0.          0.          0.          0.
 .2859  2.9290E+02  0.          0.          0.          0.          0.
```

TABLE 2 (CONTINUED)

```
    VB =    0.                XB =    0.            INCIDENT FLUX =    0.
  X(I)          PI               EP             P                A2            THETA             V1
0.0000   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0095   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0191   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0286   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0381   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0477   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0572   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0667   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0762   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0858   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .0953   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1048   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1144   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1239   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1334   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1430   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1525   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1620   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1715   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1811   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .1906   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2001   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2097   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2192   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2287   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2383   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2478   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2573   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2668   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2764   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
 .2859   1.1488E+05   1.0133E+05   2.1621E+05   0.                     4.5000E-02   0.
EXP. TIME LOCATION   EPR(IC,JJ)       PINT        PRDIF        SUM
   1800.00     .03505     .101E+06    .191E+06   -.903E+05    .815E+00
   1800.00     .17770     .101E+06    .115E+06   -.141E+05    .835E+00
EXP. TIME   EINTWR(IC)     WATREL    WATDIF          SUM
    1800.0     .093000  1.147883 -1.054883      .19480E+01
```

TABLE 3

OUTPUT FROM USINT FOR TEST CASE. TIME EQUALS 3600 S

```
 FIELD QUANTITIES AT N =  60  AND T = 3.6000E+03 SEC = 6.0000E+01 MIN
 X(I)        U          QDOT            AI         S1DOT(STM)  S2DOT(CO2)   S3DOT(LIQ)
0.0000  4.8048E+02 -3.1894E+00  1.0000E+00  5.4896E-07  0.            0.
 .0095  4.4114E+02 -7.0148E-02  1.0000E+00  1.2074E-08  0.            0.
 .0191  4.1003E+02 -5.9452E+04  1.0000E+00  3.5112E-10  0.          -2.62E-02
 .0286  3.8672E+02  1.3218E+04  9.9893E-01  2.0624E-03  0.           8.36E-03
 .0381  3.6751E+02 -1.1843E+04  9.0084E-01  7.3335E-02  0.           8.49E-02
 .0477  3.5223E+02 -5.6007E+05  1.5995E-01  2.9750E-01  0.           1.19E-01
 .0572  3.3984E+02  4.5128E+01  0.          0.          0.           1.83E-05
 .0667  3.2988E+02  6.0036E+00  0.          0.          0.           1.43E-06
 .0762  3.2188E+02  5.2332E-01  0.          0.          0.          -6.89E-07
 .0858  3.1547E+02 -2.1342E+00  0.          0.          0.          -1.64E-06
 .0953  3.1036E+02 -3.2832E+00  0.          0.          0.          -1.99E-06
 .1048  3.0630E+02 -3.6191E+00  0.          0.          0.          -2.02E-06
 .1144  3.0310E+02 -3.5156E+00  0.          0.          0.          -1.89E-06
 .1239  3.0060E+02 -3.1866E+00  0.          0.          0.          -1.67E-06
 .1334  2.9868E+02 -2.7629E+00  0.          0.          0.          -1.43E-06
 .1430  2.9722E+02 -2.3241E+00  0.          0.          0.          -1.19E-06
 .1525  2.9613E+02 -1.9158E+00  0.          0.          0.          -9.75E-07
 .1620  2.9534E+02 -1.5605E+00  0.          0.          0.          -7.91E-07
 .1715  2.9478E+02 -1.2662E+00  0.          0.          0.          -6.40E-07
 .1811  2.9441E+02 -1.0328E+00  0.          0.          0.          -5.21E-07
 .1906  2.9418E+02 -8.5551E-01  0.          0.          0.          -4.31E-07
 .2001  2.9408E+02 -7.2768E-01  0.          0.          0.          -3.66E-07
 .2097  2.9409E+02 -6.4198E-01  0.          0.          0.          -3.23E-07
 .2192  2.9419E+02 -5.9114E-01  0.          0.          0.          -2.98E-07
 .2287  2.9437E+02 -5.6833E-01  0.          0.          0.          -2.87E-07
 .2383  2.9464E+02 -5.6730E-01  0.          0.          0.          -2.87E-07
 .2478  2.9499E+02 -5.8238E-01  0.          0.          0.          -2.95E-07
 .2573  2.9543E+02 -6.0838E-01  0.          0.          0.          -3.09E-07
 .2668  2.9595E+02 -6.3423E-01  0.          0.          0.          -3.24E-07
 .2764  2.9658E+02 -1.7012E+02  0.          0.          0.          -7.50E-05
 .2859  2.9732E+02  0.          0.          0.          0.            0.
```

TABLE 3 (CONTINUED)

```
   VB =   0.            XB =   0.          INCIDENT FLUX =   9.2300E+03
IGPM=    2  IWI =    3  IWDF =    0  ITHI =    3  IPIDM =    2
INTEGRATED WATER RELEASE= 2.279E+00KG/M2 WATER REL. RATE= 2.527E-03KG/M2-SEC
 X(I)        PI          EP           P            A2          THETA          VI
0.0000  0.          1.5860E-01  0.          1.7662E-06  1.5860E-01  0.
