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TOM MIX: A Computer Code for Calculating Steam Explosion Phenomena

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ABSTRACT

A mathematical model for a mixture of hot liquid drops mixed and in film boiling with water is developed. It is used to examine the propagation and growth of pressure disturbances which result in a steam explosion.

The model is incorporated into a wave-propagation computer code and an example problem is examined. These calculations suggest that pressure disturbances will propagate and grow in the mixture even if the drops do not fragment. These pressure pulses initiate fragmentation which ultimately controls the release of energy during a steam explosion.

PREFACE

The purpose of this report is to present a mathematical model to describe steam explosions and to document its implementation into a computer code. This report does not contain a review of the extensive literature on the subject. For such reviews, the reader is referred to Croneberg and Benz¹ and to Nelson and Duda.² The limited references recorded in this work are specific to the construction of the theory and the computer code.

The reader is warned that this code is still experimental. Errors may still exist in the program logic.

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I. INTRODUCTION

When hot molten materials are mixed with a more volatile fluid, a sudden and violent vaporization of the fluid sometimes occurs. Such events present a potential hazard to the safe operation of water-cooled nuclear power reactors.¹

The accidental melting of a reactor core can introduce a large number of molten drops into the reactor coolant. In a pressurized water reactor these drops go into stable film boiling with the coolant. The resulting vapor films which surround each drop effectively insulate the drops from additional loss of heat by thermal conduction to the coolant; however, small disturbances can disrupt these films causing a sudden and explosive vaporization of the coolant.²

Board and Hall³ propose that this event behaves as a detonation wave propagating through a high explosive. They surmise that the initial disturbance fragments a small number of drops which results in increased contact area and vaporization of the coolant. This process in turn fragments neighboring drops and causes the disturbance to propagate and grow. Board and Hall do not offer a quantitative description of the fragmentation process.

Recently, Drumheller⁴ proposed a film collapse model which describes the fragmentation process. In this model, the disturbance elevates the pressure locally in the coolant. Some of the vapor films are compressed and condensed. As a result, the coolant impacts and fragments some of the drops. Thus, the coolant acts like a "hydraulic hammer" applied in a spherically symmetric fashion to the surface of the drop.

A model to describe the propagation of a steam explosion through an array of molten drops in water can be constructed by incorporating

the single-drop model of Drumheller into a mixture theory. The mixture theory of Bedford and Drumheller^{5,6,7} is used since it easily accommodates the microstructural phenomena associated with the vapor-film collapse.

Each constituent is assigned a balance of mass equation, and exchange of mass between the vapor and coolant is allowed. The model ignores relative translation of the melt, vapor, and coolant. Consequently, only one balance of momentum equation is used.* Each constituent is assigned an individual temperature and is described by a separate balance of energy equation which accounts for the exchange of thermal and mechanical energy between the constituents.

In addition to these equations which account for changes in mass density, velocity, and temperature, auxiliary equations are employed to compute changes in the drop radii and vapor-film thicknesses. These relations have the form of the classical Rayleigh cavitation equation for a bubble in an infinite fluid. The structure of the completed theory is similar to those constructed for bubbly liquids.^{8,9,10} A brief derivation of the theory will be given in the next section. This will be followed by a description of the constitutive assumptions.

Section IV contains a description of the numerical solution procedure. The theory is incorporated into a conventional, one-dimensional, wave propagation code, WONDY IV.¹¹ The method is similar to that described in Ref. 10.

An example problem is worked in Section V. In this problem a weak trigger pulse is applied to the boundary of a mixture of molten iron drops in water.

*The spherically symmetric collapse of the vapor film does not result in a net translation of the coolant with respect to the drops.

II. FIELD EQUATIONS

The equations of balance of mass, momentum, and energy are derived by a method employing Hamilton's variational principle. This method is described in several papers by Bedford and Drumheller.⁵⁻⁷

These papers also outline the basic motivations behind the mixture theory used in this work; that is, this theory preserves the identity and internal structure of each constituent in the mixture. The constitutive relations for water, steam, and molten drops are used unaltered in the theory; the theory explicitly accounts for the volume fractions occupied by each constituent; and information about the geometry of the individual molten drops and their vapor films is preserved.

The particular microstructural model used in this work is described in Drumheller.⁴ The works of Drumheller and Bedford^{8,9} give details on how a similar microstructural model for gas bubbles in a liquid is incorporated into a mixture theory.

These works on bubbly liquids have particular relevance to the present problem since the basic microstructure of the steam explosion is viewed as a mixture of steam bubbles in water. The steam bubbles exist because each bubble contains a drop of hot molten material. Pressure disturbances cause condensation and evaporation as well as mechanical oscillation of the steam bubbles. When sufficient pressure is applied to an individual steam bubble, the bubble collapses and the coolant impacts and fragments the molten drop inclusion.

Hamilton's variational principle is based on an energy postulate. As shown in Refs. 5-7, various kinematical constraints can be embedded into this energy postulate. Application of the variational procedure then yields

equations of motion which are consistent with the combined energy and kinematical statements. The derivation of the equations of motion will be outlined by first postulating the form of the kinematical constraints.

To begin, in one spatial dimension the original position of a material particle is given by X and the current position is given by x .[†] The variable J , called the Jacobian of the motion, is given by

$$J = \partial x / \partial X \quad . * \quad (1)$$

The mass densities and volume fractions of the molten material, vapor, and coolant are given by $\bar{\rho}_f$, $\bar{\rho}_v$, $\bar{\rho}_c$, ϕ_f , ϕ_v , and ϕ_c . The density of the mixture, ρ , is given as

$$\rho = \phi_f \bar{\rho}_f + \phi_v \bar{\rho}_v + \phi_c \bar{\rho}_c \quad (2)$$

where

$$\phi_f + \phi_v + \phi_c = 1 \quad . \quad (3)$$

The balance of mass postulate for the mixture is

$$\rho J = \rho_0 \quad (4)$$

where ρ_0 is the original value of ρ . A more familiar form of Eqn. (4) is

$$\dot{\rho} + \rho \partial v / \partial x = 0 \quad (5)$$

where the dot denotes the material time derivative and v is the particle velocity

[†]A nomenclature is included in Appendix A.

*This work does not contain a rigorous derivation of the theory. Rather, only an outline is presented. A more precise derivation is given in Refs. 5-7.

$$v = \partial x / \partial t \quad . \quad (6)$$

Similarly, the balance of mass postulates for the constituents are

$$\phi_f \bar{\rho}_f J = \phi_{f0} \bar{\rho}_{f0} \quad , \quad (7)$$

$$\phi_v \bar{\rho}_v J = \phi_{v0} \bar{\rho}_{v0} + c_v \quad , \quad (8)$$

and

$$\phi_c \bar{\rho}_c J = \phi_{c0} \bar{\rho}_{c0} - c_v \quad . \quad (9)$$

Note that Eqn. (4) can be recovered by adding Eqns. (7), (8), and (9). In the above equations c_v represents the exchange of mass between the vapor and the coolant. During evaporation, c_v is positive. Furthermore, these equations imply absence of relative translational motion between the constituents.

If R_f , R_v , and R_c represent the radii of the molten drop, the vapor film, and the unit cell of coolant which encloses the drop (see Fig. 1) then another set of constraints is obtained. These constraints are

$$\phi_c = 1 - R_v^3 / JR_{c0}^3 \quad , \quad (10)$$

$$\phi_f = R_f^3 / JR_{c0}^3 \quad , \quad (11)$$

and

$$\phi_v = (R_v^3 - R_f^3) / JR_{c0}^3 \quad . \quad (12)$$

Note that these relations satisfy Eqn. (3). Also

$$R_c^3 = JR_{c0}^3 \quad . \quad (13)$$

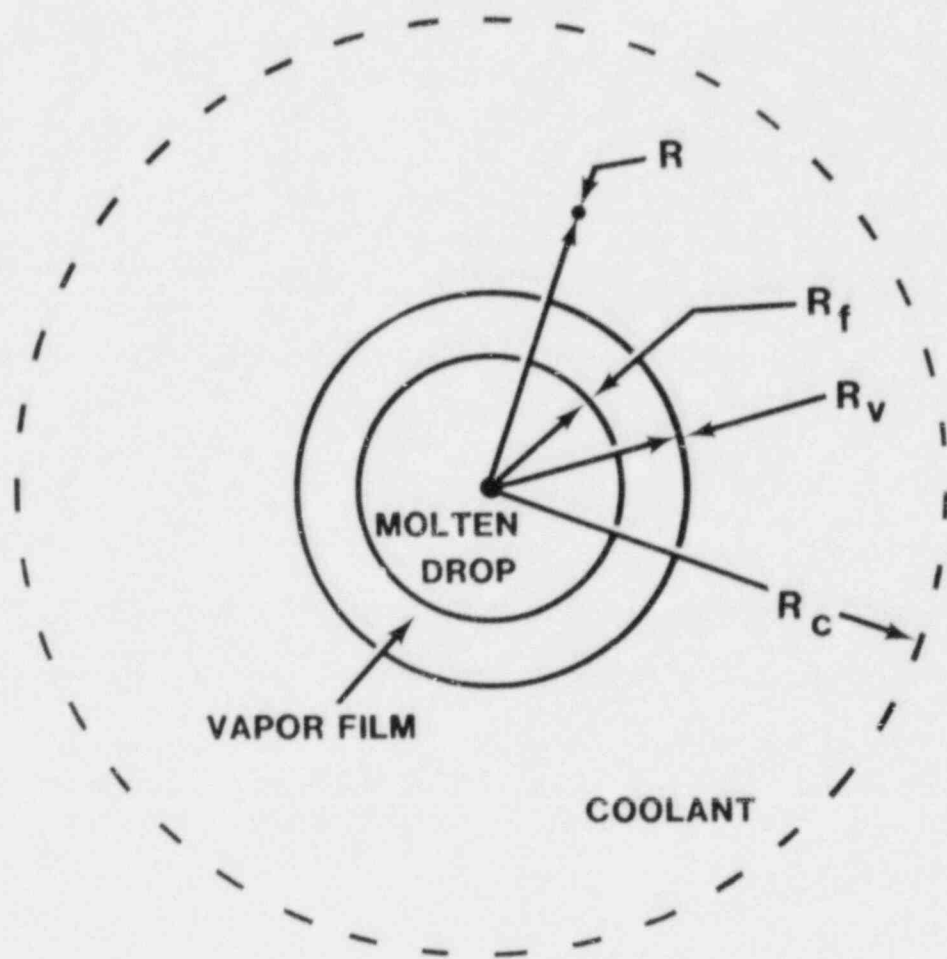


FIGURE 1. The Unit Cell

Next, if m_v is the mass of vapor in a given vapor film, the particle velocity of the coolant at $R = R_v$ relative to drop center is

$$V_R = \dot{R}_v - \dot{m}_v / 4\pi R_v^2 \bar{\rho}_c \quad (14)$$

Noting that the number of drops per unit mixture volume is

$$N = \phi_f / 4 \pi R_f^3 \quad (15)$$

and

$$\dot{c}_v / J = \phi_f \dot{m}_v / 4 \pi R_f^3 \quad , * \quad (16)$$

then

$$V_R = \dot{R}_v - \dot{c}_v R_f^3 / 3J \phi_f \bar{\rho}_c R_v^3 \quad (17)$$

This completes the kinematical description of the problem. The kinetic energy statement will be considered next.

The kinetic energy of the mixture due to translational motion is

$$\int_{\#} \frac{1}{2} \rho v^2 d\# \quad (18)$$

where $\#$ is the volume occupied by the mixture. Now consider a single unit cell of the mixture. The kinetic energy of this cell is not simply described by the translational motion of the cell. If the cell has a radial oscillation, this will also contribute to the kinetic energy by an amount

$$2\pi R_v^3 \bar{\rho}_c V_R^2 \quad (19)$$

*Note from Eqn. (11) that $\phi_f J / R_f^3$ is a constant.

This expression which is derived in Ref. 8 ignores kinetic energy contributions of the radial motions of the drop and vapor, and only considers contributions of the radial oscillation of the coolant.

By using Eqns. (15), (18), and (19), the total kinetic energy expression is

$$T = \int_{\theta} \left[\frac{1}{2} \rho v^2 + \frac{3}{2} \bar{\rho}_C \phi_f v_R^2 \frac{R_V^3}{R_f^3} \right] d\theta \quad (20)$$

The final postulate required for the variational principle is the virtual work statement. It is assumed to be

$$\delta W = \int_{\theta} \left[-\phi_f P_f \delta \bar{\rho}_f / \bar{\rho}_f - \phi_v P_v \delta \bar{\rho}_v / \bar{\rho}_v - \phi_c P_c \delta \bar{\rho}_c / \bar{\rho}_c + L_v \delta c_v / J - L_c \delta c_v / J + \rho f \delta x \right] d\theta + \int_S \bar{\sigma} \delta x ds \quad (21)$$

The postulated forces P_f , P_v , and P_c are the average pressures in each constituent. The forces L_v and L_c drive the phase change. The function f is the specific external body force, and $\bar{\sigma}$ is the applied surface traction on the boundary s of the mixture.

When Hamilton's principle is applied to relations (20) and (21) subject to the constraints (3), (7), (8), (9), (11), and (12), the following equations of motion are obtained:

$$\rho \dot{v} = -\partial \lambda / \partial x + \rho f \quad (22)$$

$$R_V \dot{v}_R + \frac{3}{2} [1 - (1 - \phi_c) / \phi_c] v_R^2 + R_V v_R \dot{\bar{\rho}}_c / \bar{\rho}_c + [1/3(1 - \phi_c) - 1/\phi_c + 1/\phi_f] \dot{c}_v R_V v_R / J \bar{\rho}_c = (P_f - P_c) / \bar{\rho}_c \quad (23)$$

$$R_V \dot{c}_V V_R / \phi_C J = P_f - P_V \quad , \quad (24)$$

$$\lambda = P_C - R_V \dot{c}_V V_R / \phi_C J + \frac{3}{2} \phi_f R_V^3 \rho_C V_R^2 / \phi_C R_f^3 \quad , \quad (25)$$

and

$$\phi_f \bar{\rho}_f \overline{\dot{R}_V V_R / \bar{\rho}_f} - P_V / \bar{\rho}_V + P_C / \bar{\rho}_C + L_V - L_C = 0 \quad (26)$$

in the volume v ; and

$$\lambda = - \bar{\sigma} \quad (27)$$

on the boundary surface s .

Because Hamilton's principle is an energy statement, it implies the following energy balance statements:

$$\phi_f \bar{\rho}_f \dot{E}_f = \phi_f P_f \dot{\bar{\rho}}_f / \bar{\rho}_f + \phi_f \bar{\rho}_f r_f + \epsilon_f^+ \quad , \quad (28)$$

$$\phi_V \bar{\rho}_V \dot{E}_V + \dot{c}_V E_V / J = \phi_V P_V \dot{\bar{\rho}}_V / \bar{\rho}_V - L_V \dot{c}_V / J + \phi_V \bar{\rho}_V r_V + \epsilon_V^+ \quad , \quad (29)$$

and

$$\phi_C \bar{\rho}_C \dot{E}_C - \dot{c}_V E_C / J = \phi_C P_C \dot{\bar{\rho}}_C / \bar{\rho}_C + L_C \dot{c}_V / J + \phi_C \bar{\rho}_C r_C + \epsilon_C^+ \quad (30)$$

where E_f , E_V and E_C are the internal energies, r_f , r_V , and r_C are the specific external heat supplies, and ϵ_f^+ , ϵ_V^+ , and ϵ_C^+ are the energy exchange functions which are subject to the constraint

$$\epsilon_f^+ + \epsilon_V^+ + \epsilon_C^+ = 0 \quad . \quad (31)$$

Equations (1), (3), (4), (7), (8), (9), (11), (12), (17), (22), (23), (24), (25), (26), (28), (29), (30), and (31) form a system of 18 equations in the 32 variables $\bar{\rho}_V$, $\bar{\rho}_C$, $\bar{\rho}_f$, ϕ_V , ϕ_C , ϕ_f , v , R_f , R_V , V_R , J , λ , P_C , P_f , P_V , L_C , L_V , ρ , ϵ_f^+ , ϵ_V^+ , ϵ_C^+ , f , E_f , E_C , E_V , θ_f , θ_C , θ_V , r_f , r_V , r_C , and

c_v . The variables θ_f , θ_c , and θ_v are the constituent temperatures. In order to form a determined system of equations, constitutive relations must be specified for P_c , P_f , P_v , L_v , ϵ_f^+ , ϵ_v^+ , f , E_f , E_c , E_v , r_f , r_v , r_c , and c_v .

III. CONSTITUTIVE RELATIONS

Constitutive relations are required for the variables P_C , P_f , P_V , L_V , ϵ_f^+ , ϵ_V^+ , f , E_f , E_C , E_V , r_f , r_V , r_C , and \dot{c}_V . The body force f and specific external heat supplies r_f , r_V , and r_C are assumed to be zero. The vapor and coolant pressures, P_V and P_C , and specific internal energies, E_V and E_C are given by a tabular "steam-table" subroutine listed in Appendix B. The pressure and specific internal energy of the molten drops are given by the relations

$$P_f = S_f(1 - \bar{\rho}_{fr}/\bar{\rho}_f) + Q\dot{\bar{\rho}}_f \quad (32)$$

and

$$E_f = c_{pf}\theta_f \quad (33)$$

where the bulk modulus S_f , reference mass density $\bar{\rho}_{fr}$, damping factor Q , and specific heat c_{pf} are specified constants.

The damping term in Eqn. (32) is introduced to model fragmentation of the molten drops. When vapor separates the drop from the coolant, $\dot{\bar{\rho}}_f$ is small; however, when the coolant impacts the drop, large values of $\dot{\bar{\rho}}_f$ result. Previous calculations on the behavior of single fluid drops subjected to spherically symmetric impacts indicate that the resulting motion is quickly damped due to the energy absorbed by fragmentation of the drop.⁴

From Eqn. (32), the energy available to fragment the drop E_d can be computed from the relation

$$\bar{\rho}_f \dot{E}_d = Q\dot{\bar{\rho}}_f^2/\bar{\rho}_f \quad (34)$$

Given the surface tension coefficient of the molten material, denoted as σ ,

the potential increase in the surface area of a drop is $\phi_f \bar{\rho}_f E_d / N\sigma$ where the number of drops per unit volume N is given by Eqn. (15). Only a fraction of this energy will actually result in new contact area between the drop and the coolant. If γ denotes the efficiency of this process, the increase in contact area A_d is

$$A_d = \phi_f \bar{\rho}_f E_d \gamma / N\sigma \quad (35)$$

The current contact area is $4\pi R_f^2$ plus A_d . If A represents the current contact area per unit volume of the mixture

$$A = 4\pi R_f^2 N + \phi_f \bar{\rho}_f E_d \gamma / \sigma = 3\phi_f / R_f + \phi_f \bar{\rho}_f E_d \gamma / \sigma \quad .$$

The mass exchange rate per unit contact area between the vapor and the coolant is

$$\dot{U} = \alpha (M_v / 2\pi R_u)^{1/2} (P_v / \theta_s)^{1/2} - P_w / \theta_w^{1/2} \quad (37)$$

(see Ref. 9). The accommodation coefficient is denoted by α and is a specified constant (normally 0.2 for a water-steam phase transition); M_v is the molecular weight of the vapor; R_u is the universal gas constant; θ_s is the saturation temperature at P_v ; θ_w is the temperature of the coolant at the vapor interface; and P_w is the pressure of the vapor when its temperature is θ_w instead of θ_s . It is assumed that

$$P_w / \theta_w = P_v / \theta_s \quad (38)$$

The required constitutive expression for \dot{c}_v is

$$\begin{aligned} \dot{c}_v / J &= - \dot{A} U \\ &= - (3\phi_f / R_f + \phi_f \bar{\rho}_f E_d \gamma / \sigma) \\ &\quad \times \alpha (M_v / 2\pi R_u)^{1/2} P_v (\theta_s^{-1/2} - \theta_w^{1/2} / \theta_s) \end{aligned} \quad (39)$$

where Eqns. (36-38) have been used.

The variables θ_w , ϵ_f^+ , and ϵ_v^+ are specified through consideration of the local temperature profile in the neighborhood of a single drop.

Figure 2 is a schematic illustration of the temperature profile assumed in this work.* The heat flux in the drop due to the temperature gradient at $R = R_f$ is given as

$$q_f = K_f \left[\frac{\alpha_f R_f + 1}{R_f} (\theta_f - \theta_\ell) \right] \quad (40)$$

where

$$\alpha_f^2 = \omega \bar{\rho}_f c_{pf} / K_f \quad (41)$$

K_f is the thermal conductivity of the drop, θ_ℓ is the temperature at the drop-vapor interface, and ω is the dominant frequency associated with the mechanical deformation in the mixture. It is assumed that

$$\omega = |\dot{R}_v / (R_v - R_f)| \quad (42)$$

Discussion of these assumptions can be found in Drumheller, Kipp and Bedford.¹⁰

Similarly, the heat flux into the vapor at this interface is

$$q_{fv} = K_v \left[\frac{\theta_\ell - \theta_s}{R_v - R_f} + \frac{\alpha_v R_f + 1}{R_f} \left(\theta_v - \frac{\theta_\ell + \theta_s}{2} \right) \right] \quad (43)$$

*During solution of an explicit problem, the values of θ_f , θ_v , θ_ℓ , θ_s , θ_w , and θ_c change continuously in both time and space. The situation illustrated in Fig. 2 (especially the dome in the temperature profile of the vapor) is highly transient. Depending on the computed values of θ_v , θ_ℓ , θ_s , a well could appear in the temperature profile for the vapor.