 .0095  2.7331E+05  1.5860E-01  3.7464E+05  3.8560E-08  1.5860E-01 -1.28E-04
 .0191  5.4395E+05  1.5860E-01  6.4528E+05  7.8450E-10  1.4564E-01 -2.70E-05
 .0286  4.3034E+05  1.5848E-01  5.3166E+05  0.          1.0847E-02  0.
 .0381  3.4693E+05  1.4753E-01  4.4825E+05  0.          9.7937E-03  1.79E-06
 .0477  2.8741E+05  6.4850E-02  3.8874E+05  0.          5.1233E-02  9.46E-07
 .0572  2.4372E+05  4.7000E-02  3.4505E+05  0.          4.4965E-02  4.01E-07
 .0667  2.1152E+05  4.7000E-02  3.1285E+05  0.          4.4981E-02  3.08E-07
 .0762  1.8759E+05  4.7000E-02  2.8891E+05  0.          4.4988E-02  2.37E-07
 .0858  1.6964E+05  4.7000E-02  2.7096E+05  0.          4.4993E-02  1.83E-07
 .0953  1.5608E+05  4.7000E-02  2.5741E+05  0.          4.4996E-02  1.41E-07
 .1048  1.4581E+05  4.7000E-02  2.4713E+05  0.          4.4998E-02  1.09E-07
 .1144  1.3802E+05  4.7000E-02  2.3934E+05  0.          4.4999E-02  8.33E-08
 .1239  1.3213E+05  4.7000E-02  2.3345E+05  0.          4.4999E-02  6.35E-08
 .1334  1.2770E+05  4.7000E-02  2.2902E+05  0.          4.5000E-02  4.79E-08
 .1430  1.2439E+05  4.7000E-02  2.2572E+05  0.          4.5000E-02  3.58E-08
 .1525  1.2196E+05  4.7000E-02  2.2329E+05  0.          4.5000E-02  2.62E-08