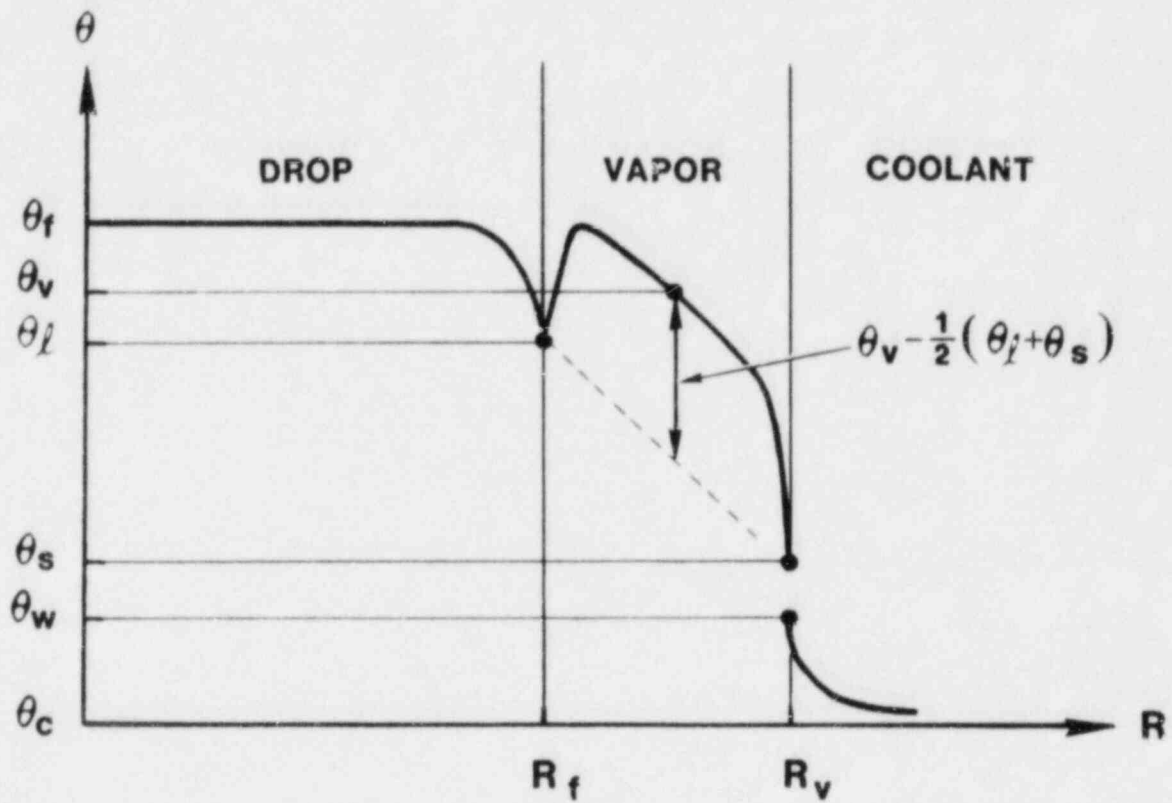


FIGURE 2. Local Temperature Profile

where K_v and α_v are defined in the same manner as K_f and α_f . It is noted that

$$q_f = q_{fv} \quad (44)$$

must hold.

At $x = R_v$, the vapor-coolant interface, the heat flux from the vapor film is

$$q_{vc} = K_C \left[\frac{\theta_\ell - \theta_s}{R_v - R_f} + \frac{\alpha_v R_v + 1}{R_v} \left(\theta_v - \frac{\theta_f + \theta_s}{2} \right) \right], \quad (45)$$

and heat flux into the coolant is

$$q_C = K_C \left[\frac{\alpha_C R_v + 1}{R_v} (\theta_w - \theta_C) \right]. \quad (46)$$

At this interface the following relation must hold

$$q_{vc} - h_v \dot{U} = q_C + h_C \dot{U} \quad (47)$$

where U is given by Eqns. (37-38) and h_v and h_C are the enthalpies of the vapor and the coolant.

Equations (44) and (47) can be solved to obtain

$$\begin{aligned} \theta_\ell = & \left[K_f \left(\frac{\alpha_f R_f + 1}{R_f} \right) \theta_f + K_v \left(\frac{\alpha_v R_f + 1}{R_f} \right) \theta_v \right. \\ & \left. + K_v \left(\frac{1}{R_v - R_f} - \frac{\alpha_v R_f + 1}{2R_f} \right) \theta_s \right] \left[K_f \left(\frac{\alpha_f R_f + 1}{R_f} \right) \right. \\ & \left. + K_v \left(\frac{1}{R_v - R_f} + \frac{\alpha_v R_f + 1}{2R_f} \right) \right]^{-1} \end{aligned} \quad (48)$$

and

$$\theta_w = \left[(-b + \sqrt{b^2 + 4ac})/2a \right]^2 \quad (49)$$

where

$$a = K_C \left(\frac{\alpha_C R_V + 1}{R_V} \right) , \quad (50)$$

$$b = (h_V - h_C) \alpha (M_V/2\pi R_U)^{1/2} P_V/\theta_S , \quad (51)$$

and

$$c = K_C \left(\frac{\alpha_C R_V + 1}{R_V} \right) \theta_C + q_{VC} + b\theta_S^{1/2} . \quad (52)$$

Equations (48) and (49) determine θ_w and θ_s in terms of the system variables. Consequently, the local heat fluxes are also determined by the system variables.

The required expressions for ϵ_f^+ and ϵ_v^+ are

$$\epsilon_f^+ = -\Lambda q_f \quad (53)$$

and

$$\epsilon_v^+ = -\epsilon_f^+ - \Lambda q_{VC} + h_V \dot{c}_V/J . \quad (54)$$

Finally, L_V is assumed to always be given by its equilibrium value

$$L_V = P_V/\bar{\rho}_V \quad (55)$$

(see Ref. 7; Eqn. (4.23)).

This completes the constitutive description for the mixture under conditions of relatively thick vapor films; however, as complete collapse of a

vapor film approaches, two auxiliary conditions are applied. Both E_v and ω are limited in magnitude. After collapse and until a relatively thick vapor film is reestablished, $\dot{E}_v = 0$ and \dot{c}_v is either zero or positive.

IV. NUMERICAL ANALYSIS

Transient numerical solutions to the equations presented in the previous two sections are obtained by incorporating the model into the explicit - Lagrangian finite-difference code WONDY IV.¹¹ The mass and momentum equations of this code are identical to Eqns. (4) and (22). In the structure of this code, the constitutive equations as well as the energy equations are solved in the material description subroutine.

The code generates solutions by first advancing the values of ρ and v in time through explicit finite-differenced forms of the relations (4) and (22). Next, the pressure λ is advanced through the material subroutine. In this subroutine the density ρ is linearly interpolated between the old-time and new-time values. This interpolation is substituted into the remaining system equations, Eqns. (1), (3), (7), (8), (9), (11), (12), (17), (23), (24), (25), (26), (28), (29), (30), and (31). These equations then reduce to a set of ordinary differential equations in time which are integrated to the new time using an auxiliary integrator DE.¹² The system is recast into eight first-order ordinary differential equations in the variables

$$[c_v, R_f, R_v, \psi, E_d, E_f, E_v, E_c] \quad (56)$$

where

$$\psi = \bar{\rho}_c V_R \quad (57)$$

The update coding required to incorporate this mixture model into WONDY IV is included in Appendix B. A key relating the coding variable names to the mathematical symbols is included in Appendix A. The input instructions are given in Appendix C.

V. EXAMPLE PROBLEM

In this section the code input for an example problem will be presented. A sample of the computed results is also given.

This problem involves a mixture of water and molten iron. The temperature of the water is 303.2 K and of the iron is 2443.2 K. The coolant occupies 80 percent of the mixture volume. Each drop of iron has a radius of 10 μm and a vapor film 0.2- μm thick. The mixture is at an ambient pressure of 0.1 MPa and the left boundary pressure is instantaneously raised to 2.1 MPa for 30 μs and then lowered to 0.1 MPa.

A list of code input values is contained in Appendix D. Several points about this list should be noted. The stability sound speed is 5 km/s which is well above the sound speed of water. The efficiency factor for fragmentation is set at zero. Thus, film collapse and fragmentation will not increase the contact area between the drop and the coolant. The mesh dimension is quite small, one quarter of the drop radius. This can be increased without affecting the results, but experience indicates it should not exceed the drop radius. The viscosity coefficients, B1 and B2 on card number 4, are smaller than the values normally used in this code because of the low pressures incurred in the calculations.

The value of Q , Eqn. (32), is evaluated through consideration of Eqn. (23). If it is assumed that $R_v \approx R_f$ and mass exchange is ignored, then Eqn. (23) can be linearized to obtain

$$(\bar{\rho}_c R_f^2 / 3\bar{\rho}_f) \ddot{\epsilon} + Q\dot{\epsilon} + S_f \epsilon / \bar{\rho}_f = 0 \quad (58)$$

where Eqn. (32) is used and ϵ represents a small perturbation of $\bar{\rho}_f$ so that

$$\bar{\rho}_f = \bar{\rho}_{f0} + \epsilon \quad (59)$$

Equation (58) describes a damped oscillator. Critical damping occurs when

$$Q^2 = 4R_f^2 \bar{\rho}_c S_f / 3\bar{\rho}_f^2 \quad (60)$$

The listed value of Q was computed from Eqn. (60).

Computed results are plotted in Figs. (3) through (6). The evolution and growth of the pressure wave is evident. The peak pressure in the wave profile occurs simultaneously with the film collapse. The initial film collapse at the left boundary occurs approximately 55 μ s into the problem. Successive collapses propagate to the right at an average rate of approximately 900 m/s. The peak pressure quickly reaches values which exceed the limits of the steam and water constitutive expressions used in the calculations.

The pressure disturbance which is applied to the left boundary will not grow unless the initial disturbance is of sufficient strength to cause film collapse. If the initial collapse occurs, the disturbance propagates and grows even if fragmentation is completely suppressed.

In previous work on bubbly liquids,^{8,9,10} it was observed that pressure disturbances resulted in irreversible flow of heat from the bubble to the liquid. This flow of heat was driven by the pressure disturbance which heated the gas in the bubble more than the surrounding liquid. Consequently, the flow of heat represented a drain of energy from the pressure disturbance and provided the dominant wave attenuating mechanism in these types of problems.

In the present problem, irreversible flow of heat to the coolant is also triggered by the pressure disturbance. In this case however, a natural source of heat is present in the bubble. The flow of this heat causes additional vaporization of the coolant which adds to the energy of the pressure disturbance. Any fragmentation which occurs enhances this process, but

fragmentation does not appear to be necessary to the early development of the steam explosion. At later times fragmentation plays a far more important role in the release of energy.

The rapid growth of the amplitude of the computed pressure pulse may be an artifact of this particular calculation. Physical situations usually involve the growth of pressure pulses in an expanding spherical geometry through a medium containing a range of drop sizes and vapor film thicknesses. These effects tend to limit the growth and coherence of the pressure pulse. Future work could investigate these effects through modifications of this computer code.