 .1620  1.2021E+05  4.7000E-02  2.2153E+05  0.          4.5000E-02  1.87E-08
 .1715  1.1898E+05  4.7000E-02  2.2031E+05  0.          4.5000E-02  1.29E-08
 .1811  1.1817E+05  4.7000E-02  2.1949E+05  0.          4.5000E-02  8.19E-09
 .1906  1.1768E+05  4.7000E-02  2.1901E+05  0.          4.5000E-02  4.41E-09
 .2001  1.1747E+05  4.7000E-02  2.1880E+05  0.          4.5000E-02  1.27E-09
 .2097  1.1748E+05  4.7000E-02  2.1881E+05  0.          4.5000E-02 -1.44E-09
 .2192  1.1770E+05  4.7000E-02  2.1902E+05  0.          4.5000E-02 -3.88E-09
 .2287  1.1810E+05  4.7000E-02  2.1942E+05  0.          4.5000E-02 -6.19E-09
 .2383  1.1868E+05  4.7000E-02  2.2000E+05  0.          4.5000E-02 -8.48E-09
 .2478  1.1944E+05  4.7000E-02  2.2077E+05  0.          4.5000E-02 -1.08E-08
 .2573  1.2040E+05  4.7000E-02  2.2172E+05  0.          4.5000E-02 -1.33E-08
 .2668  1.2156E+05  4.7000E-02  2.2289E+05  0.          4.5000E-02 -1.60E-08
 .2764  1.2295E+05  4.7000E-02  2.2428E+05  0.          4.5150E-02  7.63E-07
 .2859  0.          4.7000E-02  1.0133E+05  0.          4.5000E-02  0.
  EXP. TIME  LOCATION  EU(IC,JJ)      TINT       TDIF        SUM
   3600.00        .04     384.82    373.60      11.22    .32067E+01
   3600.00        .09     321.71    314.70       7.00    .36968E+01
   3600.00        .13     314.26    298.67      15.59    .61273E+01
   3600.00        .18     298.32    294.54       3.78    .62701E+01
   3600.00        .24     298.26    294.59       3.67    .64048E+01
 EXP. TIME LOCATION  EPR(IC,JJ)     PINT      PRDIF       SUM
   3600.00     .03505   .411E+06   .374E+06   .372E+05   .654E+01
   3600.00     .17770   .101E+06   .118E+06  -.175E+05   .657E+01
 EXP. TIME  EINTWR(IC)   WATREL    WATDIF       SUM
    3600.0  1.133000  2.279463 -1.146463     .78881E+01
 EXP. TIME LOCATION  EPR(IC,JJ)     PINT      PRDIF       SUM
   5400.00     .03505   .443E+06   .566E+06  -.123E+06   .941E+01
   5400.00     .17770   .101E+06   .129E+06  -.282E+05   .949E+01
 EXP. TIME  EINTWR(IC)   WATREL    WATDIF       SUM
    5400.0  2.749000  3.145776  -.396776     .96460E+01
```

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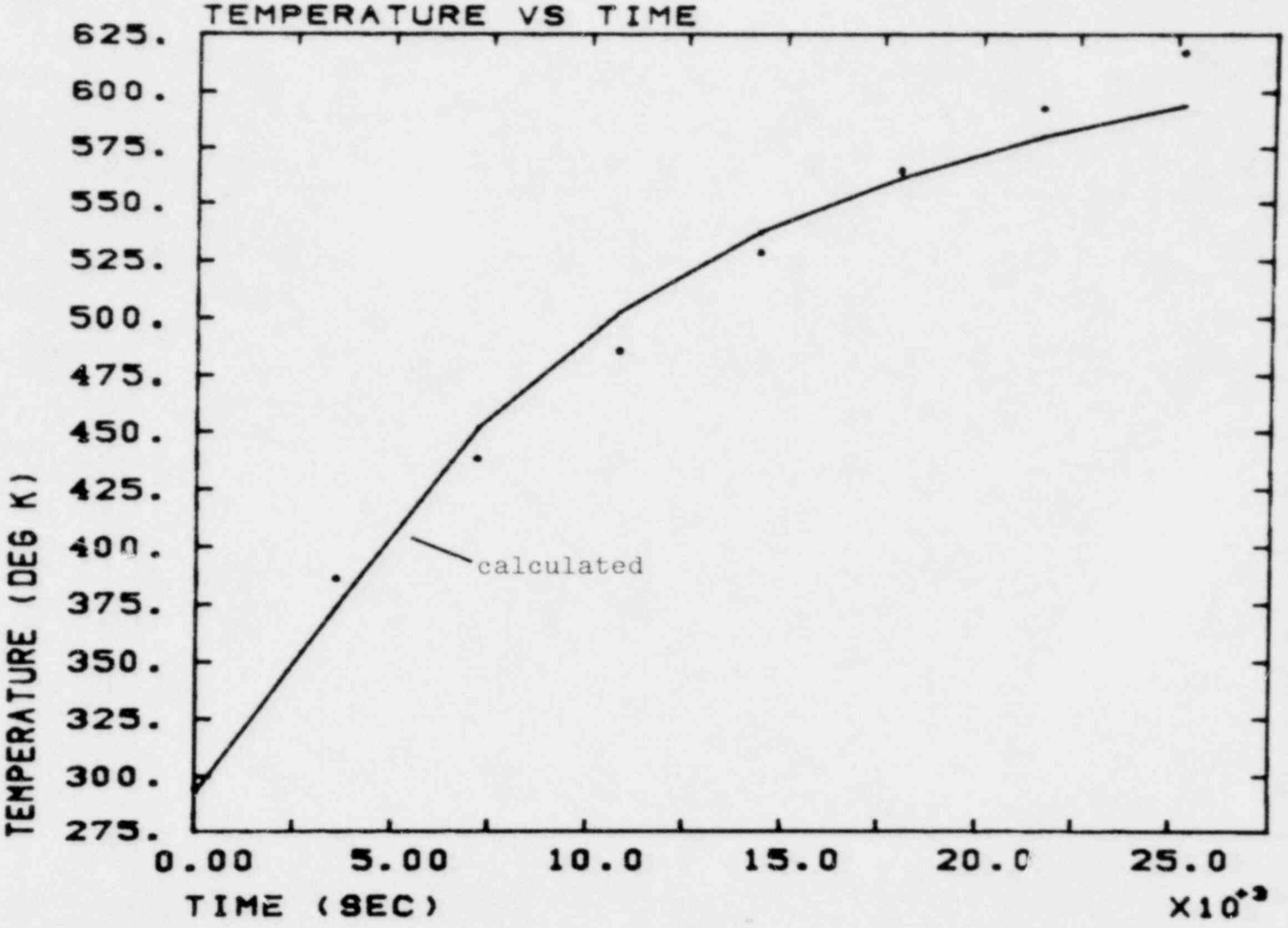

Fig. 1 Plot of calculated and measured temperatures at x=.0351m for HEDL Test No. 1 data [7].

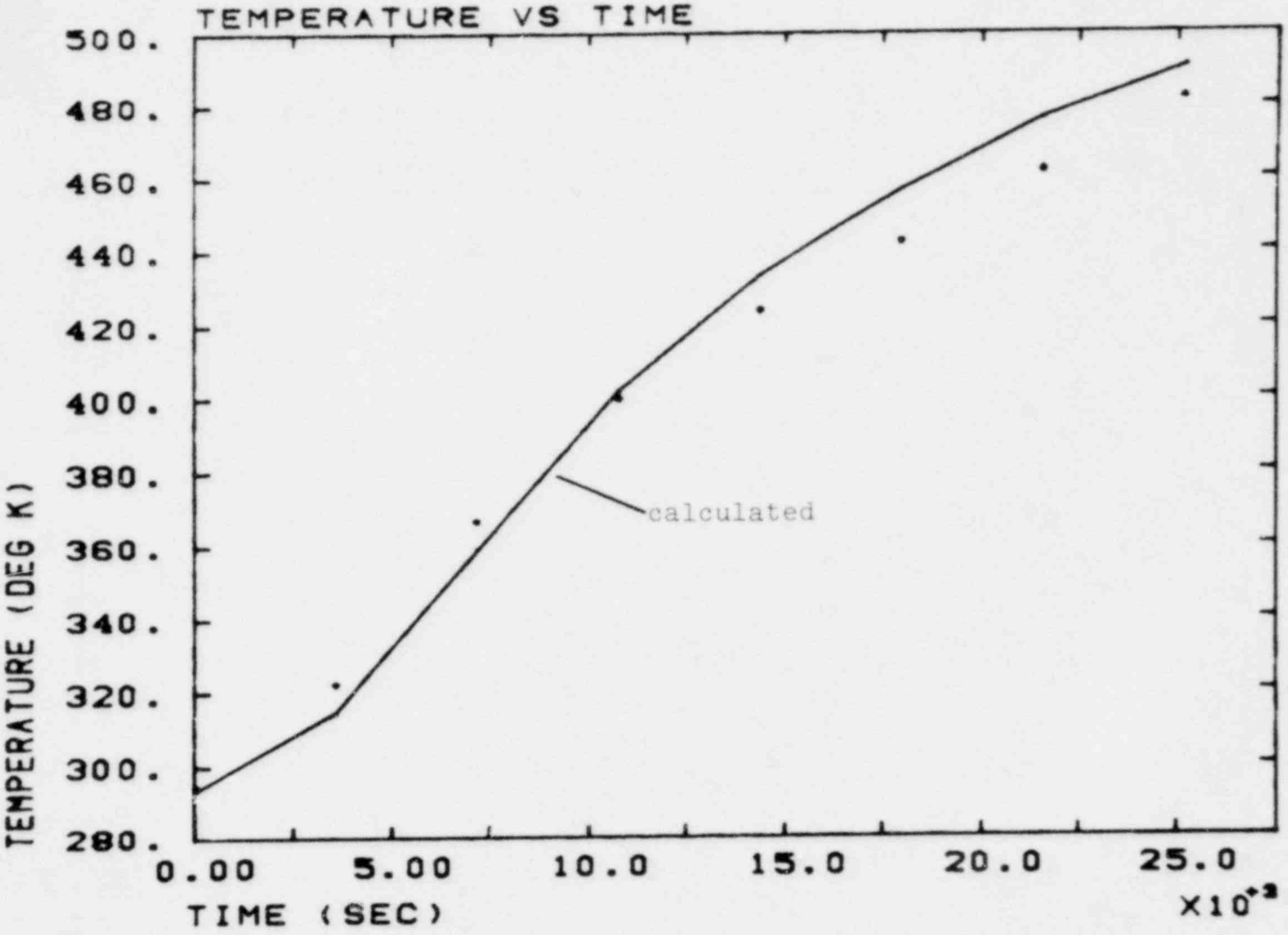

Fig. 2 Plot of calculated and measured temperatures at x=.0872m for HEDL Test No. 1 data [7].

9

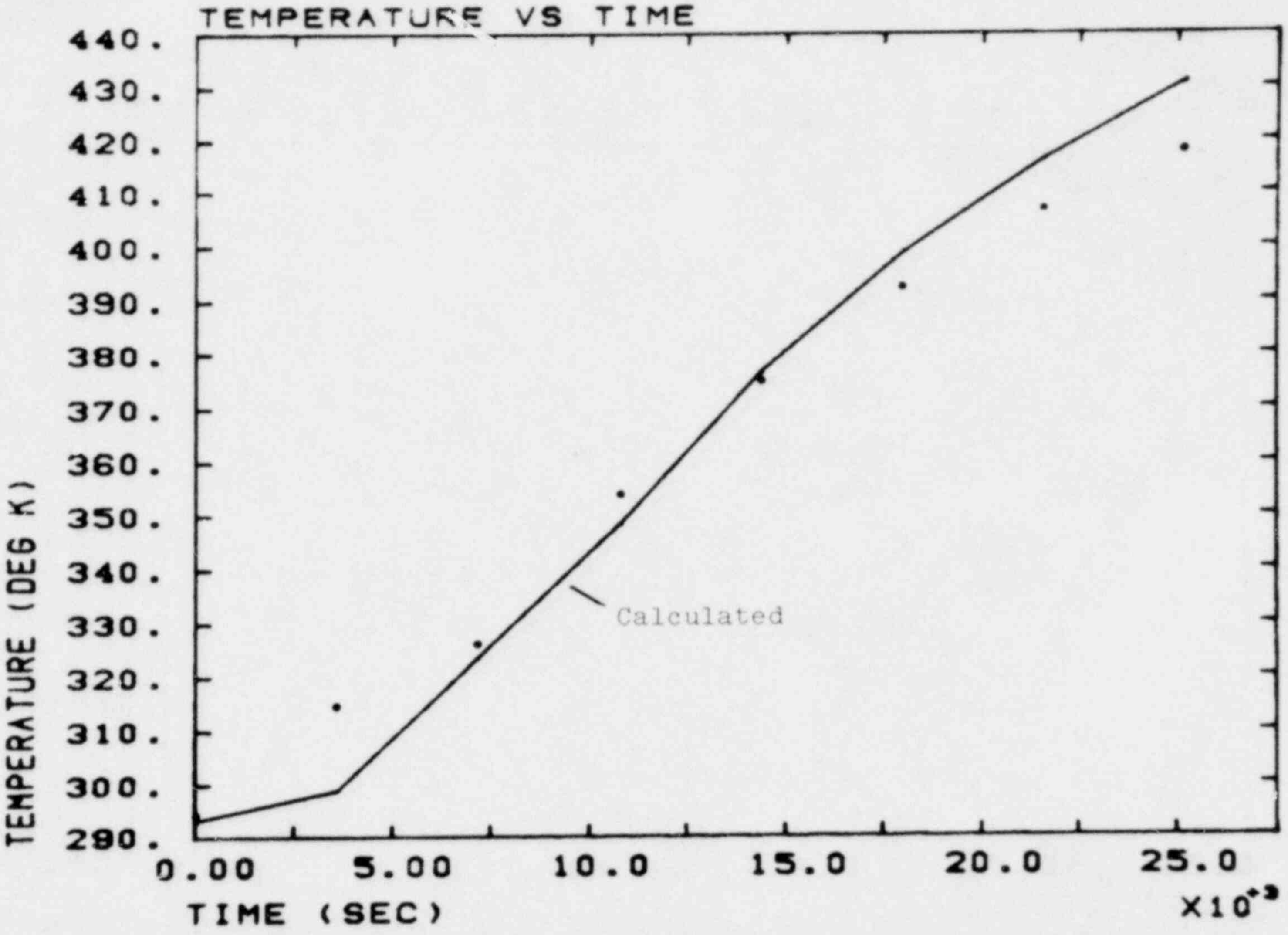

Fig. 3 Plot of calculated and measured temperatures at x=.1335m for HEDL Test No. 1 data [7].