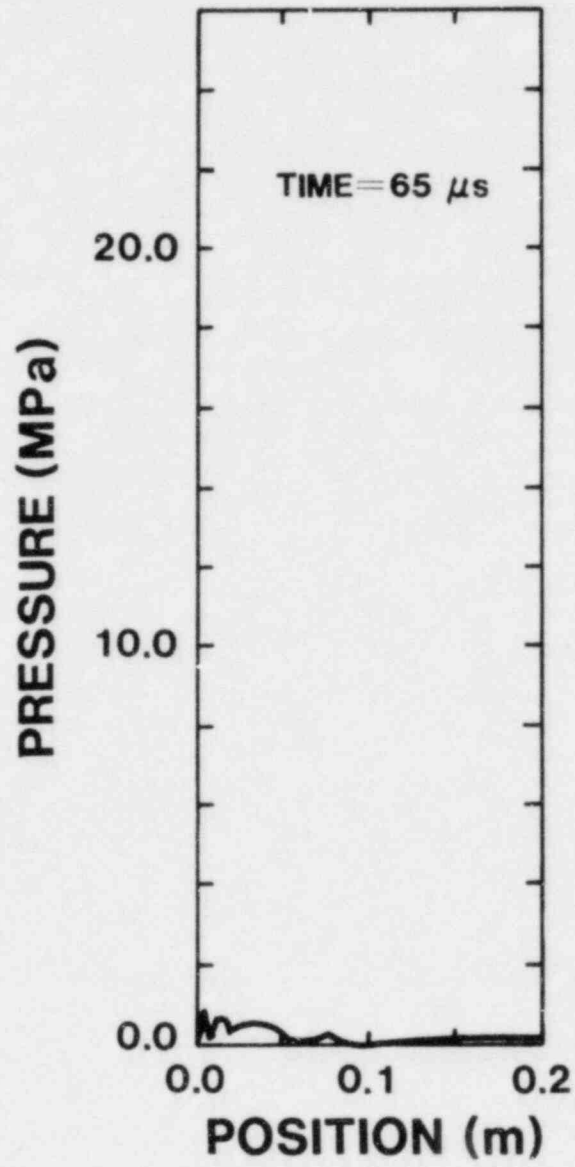


FIGURE 3. Example Calculation

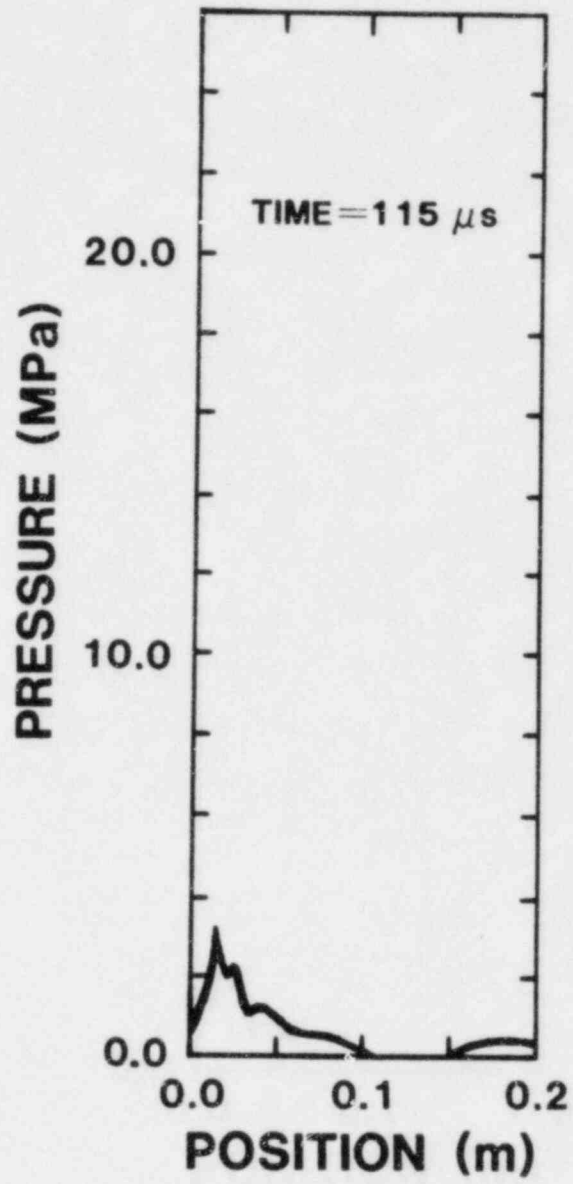


FIGURE 4. Example Calculation

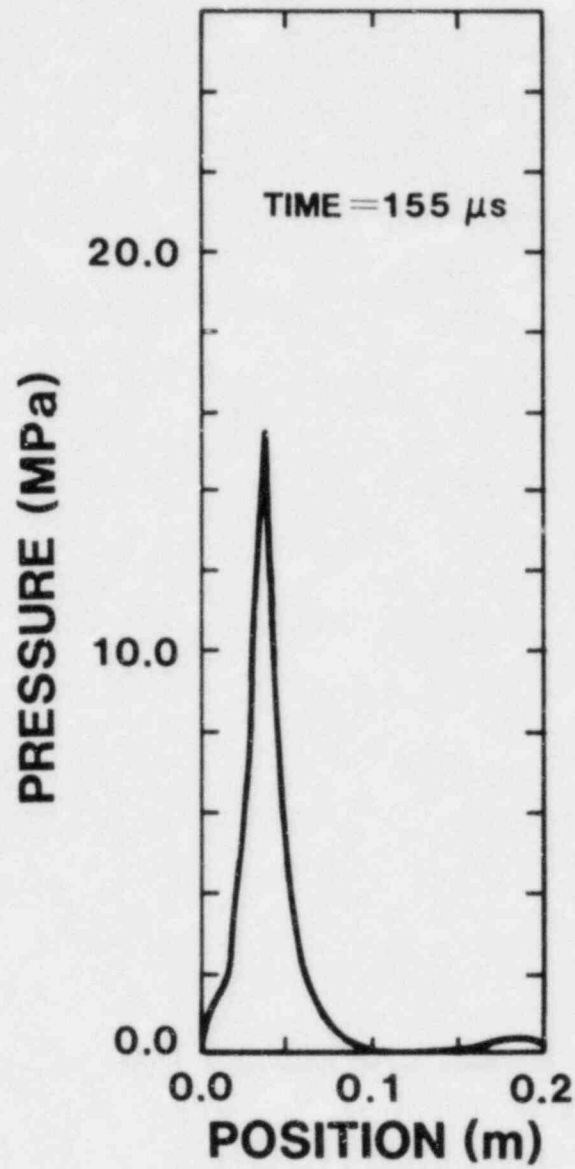


FIGURE 5. Example Calculation

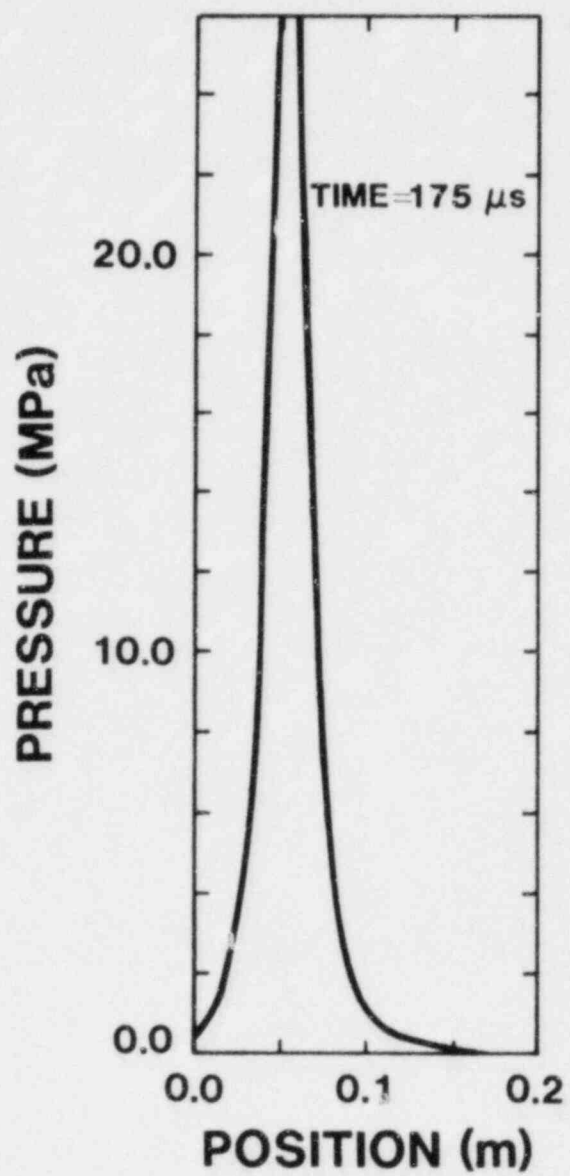


FIGURE 6. Example Calculation

REFERENCES

1. A. W. Cronenberg and R. Benz, "Vapor Explosion Phenomena with Respect to Nuclear Reactor Safety Assessment," Adv. Nucl. Sci. Technol. 12, 247-334 (1980).
2. L. S. Nelson and P. M. Duda, "Steam Explosion Experiments with Single Drops of Iron Oxide Melted with a CO₂ Laser," NUREG/CR-2295, Sandia National Laboratories (1981).
3. S. J. Board and R. W. Hall, "Thermal Explosions at Molten Tin/Water Interfaces," Moving Boundary Problems in Heat Flow and Diffusion, J. R. Ockendon and W. R. Hodgkins, Eds., Clarendon Press, Oxford (1975).
4. D. S. Drumheller, "The Initiation of Melt Fragmentation in Fuel-Coolant Interactions," Nucl. Science Engr. 72, 347-356 (1979).
5. A. Bedford and D. S. Drumheller, "A Variational Theory of Immiscible Mixtures," Arch. Rat. Mech. Anal. 68, 37-51 (1978).
6. D. S. Drumheller and A. Bedford, "On the Mechanics and Thermodynamics of Fluid Mixtures," Arch. Rat. Mech. Anal. 71, 345-355 (1979).
7. D. S. Drumheller and A. Bedford, "A Thermomechanical Theory for Reacting Immiscible Mixtures," Arch. Rat. Mech. Anal. 73, 257-284 (1980).
8. D. S. Drumheller and A. Bedford, "A Theory of Bubbly Liquids," J. Acoust. Soc. Am. 66, 197-208 (1979).
9. D. S. Drumheller and A. Bedford, "A Theory of Liquids with Vapor Bubbles," J. Acoust. Soc. Am. 67, 186-200 (1980).
10. D. S. Drumheller, M. E. Kipp and A. Bedford, "Transient Wave Propagation in Bubbly Liquids," J. Fluid Mech. 119, 347-365 (1982).
11. R. J. Lawrence and D. S. Mason, "WONDY IV -- A Computer Program for One-Dimensional Wave Propagation with Rezoning," SC-RR-71-0284, Sandia National Laboratories (1971).
12. L. F. Shampine and M. K. Gordon, Computer Solution of Ordinary Differential Equations: The Initial Value Problem, Freeman, San Francisco (1974).
13. K. H. Haskell and W. H. Vandevender, "Brief Instructions for Using the Sandia Mathematical Subroutine Library (Version 8.0)," SAND79-2382, Sandia National Laboratories (1979).
14. R. K. Cole, Sandia National Laboratories, (private communication).