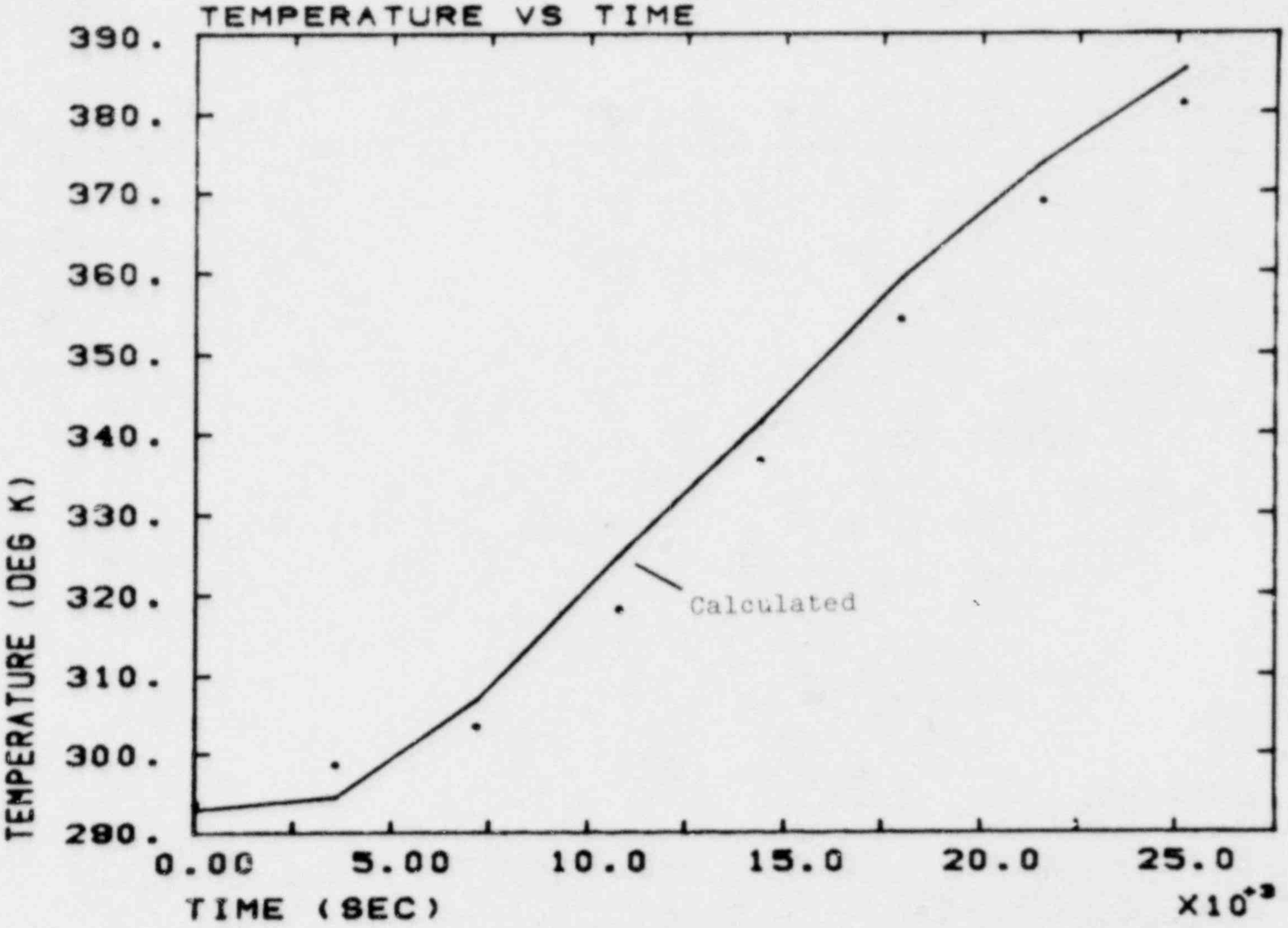

Fig. 4 Plot of calculated and measured temperatures at x=.1777m for HEDL Test No. 1 data [7].

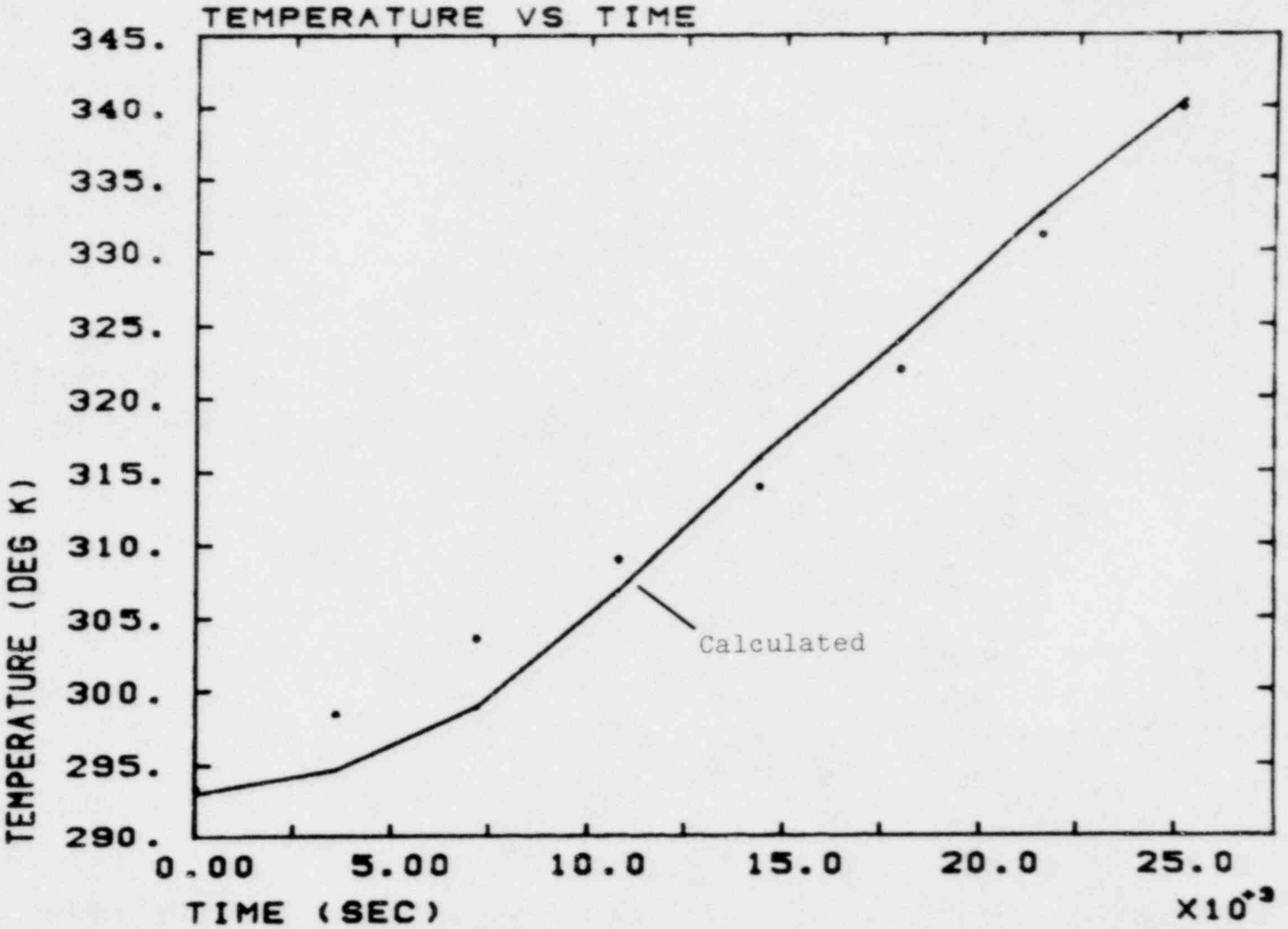

Fig. 5 Plot of calculated and measured temperatures at x=.2365m for HEDL Test No. 1 data [7].