APPENDIX A: NOMENCLATURE

This appendix contains two lists. The first list gives the definition of the mathematical symbols used in the derivation of the theory. This list also contains the equation number where the symbol is first used and the corresponding code variable name. The second list gives the definitions of the code variable names:

i) Mathematical Symbols:

<u>Symbol</u>	<u>Code Name</u>	<u>Definition</u>
A		contact area, Eqn. (36)
A_d		increase in contact area, Eqn. (35)
a		parameter, Eqn. (50)
b		parameter, Eqn. (51)
c_{pc}	CPC	specific heat capacity of coolant
c_{pf}	CPF	specific heat capacity of drop, Eqn. (33)
c_{pv}	CPV	specific heat capacity of vapor
c_v	Y(1)	mass exchange parameter, Eqn. (8)
c		parameter, Eqn. (52)
E_C	Y(8)	specific internal energy of coolant, Eqn. (30)
E_d	Y(5)	fragmentation energy, Eqn. (34)
E_f	Y(6)	specific internal energy of drop, Eqn. (28)
E_v	Y(7)	specific internal energy of vapor, Eqn. (29)
f		specific external body force, Eqn. (21)
h_C	HC	enthalpy of coolant, Eqn. (47)
h_v	HV	enthalpy of vapor, Eqn. (47)
J	ROR	Jacobian of the deformation, Eqn. (1)
K_C	AKC	thermal conductivity of the coolant, Eqn. (45)

<u>Symbol</u>	<u>Code Name</u>	<u>Definition</u>
K_f	AKF	thermal conductivity of the drop, Eqn. (40)
K_v	AKV	thermal conductivity of the vapor, Eqn. (43)
L_c	AALC	mass exchange force, Eqn. (21)
L_v	AALV	mass exchange force, Eqn. (21)
M_v		molecular weight of vapor, Eqn. (37)
m_v		mass of vapor in a film, Eqn. (14)
N		drop number density, Eqn. (15)
P_c	PC	coolant pressure, Eqn. (21)
P_f	PF	drop pressure, Eqn. (21)
P_v	PV	vapor pressure, Eqn. (21)
P_w		interface pressure, Eqn. (37)
Q		damping coefficient, Eqn. (32)
q_c		heat flux, Eqn. (46)
q_f		heat flux, Eqn. (40)
q_{fv}	QV	heat flux, Eqn. (43)
q_{vc}		heat flux, Eqn. (45)
R		radial coordinate
R_c		unit cell radius, Eqn. (13)
R_{co}		initial R_c , Eqn. (10)
R_f	Y(2)	drop radius, Eqn. (11)
r_v	Y(3)	vapor film radius, Eqn. (10)
R_u		universal gas constant, Eqn. (37)
r_c		specific external heat supply of coolant, Eqn. (30)
r_f		specific external heat supply of drop, Eqn. (28)
r_v		specific external heat supply of vapor, Eqn. (29)

<u>Symbol</u>	<u>Code Name</u>	<u>Definition</u>
s		mixture surface, Eqn. (21)
S _f		bulk modulus of drop, Eqn. (32)
T		kinetic energy, Eqn. (20)
t		time, Eqn. (6)
U		mass exchange parameter, Eqn. (37)
v		mixture volume, Eqn. (18)
V _R		radial velocity, Eqn. (14)
v		translational velocity, Eqn. (6)
δW		virtual work, Eqn. (21)
X		original position, Eqn. (1)
x		current position, Eqn. (1)
α		accommodation coefficient, Eqn. (37)
α _C	ALC	thermal diffusivity of coolant, Eqn. (45)
α _f	ALF	thermal diffusivity of drop, Eqn. (41)
α _v	ALV	thermal diffusivity of vapor, Eqn. (43)
γ		fragmentation efficiency parameter, Eqn. (35)
δ		variational operator, Eqn. (21)
ε _C ⁺	ECP	energy exchange of coolant, Eqn. (30)
ε _f ⁺	EFP	energy exchange of drop, Eqn. (28)
ε _v ⁺	EVP	energy exchange of vapor, Eqn. (29)
θ _C	THC	coolant temperature, Eqn. (46)
θ _f	THF	drop temperature, Eqn. (33)
θ _l	TF	drop-vapor interface temperature, Eqn. (40)
θ _S	TSAT	vapor saturation temperature, Eqn. (37)
θ _v	THV	vapor temperature, Eqn. (43)
θ _w	TW	vapor-coolant interface temperature, Eqn. (37)

<u>Symbol</u>	<u>Code Name</u>	<u>Definition</u>
λ		mixture pressure, Eqn. (22)
ρ	DENS	mixture density, Eqn. (2)
$\bar{\rho}_c$	RC	coolant density, Eqn. (2)
$\bar{\rho}_f$	RF	drop density, Eqn. (2)
$\bar{\rho}_v$	RV	vapor density, Eqn. (2)
σ		drop surface tension, Eqn. (35)
$\bar{\sigma}$		surface traction, Eqn. (21)
ϕ_c	PHV	coolant volume fraction, Eqn. (2)
ϕ_f	PHF	drop volume fraction, Eqn. (2)
ϕ_v	PHV	vapor volume fraction, Eqn. (2)
ψ	Y(4)	parameter, Eqn. (57)
ω	OMG	heat conduction parameter, Eqn. (41)

ii) Code Variable Names:

<u>Code Name</u>	<u>Mathematical Symbol</u>
AKC	K_c
AKF	K_f
AKV	K_v
ALS	$h_v - h_c$
CPC	c_{pc}
CPF	c_{pf}
CPV	c_{pv}
DJ	\dot{J}
DPHC	$\dot{\phi}_c$
DPHF	$\dot{\phi}_f$
DPHV	$\dot{\phi}_v$

<u>Code Name</u>	<u>Mathematical Symbol</u>
DRC	$\dot{\bar{\rho}}_c$
DRF	$\dot{\bar{\rho}}_f$
DRV	$\dot{\bar{\rho}}_v$
ECP	ε_c^+
EFP	ε_f^+
FAC	$1 + A_d/A$
HC	h_c
HV	h_v
OMG	ω
PC	P_c
PF	P_f
PHC	ϕ_c
PHF	ϕ_f
PHV	ϕ_v
PRC	$\phi_c \bar{\rho}_c$
PRF	$\phi_f \bar{\rho}_f$
PRV	$\phi_v \bar{\rho}_v$
PV	P_v
QV	q_v
RC	$\bar{\rho}_c$
RF	$\bar{\rho}_f$
ROR	J
RV	$\bar{\rho}_v$
TF	θ_l
THC	θ_c
THF	θ_f

<u>Code Name</u>	<u>Mathematical Symbol</u>
THV	θ_v
TSAT	θ_s
TW	θ_w
Y(1)	c_v
Y(2)	R_f
Y(3)	R_v
Y(4)	ψ
Y(5)	E_d
Y(6)	E_f
Y(7)	E_v
Y(8)	E_c

APPENDIX B: CODE LISTING

This appendix contains a listing of the code updates for WONDY IV.¹¹ The STAT5 subroutine modifications require a call to the ODE subroutine. This is a library subroutine¹³ which is based on the DE scheme of Shampine and Gordon.¹² The ODE subroutine requires the F subroutine which computes the material derivatives of the array in Eqn. (56). Function TEXTND computes values of θ_3 above the critical point for purposes of continuity in the heat conduction and mass exchange calculations. Subroutine COND computes values of K_f , K_v , and K_c . The remaining routines describe the behavior of water and were supplied by Cole.¹⁴

The update listing follows:

```

*IDENT,BNDLFT
*D ONEDY.1056,1057
  IF(NONE) B=ADDA(8)
  BN=ADDA(8)
  IF(T.GE.ADDA(10)) BN=ADDA(9)
*IDENT,ARTVIS
*I ONEDY.1126
  GO TO 5008
*IDENT,MEKST5
*D MAXPA.16,338
C
C   STAT5 MODIFICATIONS
C
  DIMENSION Y(8),YPOUT(8),WORK(268),IWORK(6)
  COMMON/WITHF/PC,VR,PHF,PHC,RC,PF,PV,PRC,PRF,PRV,ROR,THCO,THVO
1  ,THFO,AKF,AKC,AKV
  COMMON/TIMESF/ DELTIM,TZERO,TEND
  COMMON/ARGLST/ TE,RHO,PR,ER,SY,CV,DRT,DPR
  TYPE INTEGER PLATE,W4020
  EXTERNAL F
  DELTIM=DELT(1)
  TZERO=T-DELTIM
  TEND=T
  DO 10 I=1,8
10  Y(I)=DATB(I)
  THVO=DATB(9)
  THCO=DATB(10)
  TPRES=TZERO
  NEQN=8
  EPS=CES(26,PLATE)
  EP2=EPS
  IFLAG=-1
206 CONTINUE
  CALL ODE(F,NEQN,Y,TPRES,TEND,EPS,EP2,IFLAG,WORK,IWORK)
  IF(IFLAG.LT.-2) PRINT 205,N,L,IFLAG
205 FORMAT(10X,*N=* I5,* L=* I5,*IFLAG=* I5)
  IF(TPRES.LT.TEND) GO TO 206
  DO 11 I=1,8
11  DATB(I)=Y(I)
  DATB(9)=THVO
  DATB(10)=THCO
  CALL F(TEND,Y,YPOUT)
  PN=PC-Y(3)/PHC*YPOUT(1)/ROR*VR-1.5*PHF/PHC*(Y(3)/Y(2))**3.*RC
  1*VR**2.
  BN=PN
  ZN=0.
  EN=(PRF*Y(6)+PRV*Y(7)+PRC*Y(8))/(PRF+PRV+PRC)
  CN=CES(2,PLATE)
  DATB(11)=PV
  RETURN
C
C   STAT5 INITIALIZATION
C
  ENTRY STIN5
  NINT=0

```



```

TE=CES(7,PLATE)
RHO=CES(1,PLATE)/1000.
55 CALL STMTBL
RHA=RHO+(CES(28,PLATE)*10.-PR)/DPR
AB=ABS((RHA-RHO)/RHO)
IF(AB.LE.1.OE-7) GO TO 12
RHO=RHA
NINT=NINT+1
IF(NINT.LT.10) GO TO 55
PRINT 14
14 FORMAT(* COOLANT INITIALIZATION DID NOT CONVERGE*)
12 CES(1,PLATE)=RHA*1000.
NINT=0
TE=CES(8,PLATE)
RHO=CES(3,PLATE)/1000.
20 CALL STMTBL
RHA=RHO+(CES(29,PLATE)*10.-PR)/DPR
AB=ABS((RHA-RHO)/RHO)
IF(AB.LE.1.OE-7) GO TO 22
RHO=RHA
NINT=NINT+1
IF(NINT.LT.10) GO TO 20
PRINT 24
24 FORMAT(* VAPOR INITIALIZATION DID NOT CONVERGE*)
22 CES(3,PLATE)=RHA*1000.
CES(15,PLATE)=CES(10,PLATE)**3./(1.-CES(5,PLATE))
CES(6,PLATE)=(CES(10,PLATE)**3.-CES(11,PLATE)**3.)/CES(15,PLATE)
DO 40 LA=L0L,L0R
JA=(LA-1)*NVAR
TE=CES(8,PLATE)
RHO=CES(3,PLATE)/1000.
CALL STMTBL
STORE(JA+17)=ER*1.OE-4
PRESS=PR*0.1
TE=CES(7,PLATE)
RHO=CES(1,PLATE)/1000.
CALL STMTBL
STORE(JA+18)=ER*1.OE-4
STORE(JA+16)=CES(16,PLATE)*CES(9,PLATE)
CES(4,PLATE)=CES(18,PLATE)/(1.-PRESS/CES(17,PLATE))
CES(12,PLATE)=CES(1,PLATE)*CES(5,PLATE)
CES(13,PLATE)=CES(4,PLATE)*(1.-CES(5,PLATE)-CES(6,PLATE))
CES(14,PLATE)=CES(3,PLATE)*CES(6,PLATE)
CES(27,PLATE)=CES(12,PLATE)+CES(13,PLATE)+CES(14,PLATE)
STORE(JA+11)=0.
STORE(JA+12)=CES(11,PLATE)
STORE(JA+13)=CES(10,PLATE)
STORE(JA+14)=0.
STORE(JA+15)=0.
STORE(JA+6)=CES(27,PLATE)
STORE(JA+7)=PRESS
STORE(JA+19)=CES(8,PLATE)
STORE(JA+20)=CES(7,PLATE)
40 CONTINUE
RETURN

```

```

      END
      SUBROUTINE F(TB,Y,YP)
*CALL, SHORTEN
      COMMON/HDOG/REXTND
      COMMON/TIMESF/ DELTIM, TZERO, TEND
      COMMON/ARGLST/ TE, RHO, PR, ER, SY, CV, DPT, DPR
      COMMON/THERMO/PM, EM, SM, CVM, DPTM, DPRM, KPA, RVV, EV, SV, CVV, DPTV, DPRV
1, RLL, EL, SL, CVL, DPTL, DPRL
      COMMON/WITHF/PC, VR, PHF, PHC, RC, PF, PV, PRC, PRF, PRV, ROR, THC, THV
1, THF, AKF, AKC, AKV
      DIMENSION Y(8), YP(8)
      TYPE INTEGER PLATE, W4020
      LOGICAL ERR
      DENS=((RN-R)*TB+R*TEND-RN*TZERO)/DELTIM
      RDT=(RN-R)/DELTIM
      ROR=CES(27, PLATE)/DENS
      RDOT=RDT/DENS
C
C      CHECK FOR IMPACT OR TOTAL EVAPORATION
C
      IF(Y(3).LE.Y(2)) GO TO 601
      IF(-Y(1).GE.CES(14, PLATE)) GO TO 601
C      USE SI UNITS
C
C      COMPUTE VOL FRACT
C
      PHC=1.-Y(3)**3./ROR/CES(15, PLATE)
      PHF=Y(2)**3./ROR/CES(15, PLATE)
      PHV=1.-PHC-PHF
      DDFP=Y(3)-Y(2)
      IF(PHV.LE.0.0) PRINT 151, PHV, DDFP
151  FORMAT(* PHV=*, E10.3, * Y3-Y2=*, E10.3)
C
C      COMPUTE DENSITIES
C
      RC=(CES(12, PLATE)-Y(1))/PHC/ROR
      RF= CES(13, PLATE)/PHF/ROR
      RV=(CES(14, PLATE)+Y(1))/PHV/ROR
      IF(RV.GT.RC) GO TO 601
      IF(RV.LE.0.0) PRINT 152, RV, Y(1), CES(14, PLATE)
152  FORMAT(* RV=*, E10.3, * Y(1)=*, E10.3, * CES14=*, E10.3)
224  CONTINUE
C
C      COMPUTE TEMPS
C      START WITH OLD TEMP
C
      NINT=0
      TE=THC
      RHO=RC/1000.
51  CALL STMTBL
      THA=TE-(ER-Y(8)*1.0E4)/CV
      AB=ABS((THA-TE)/TE)
      IF(AB.LE.1.0E-6) GO TO 50
      TE=THA
      NINT=NINT+1

```

```

      IF(NINT.LT.50) GO TO 51
      PRINT 52,RC,TE
52   FORMAT(* COOLANT TEMP DID NOT CONVERGE RC=*,E10.3,
1    * THC=*,E10.3)
50   THC=TE
      PC=PR*0.1
      CPC=(CV+1.1/DPR*(DPT/RHO)**2.)*1.0E-4
      NINT=0
      TE=THV
      RHO=RV/1000.
55   CALL STMTBL
      THA=TE-(ER-Y(7)*1.0E+4)/CV
      AB=ABS((THA-TE)/TE)
      IF(AB.LE.1.0E-5) GO TO 56
      TE=THA
      IF(TE.LT.274.) GO TO 58
      NINT=NINT+1
      IF(NINT.LT.50) GO TO 55
      PRINT 57,RV,TE
57   FORMAT(* VAPOR TEMP DID NOT CONVERGE RV=*,E10.3,
1    * THV=*,E10.3)
      GO TO 601
56   THV=TE
      GO TO 59
58   TE=274
      THV=TE
      GO TO 601
59   CONTINUE
      PV=PR/10.
      CPV=(CV+TE/DPR*(DPT/RHO)**2.)*1.0E-4
      THF=Y(6)/CES(16,PLATE)
      PF=CES(17,PLATE)*(1.-CES(18,PLATE)/RF)
C
C   COMPUTE THERMAL DIFUSIVITY
C
      CALL COND
      ABC=Y(3)-Y(2)
      IF(ABC.LT.CES(25,PLATE)) ABC=CES(25,PLATE)
      OMG=ABS(Y(4)/RC/ABC)
      IF(AKV.LE.0.0) PRINT 400,AKV
      IF(RV.LE.0.0) PRINT 401,RV
      IF(CPV.LE.0.0) PRINT 402,CPV
      IF(CPV.LE.0.0) GO TO 601
400  FORMAT(* AKV=*,E15.8)
401  FORMAT(* RV=*,E15.8)
402  FORMAT(* CPV=*,E15.8)
      FAC=1.+Y(2)*RF*Y(5)/3./CES(22,PLATE)*CES(21,PLATE)
      AKF=AKF*FAC
      AKC=AKC*FAC
      AKV=AKV*FAC
      ALF=SQRT(OMG*RF*CES(16,PLATE)/AKF)
      ALC=SQRT(OMG*RC*CPC/AKC)
      ALV=SQRT(OMG*RV*CPV/AKV)
C
C   COMPUTE SATURATION PROPERTIES

```

```

C      TSAT=TBND(PR,ERR)
      IF(ERR) GO TO 66
      GO TO 60
66     CONTINUE
      TSAT=TEXTND(PV)
      ALS=CES(19,PLATE)
      NINT=0
      TE=TSAT
      RHO=REXTND/1000.
      IF(RHO.LT.0.) GO TO 601
81     CALL STMTBL
      RACT=RHO+(PV*10.-PR)/DPR
      AB=ABS((RACT-RHO)/RHO)
      IF(AB.LE.1.0E-6) GO TO 86
      RHO=RACT
      NINT=NINT+1
      IF(RHO.LE.0.) GO TO 601
      IF(NINT.LT.50) GO TO 81
      PRINT 82,TE,RHO
82     FORMAT(* SAT PROPERTIES DID NOT CONVERGE TE=*,E10.3,* RHO=*,
1 E10.3)
86     HV=ER*1.0E-4+PV/RHO/1000.
      HC=HV
      GO TO 61
60     CALL WATER(.31681699395231 ,TSAT)
      HV=(EV+PM/RVV)*1.0E-4
      HC=(EL+PM/RLL)*1.0E-4
61     ALS=HV-HC
      IF(ALS.LT.CES(19,PLATE)) ALS=CES(19,PLATE)
C
C     COMPUTE WALL TEMPS
C
      C1=AKF/Y(2)*(ALF*Y(2)+1.)
      C2=AKV/Y(2)*(ALV*Y(2)+1.)
      C3=AKV/(Y(3)-Y(2))
      CC1=1.+Y(2)*RF*Y(5)/3./CES(22,PLATE)*CES(21,PLATE)
      TF=(C1*THF+C2*THV+(C3-C2/2.)*TSAT)/(C1+C3+C2/2.)
      ALPHAC=CES(20,PLATE)+(1.-CES(20,PLATE))*PV/22.09E6
      ALPHAC=AMIN1(1.,ALPHAC)
      AL=ALS*ALPHAC*CC1*SQR(CES(23,PLATE)/51604.43)
      C1=AKC*(ALC*Y(3)+1.)/Y(3)
      C2= AL*PV/TSAT
      QV=AKV*((TF-TSAT)/( ABC )+(THV-0.5*(TF+TSAT))*(ALV*Y(3)+1.)/
1Y(3))
      C3=C1*THC+QV+AL*PV/SQR(TSAT)
      TW=(((-C2+SQR(C2**2.+4.*C1*C3))/2./C1)**2.
C
C     COMPUTE D(CV)/DT
C
      YP(1)=-ROR*(PHV+PHF)/Y(3)*AL/ALS*PV*(1./SQR(TSAT)-SQR(TW)/TSAT)
1*3.
      IF(YP(1).GT.10.) YP(1)=10.
      IF(YP(1).LT.-10.) YP(1)=-10.
302    CONTINUE