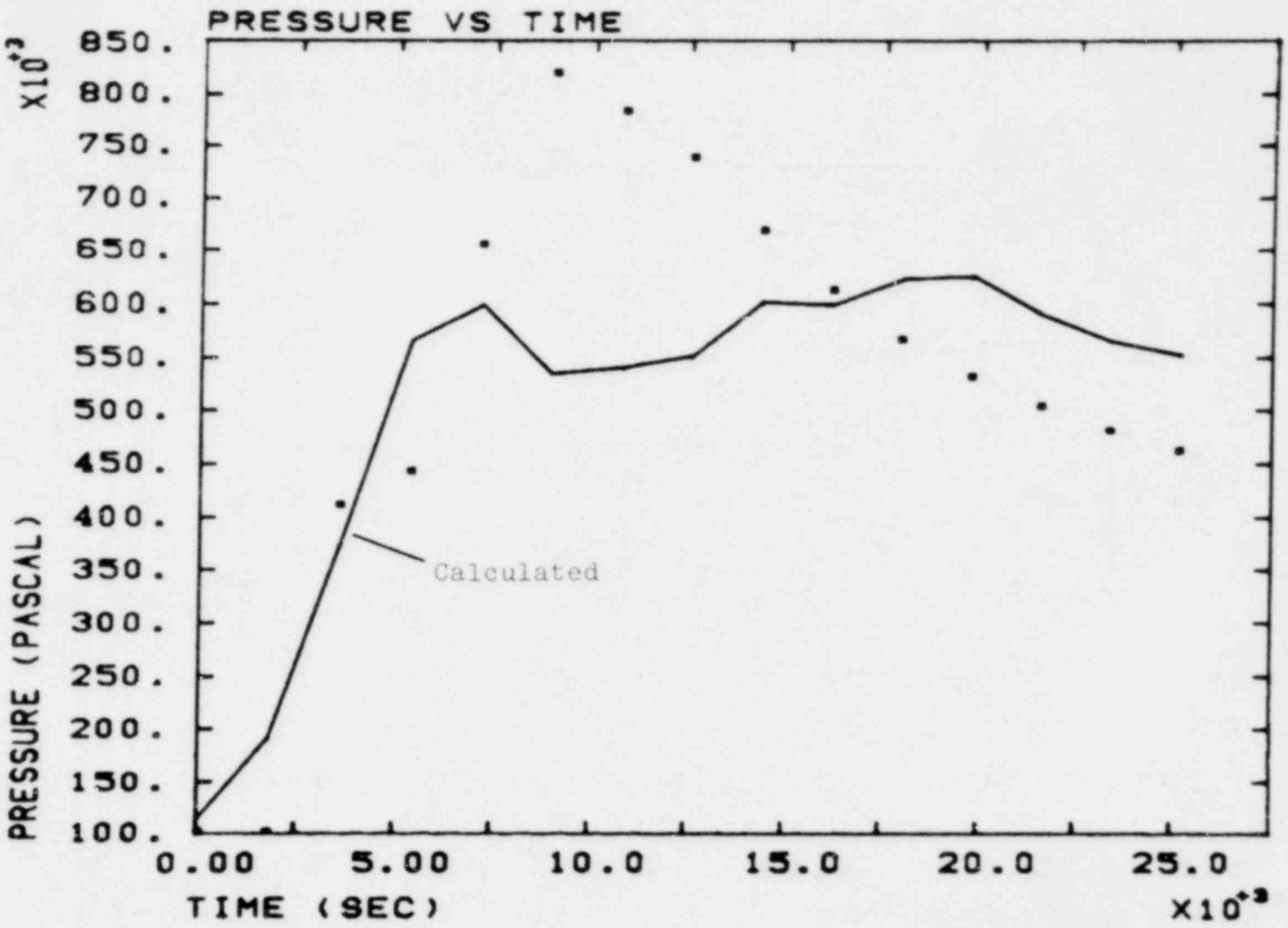

Fig. 6 Plot of calculated and measured pressures at x=.0351m for HEDL Test No. 1 data [7].

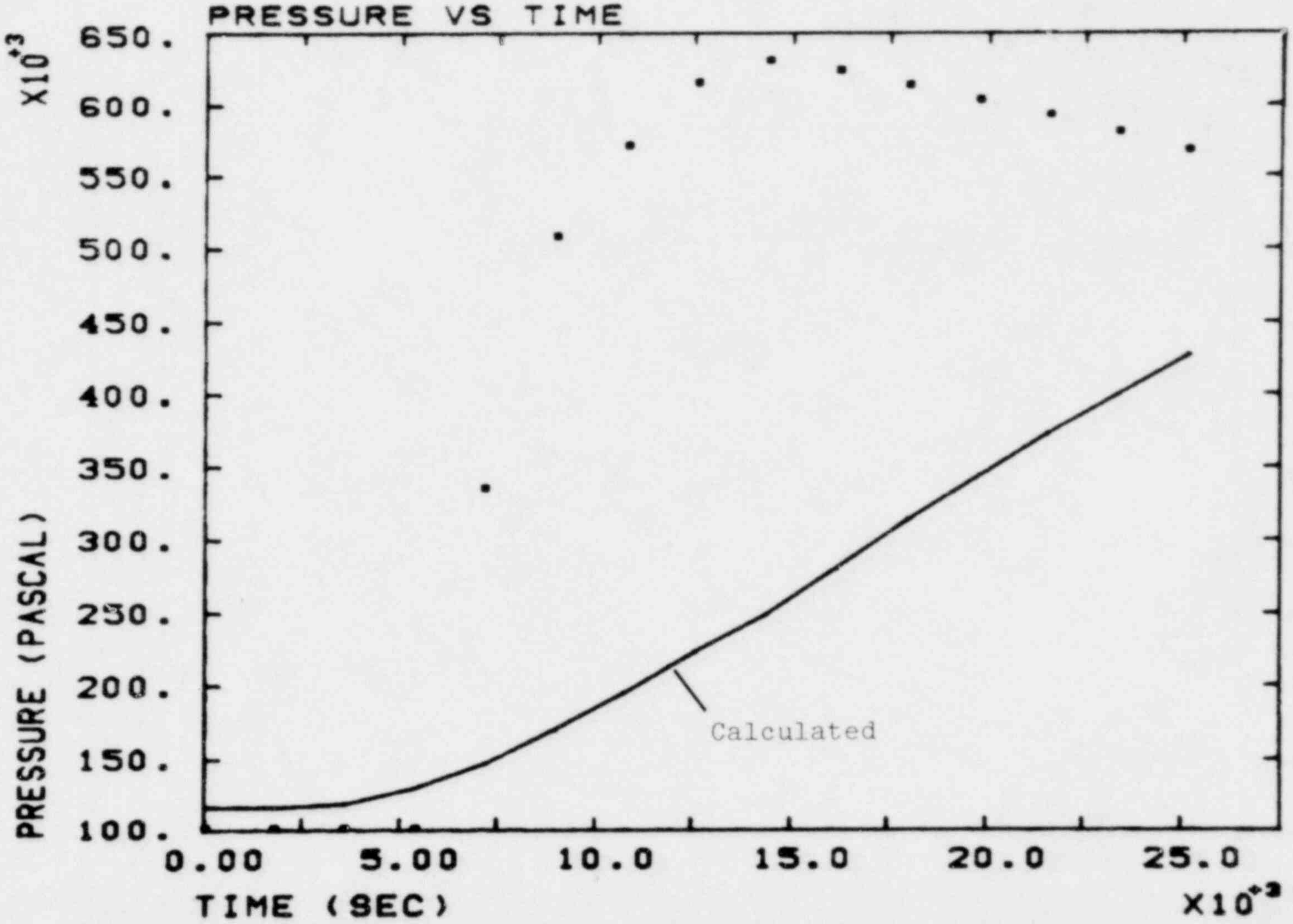

Fig. 7 Plot of calculated and measured pressures at x=.1777m for HEDL Test No. 1 data [7].