```

```

C
C   COMPUTE D(RF)/DT
C
C   YP(2)=(PF-PV+YP(1)/ROR*Y(4)/RC*Y(3)/PHF)/CES(24,PLATE)
1  / ( 3.*RF/Y(2))
C
C   COMPUTE D(R)/DT
C
C   YP(3)=Y(4)/RC+Y(2)**3./3./PHF/RC/Y(3)**2.*YP(1)/ROR
C
C   COMPUTE D(PBI)/DT
C
71  YP(4)=-1.5*(1.-(1.-PHC)/PHC)*Y(4)**2./Y(3)/RC-(1./3./(1.-PHC)-1./
1PHC+1./PHF)*YP(1)/ROR*Y(4)/RC+(PF-PC)/Y(3)
C
C   COMPUTE D(EFRACT)/DT
C
C   YP(5)=CES(24,PLATE)*9.*(YP(2)/Y(2))**2.
C
C   COMPUTE DERIVATIVES FOR ENERGY EQNS
C
EFP=-AKF*(ALF*Y(2)+1.)/Y(2)*(THF-TF)*3.*PHF/Y(2)
EVP=(TF+TSAT-2.*THV)*(ALV*Y(3)+1.)/Y(3)
1  *3.*(PHF+PHV)/Y(3)+HV*YP(1)/ROR
ECP=AKC*(TW-THC)*(ALC*Y(3)+1.)/Y(3)*3.*(PHF+PHV)/Y(3)
1  -HC*YP(1)/ROR
EXTRA=(Y(7)+PV/RV-HV)*YP(1)/ROR
EVP=EVP+EXTRA
ECP=ECP-EXTRA
DJ=-ROR*RDOT
DPHC=(-3.*YP(3)/Y(3)+DJ/ROR)*Y(3)**3./ROR/CES(15,PLATE)
DPHF=( 3.*YP(2)/Y(2)-DJ/ROR)*Y(2)**3./ROR/CES(15,PLATE)
DPHV=-DPHC-DPHF
DRC=-YP(1)/PHC/ROR-RC*(DJ/ROR+DPHC/PHC)
DRV= YP(1)/PHV/ROR-RV*(DJ/ROR+DPHV/PHV)
DRF=-3.*RF*YP(2)/Y(2)
PRC=RC*PHC
PRV=RV*PHV
PRF=RF*PHF
C
C   COMPUTE D(EF)/DT
C
C   YP(6)=EFP/PRF
VR=Y(4)/RC
DVR=YP(4)/RC-Y(4)*DRC/RC**2.
AALV=PV/RV-PC/RC+Y(3)*VR+YP(1)/PRC/ROR+1.5*PHF*(1./PHC-1.)*VR**2.
1-PRF*(YP(3)*VR/PRF+Y(3)*DVR/PRF-Y(3)*VR/PRF**2.*(DRF*PHF+RF*DPHF))
AALC=-AALV+PV/RV
AALV=PV/RV
C
C   COMPUTE D(EV)/DT
C
IF (PRV.LT.1.E-5) PRV=1.E-5
YP(7)=(-YP(1)/ROR*Y(7)+PHV*PV*DRV/RV-AALV*YP(1)/ROR+EVP)/PRV
IF (YP(7).GT.1.E11) YP(7)=1.E11

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IF (YP(7) .LT. -1.E11) YP(7)=-1.E11
C
C COMPUTE D(EC)/DT
C
YP(8)=(YP(1)/ROR*(Y(8)+AALC)+PHC*PC*DRC/RC+ECP)/PRC
GO TO 670
601 STARE=Y(3)
IF (Y(3) .LT. Y(2)) Y(3)=Y(2)
PHC=1.-Y(3)**3./ROR/CES(15,PLATE)
PHF=Y(2)**3./ROR/CES(15,PLATE)
PHV=1.-PHC-PHF
RC=(CES(12,PLATE)-Y(1))/PHC/ROR
RF= CES(13,PLATE)/PHF/ROR
RV=RC
IF (CES(14,PLATE)+Y(1) .GT. 0.) RV=2.
NINT=0
TE=THC
RHQ=RC/1000.
602 CALL STMTBL
THA=TE-(ER-Y(8)*1.0E4)/CV
AB=ABS((THA-TE)/TE)
IF (AB .LE. 1.0E-6) GO TO 650
TE=THA
NINT=NINT+1
IF (NINT .LT. 50) GO TO 602
PRINT 603,RC,TE
603 FORMAT(* COOLANT TEMP DID NOT CONVERGE AFTER IMPACT RC=*,E10.3,
1 * THC=*,E10.3)
650 CONTINUE
THC=TE
PC=PR*0.1
CPC=(CV+TE/DPR*(DPT/RHQ)**2.)*1.0E-4
THF=Y(6)/CES(16,PLATE)
PF=CES(17,PLATE)*(1.-CES(18,PLATE)/RF)
OMG=ABS(Y(4)/RC)/CES(25,PLATE)
CALL COND
FAC=1.+Y(2)*RF*Y(5)/3./CES(22,PLATE)*CES(21,PLATE)
AKC=AKC*FAC
AKF=AKF*FAC
ALF=SQRT(OMG*RF*CES(16,PLATE)/AKF)
ALC=SQRT(OMG*RC*CPC/AKC)
IF (Y(3) .GT. Y(2)) ISAT=CES(31,PLATE)
IF (Y(3) .GT. Y(2)) GO TO 604
PR=10.*PF
ISAT=TBND(PR,ERR)
IF (ERR) GO TO 605
GO TO 604
605 CONTINUE
ISAT=TEXTND(PF)
604 CONTINUE
IF ( Y(3) .GT. Y(2) ) TW=THC
IF ( Y(3) .LE. Y(2) ) TW=(AKF/Y(3))*(ALF*Y(3)+1.)*THF+
1 AKC/Y(3)*(ALC*Y(3)+1.)*THC/(AKF/Y(3))*(ALF*Y(3)+1.)+
2 AKC/Y(3)*(ALC*Y(3)+1.)
TW=THC

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```

TE=TW
RHO=RV/1000.
CALL STMTBL
PV=PR/10.
680 CONTINUE
ALPHAC=CES(20,PLATE)+(1.-CES(20,PLATE))*PV/22.09E6
ALPHAC=AMIN1(1.,ALPHAC)
AL=ALPHAC*(1.+Y(2)*RF*Y(5)/3./CES(22,PLATE)
1 *CES(21,PLATE))*
2SQRT(CES(23,PLATE)/51604.43)
YP(1)=-ROR*(PHV+PHF)/Y(3)*AL *PV*(1./SQRT(TSAT)-SQRT(TW)/TSAT)
1*3.
IF(YP(1).GT.10.) YP(1)=10.
IF(YP(1).LT.0.) YP(1)=0.
YP(2)=(PF-PV +YP(1)/ROR*Y(4)/RC*Y(3)/PHF)/
1 CES(24,PLATE)/(3.*RF/Y(2))
YP(3)=Y(4)/RC+Y(2)**3./3./PHF/RC/Y(3)**2.*YP(1)/ROR
IF(Y(3).GT.Y(2)) GO TO 733
IF(YP(3).LT.YP(2)) YP(2)=YP(3)
IF(YP(3).LT.YP(2)) PF=PF-3.*RF/Y(2)*YP(2)*CES(23,PLATE)
GO TO 734
733 PF=PF+PC
734 CONTINUE
YP(4)=-1.5*(1.-(1.-PHC)/PHC)*Y(4)**2./Y(3)/RC-(1./3./(1.-PHC)-1./
1PHC+1./PHF)*YP(1)/ROR*Y(4)/RC+(PF-PC)/Y(3)
YP(5)=CES(24,PLATE)*9.*(YP(2)/Y(2))**2.
IF(Y(3).GT.Y(2)) EFP=0
IF(Y(3).GT.Y(2)) ECP=0
IF(Y(3).LE.Y(2)) EFP=-AKF*(ALF*Y(3)+1.)/Y(3)*(THF-TW)
IF(Y(3).LE.Y(2)) ECP=AKC*(TW-THC)*(ALC*Y(3)+1.)/Y(3)
HC=0
HV=0
DJ=-ROR*RDOT
DPHC=(-3.*YP(3)/Y(3)+DJ/ROR)*Y(3)**3./ROR/CES(15,PLATE)
DPHF=(3.*YP(2)/Y(2)-DJ/ROR)*Y(2)**3./ROR/CES(15,PLATE)
DPHV=-DPHC-DPHF
DRC=-YP(1)/PHC/ROR-RC*(DJ/ROR+DPHC/PHC)
DRF=-3.*RF*YP(2)/Y(2)
PRC=RC*PHC
PRF=RF*PHF
YP(6)=EFP/PRF
YP(7)=0
YP(8)=(YP(1)/ROR*(Y(8) )+PHC*PC*DRC/RC+ECP)/PRC
Y(3)=STARE
670 CONTINUE
RETURN
END
FUNCTION TEXTND(PV)
C
C EXTENDED SATURATION LINE
C
COMMON/HDGG/REXTND
DIMENSION T(5),P(5),R(5)
DATA(T(I),I=1,5)/
* 647.206,657.1,671.89,713.96,764.28/

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DATA(P(I),I=1,5)/
*22.09E6,25.E6,30.E6,50.E6,100.E6/
DATA(R(I),I=1,5)/
* 316.96,336.95,372.60,457.47,542.38/
DO 10I=2,5
IF(PV.GT.P(I)) GO TO 10
TEXTND=T(I-1)*T(I)/(T(I-1)+(T(I)-T(I-1))*ALOG(PV/P(I))
1 /ALOG(P(I-1)/P(I)))
REXTND=R(I)+(R(I-1)-R(I))*(PV-P(I))/(P(I-1)-P(I))
RETURN
10 CONTINUE
END
SUBROUTINE COND
DIMENSION VA(6,6),FL(6,6),P(6),T(6)
COMMON/WITHF/PC,VR,PHF,PHC,RC,PF,PV,PRC,PRF,PRV,ROR,THC,THV
1 ,THF,AKF,AKC,AKV
DATA((VA(I,J),J=1,6),I=1,6)/
*.024,.0287,.0434,.0611,.0943,.0943,
*.024,.0287,.0434,.0611,.0943,.0943,
*.0261,.030,.0525,.0659,.0986,.0986,
*.125,.125,.125,.093,.113,.113,
*.300,.300,.300,.301,.148,.148,
*.600,.600,.600,.600,.170,.170/
DATA((FL(I,J),J=1,6),I=1,6)/
*.569,.681,.500,.301,.150,.150,
*.569,.681,.500,.301,.150,.150,
*.573,.690,.520,.301,.150,.150,
*.585,.700,.571,.301,.150,.150,
*.606,.720,.622,.301,.148,.148,
*.700,.700,.700,.600,.170,.170/
DATA(P(I),I=1,6)/
*0.0,0.1E5,5.0E5,20.0E5,50.0E5,100.0E5/
DATA(T(I),I=1,6)/
*273.16,423.16,573.16,723.16,973.16,5273.16/
DO 10 Y = 2,6
IF(PV.LE.P(I)) GO TO 11
10 CONTINUE
I=6
AKV=.170
GO TO 31
11 CONTINUE
DO 12 J = 2,6
IF(THV.LE.T(J)) GO TO 13
12 CONTINUE
J=6
AKV=.170
GO TO 31
13 CONTINUE
DP=P(I)-P(I-1)
DT=T(J)-T(J-1)
V1=VA(I-1,J-1)
V2=VA(I,J-1)
V3=VA(I-1,J)
V4=VA(I,J)
B=(V2-V1)/DP

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C=(V3-V1)/DT
D=(V4+V1-V3-V2)/DP/DT
AKV=V1+B*(PV-P(I-1))+C*(THV-T(J-1))+D*(PV-P(I-1))*(THV-T(J-1))
31 CONTINUE
DO 20 I = 2,6
IF(PC.LE.P(I)) GO TO 21
20 CONTINUE
I=6
AKC=.170
GO TO 32
21 CONTINUE
DO 22 J = 2,6
IF(THC.LE.T(J)) GO TO 23
22 CONTINUE
J=6
AKC=.170
GO TO 32
23 CONTINUE
DP=P(I)-P(I-1)
DT=T(J)-T(J-1)
V1=FL(I-1,J-1)
V2=FL(I,J-1)
V3=FL(I-1,J)
V4=FL(I,J)
B=(V2-V1)/DP
C=(V3-V1)/DT
D=(V4+V1-V3-V2)/DP/DT
AKV=V1+B*(PC-P(I-1))+C*(THC-T(J-1))+D*(PC-P(I-1))*(THC-T(J-1))
32 CONTINUE
AKF=12.
RETURN
END
SUBROUTINE WATER (R,TIN)

C
C THERMODYNAMIC PROPERTIES OF WATER AS A FUNCTION OF T AND RHO
C
COMMON /THERMO/ PM,EM,SM,CVM,DPTM,DPRM,KPA,RV,EV,SV,CVV,DPTV,DPRV,
COMMON /ARGLST/ T,RHO,P,E,S,CV,DPT,DPR
DIMENSION PPM(6),EEV(5),EEL(5),PA(6)
EQUIVALENCE (PPM(1),PM), (EEV(1),EV), (EEL(1),EL), (PA(1),P)
LOGICAL ERR,CLOSE
COMMON /LV2/ TCRT,TZERO,DTBL,NTBL1,PLV2(51),RVLV2(51),RLLV2(51)
EQUIVALENCE (PCRT,PLV2(1)), (RCRT,RVLV2(1))
DATA ERR,LIM,ITLIM /1.E-5,50/
DATA RMIN2P,RMAX2P,SAFEV,SAFEL /4.84E-6,1.00,.971,1.008/
DATA SAFEV1,SAFEL1 /.988,1.006/
T=TIN

C
C FAST CHECKS FOR SINGLE PHASE
C MAY WANT TO BIAS AWAY FROM TCRT
C
IF (T.GE.TCRT) GO TO 90
IF (R.LT.RMIN2P) GO TO 90
IF (R.GT.RMAX2P) GO TO 90
C

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```

C   INTERPOLATE FIRST APPROXIMATION TO PHASE DENSITIES
C
I=(T-TZERO)/DTBL
TLO=TZERO+FLOAT(I)*DTBL
THI=AMIN1(TLO+DTBL,TCRIT)
I=NTBL1-I
SF=(THI-T)/DTBL
IF (I.EQ.1) SF=(SF*DTBL/(TCRIT-TLO))**.333333333333
RV=RVLV2(I)+SF*(RVLV2(I+1)-RVLV2(I))