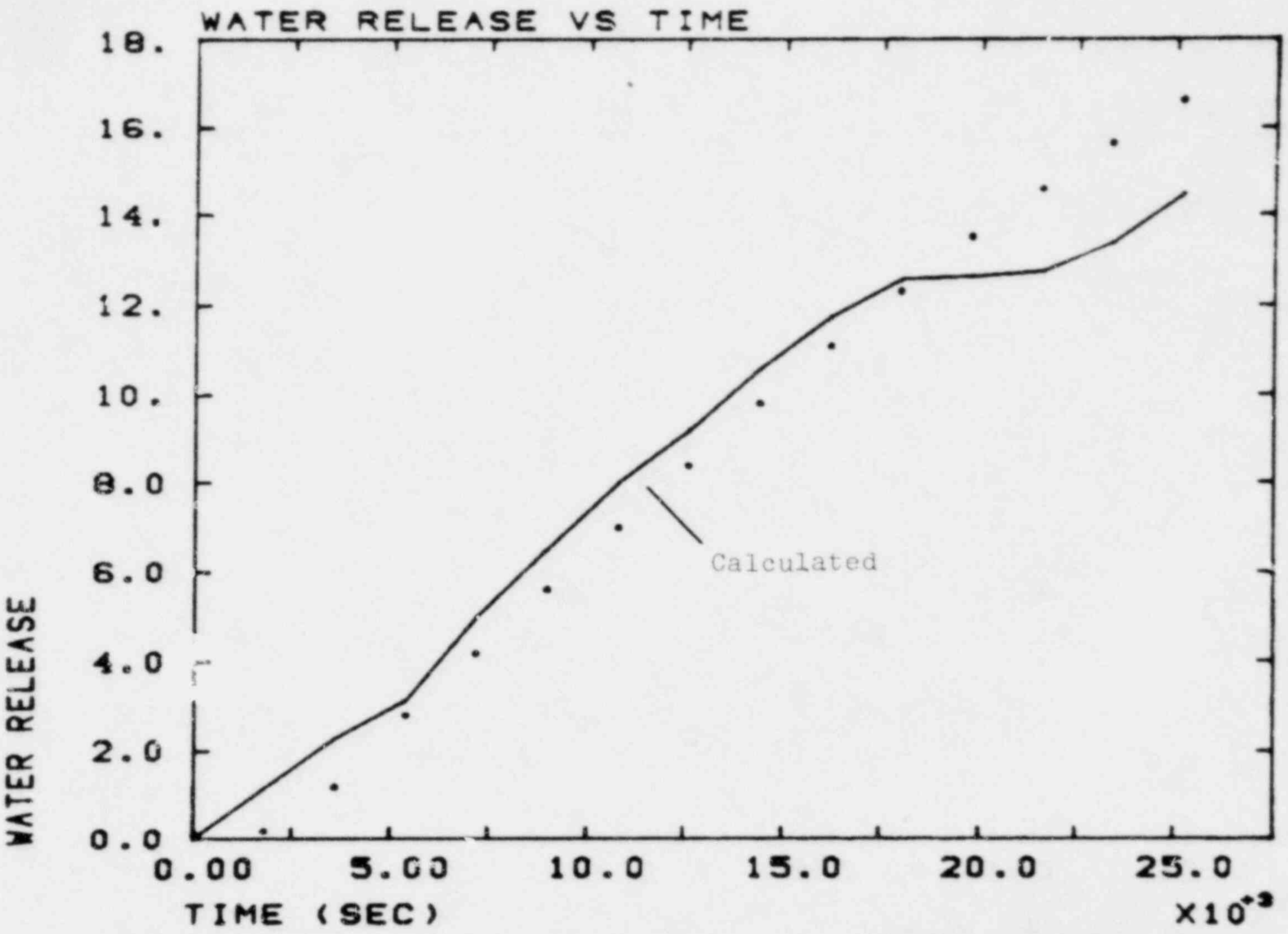

Fig. 8 Plot of calculated and measured value of integrated water release for HEDL Test No. 1 data [7].

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