RL=RLLV2(I)+SF*(RLLV2(I+1)-RLLV2(I))
C
C   CHECK DENSITY AGAINST PHASE DENSITIES WITH SAFETY FACTORS
C
IF (R.LT.SAFEV*RV) GO TO 90
IF (R.GT.SAFEL*RL) GO TO 90
PSAT=PBND(T,ERR)
IF (ERR) STOP1
C
C   IMPROVE FIRST APPROXIMATION TO PHASE DENSITIES
C   CHECK DENSITY AGAINST PHASE DENSITIES WITH SAFETY FACTORS
C
SUM=RL+RV
3F=(PLV2(I)-PSAT)/(PLV2(I)-PLV2(I+1))
IF (I.EQ.1) SF=SF**.333333333333
RV=(SF*RVLV2(I+1)*TLO/PLV2(I+1)+(1.0-SF)*RVLV2(I)*THI/PLV2(I))
1 *PSAT/T
RL=SUM-RV
IF (R.LT.SAFEV1*RV) GO TO 90
IF (R.GT.SAFEL1*RL) GO TO 90
C
C   ITERATE TO FIND LIQUID DENSITY
C
CLOSE=RL.LT.R
IF (CLOSE) RL=R
ITL=0
10 RHO=RL
ITL=ITL+1
CALL STMTBL
IF (ITL.GT.1) GO TO 20
IF (CLOSE.AND.(P.GT.PSAT)) GO TO 91
20 DP=PSAT-P
IF (ABS(DP).LT.ERR.LIM*PSAT) GO TO 30
IF (DPR.EQ.0.0) STOP2
DR=DP/DPR
RL=RL+DR
IF (ITL.LT.ITLIM) GO TO 10
STOP3
C
C   CHECK DENSITY AGAINST LIQUID DENSITY
C
30 IF (R.GT.RL) GO TO 90
DO 31 J=1,5
31 EEL(J)=PA(J+1)
C
C   ITERATE TO FIND VAPOR DENSITY

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```

C
  ITV=0
40 RHO=RV
  ITV=ITV+1
  CALL STMT9L
  DP=PSAT-P
  IF (ABS(DP).LT.ERRLIM*PSAT) GO TO 50
  IF (DPR.EQ.0.0) STOP4
  DR=DP/DPR
  RV=RV+DR
  IF (ITV.LT.ITLIM) GO TO 40
  STOP5

C
C   CHECK DENSITY AGAINST VAPOR DENSITY
C
50 IF (R.LT.RV) GO TO 90
  DO 51 J=1,5
51 EEV(J)=PA(J+1)

C
C   HAVE TWO PHASE STATE
C
  KPA=2
  PM=PSAT
  X=AMIN1(1.0,RV*(RL-R)/(R*(RL-RV)))
  EM=X*EV+(1.0-X)*EL
  SM=X*SV+(1.0-X)*SL
  DPTM=(SV-EL)*RL*RV/(RL-RV)
  FACT=PM+(EV-EL)*RL*RV/(RL-RV)
  CVM= X *(CVV+(FACT-T*DPTV)*(DPTM-DPTV)/(DPRV*RV**2))
1   +(1.0-X)*(CVL+(FACT-T*DPTL)*(DPTM-DPTL)/(DPRL*RL**2))
  DPRM=0.0
  GO TO 999

C
C   HAVE SINGLE PHASE STATE
C
90 CONTINUE
  RHO=R
  CALL STMTBL
91 KPA=1
  RV=0.0
  RL=0.0
  DO 100 J=1,5
  EEV(J)=0.0
100 EEL(J)=0.0
  DO 110 J=1,6
110 PPM(J)=PA(J)
999 RETURN
  END
  FUNCTION PBND (T,ERR)

C
C   SATURATION PRESSURE BY LINEAR INTERPOLATION OF LOG(P) VS 1/T
C
  LOGICAL ERR
  COMMON /LV2/ TCRT,TZERO,DTBL,NTBL1,PLV2(51),RVLV2(51),RLV2(51)
  EQUIVALENCE (PCRT,PLV2(1)), (RCRT,RVLV2(1))

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C TEMPERATURES ARE TCRII, (TZERO+(NTBL1-I)*DTBL ,I=0,NTBL1)
DATA TCRII,TZERO,DTBL,NTBL1 /6.4724498885354E+02,273.16,7.5,50/

C SATURATION PRESSURE
DATA (PLV2(I),I=1,51)/

* 2.2078404874679E+08,	2.0399624991274E+08,	1.8642191385428E+08,
* 1.7021255579410E+08,	1.552131494211E+08,	1.4131535874689E+08,
* 1.2843419868665E+08,	1.1649884368919E+08,	1.0544800715997E+08,
* 9.5227210688868E+07,	8.5787036358453E+07,	7.7081943660503E+07,
* 6.9069440814585E+07,	6.1709492002574E+07,	5.4964088285502E+07,
* 4.8796935477108E+	4.3173227365359E+07,	3.8059482141874E+07,
* 3.3423426109402E+07,	2.9233912958101E+07,	2.5460869865993E+07,
* 2.2075263818807E+07,	1.9049083126126E+07,	1.6355330301655E+07,
* 1.3968023381043E+07,	1.1862203438245E+07,	1.0013946575494E+07,
* 8.4003790327471E+06,	6.9996943115145E+06,	5.7911713552618E+06,
* 4.7551928909316E+06,	3.8732630329932E+06,	3.1280232026451E+06,
* 2.5032653425615E+06,	1.9839413347299E+06,	1.5561674782798E+06,
* 1.2072228766907E+06,	9.2554063696671E+05,	7.0069090921758E+05,
* 5.2335499915146E+05,	3.8529006597665E+05,	2.7928426434173E+05,
* 1.9910258410860E+05,	1.3942406296435E+05,	9.5771466827884E+04,
* 6.4434922087007E+04,	4.2391312168407E+04,	2.7221491186800E+04,
* 1.7027496270014E+04,	1.0351941204056E+04,	6.1016396936318E+03/

C SATURATED VAPOR DENSITY
DATA (RVLV2(I),I=1,51)/

* 3.1681699395231E-01,	1.8121395566705E-01,	1.4356900039010E-01,
* 1.1970972488335E-01,	1.0211953786232E-01,	8.8257487547604E-02,
* 7.6909589525150E-02,	6.7388252174886E-02,	5.9261675528176E-02,
* 5.2239044025492E-02,	4.6114240858049E-02,	4.0735327172216E-02,
* 3.5986715230857E-02,	3.1778145127381E-02,	2.8037554629907E-02,
* 2.4706296358921E-02,	2.1735831968490E-02,	1.9085389136779E-02,
* 1.6720265049647E-02,	1.4610574987901E-02,	1.2730313974087E-02,
* 1.1056642691794E-02,	9.5693366776109E-03,	8.2503561061553E-03,
* 7.0835058485399E-03,	6.0541639926657E-03,	5.1490629718466E-03,
* 4.3561116791474E-03,	3.6642499796053E-03,	3.0633292223428E-03,
* 2.5440139347520E-03,	2.0977010140221E-03,	1.7164535315528E-03,
* 1.3929468168818E-03,	1.1204248531978E-03,	8.9266524701650E-04,
* 7.0395117245265E-04,	5.4904877214249E-04,	4.2318855348588E-04,
* 3.2204937688539E-04,	2.4174371266976E-04,	1.7880295981911E-04,
* 1.3016177997187E-04,	9.3140605236117E-05,	6.5425722493264E-05,
* 4.5046609308889E-05,	3.0350482356237E-05,	1.9974300825474E-05,
* 1.2814725672404E-05,	7.9967516862289E-06,	4.8418652862328E-06/

C SATURATED LIQUID DENSITY
DATA (RLLV2(I),I=1,51)/

* 3.1681699395231E-01,	4.7682226675081E-01,	5.2816276300305E-01,
* 5.6422942547271E-01,	5.9341197447755E-01,	6.1847497657411E-01,
* 6.4071162202146E-01,	6.6084351834464E-01,	6.7932064704864E-01,
* 6.9644656042343E-01,	7.1243858270583E-01,	7.2745972023833E-01,
* 7.4163682069091E-01,	7.5507148524242E-01,	7.6784692129988E-01,
* 7.8003241180513E-01,	7.9168633197001E-01,	8.0285825310852E-01,
* 8.1359045738046E-01,	8.2391906341328E-01,	8.3387488947819E-01,
* 8.4348413643457E-01,	8.5276894513029E-01,	8.6174786548644E-01,
* 8.7043626315398E-01,	8.7884668192274E-01,	8.8698917453744E-01,
* 8.9487161026048E-01,	9.0249996385832E-01,	9.0987858730727E-01,
* 9.1701046223498E-01,	9.2389742784102E-01,	9.3054037578234E-01,
* 9.3693940030976E-01,	9.4309368886644E-01,	9.4900253548663E-01,
* 9.5466325668035E-01,	9.6007298706319E-01,	9.6522732975152E-01,

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* 9.7012003448037E-01, 9.7474227464802E-01, 9.7908169357815E-01,
* 9.8312119155402E-01, 9.8683743183067E-01, 9.9019906343171E-01,
* 9.9316471016571E-01, 9.9568091098007E-01, 9.9768056615323E-01,
* 9.9908348266566E-01, 9.9980353189992E-01, 9.9977455442334E-01/
ERR=.TRUE.
IF (T.GT.TCRIT) GO TO 99
I=(T-TZERO)/DTBL
IF (I.LT.0) GO TO 99
TLO=TZERO+FLOAT(I)*DTBL
THI=AMIN1(TLO+DTBL,TCRIT)
I=NTBL1-I
PBND=PLV2(I)*(PLV2(I+1)/PLV2(I))**
1 (TLO*(THI-T)/(T*(THI-TLO)))
ERR=.FALSE.
99 RETURN
END
FUNCTION TBND (P,ERR)
C
C SATURATION TEMPERATURE BY LINEAR INTERPOLATION OF LOG(P) VS 1/T
C
LOGICAL ERR
COMMON /LV2/ TCRIT,TZERO,DTBL,NTBL1,PLV2(51),RVLV2(51),RLLV2(51)
EQUIVALENCE (PCRIT,PLV2(1)), (RCRIT,RVLV2(1))
ERR=.TRUE.
IF (P.GT.PCRIT) GO TO 99
DO 10 I=1,NTBL1
IF (P.LT.PLV2(I+1)) GO TO 10
TLO=TZERO+(NTBL1-I)*DTBL
THI=AMIN1(TLO+DTBL,TCRIT)
TBND=THI*TLO/
1 (THI+(TLO-THI)*ALOG(P/PLV2(I+1))/ALOG(PLV2(I)/PLV2(I+1)))
ERR=.FALSE.
GO TO 99
10 CONTINUE
99 RETURN
END
SUBROUTINE STMTBL
C
C DATA FROM
C STEAM TABLES
C THERMODYNAMIC PROPERTIES OF WATER
C INCLUDING VAPOR, LIQUID, AND SOLID PHASES
C
C BY KEENAN,KEYES,HILL,AND MOORE
C WILEY (1969)
C
C WARNING THIS DATA IS ONLY GOOD FOR
C T .GE. 273.15 K
C T .LE. 1589 K
C P .LT. 15000 PSI
C
COMMON /ARGLST/ T,RHO,P,E,S,CV,DPT,DPR
EQUIVALENCE (T,TK),(RHO,R)
DIMENSION ALP(8),A(8,7),BET(7),GAM(7)
DIMENSION DTAU(7),HL(7),HLP(7),HLPP(7)

```

```

DATA DE/4.8/
DATA GASC/4.6151E6/
DATA ALP/1857.065E7,3229.12E+4,-419.465E+1,36.6649E-2,-20.5576E-5,
14.85233E-8,46.E7,-1011.249E4/
DATA A/29.492937,-132.13917,274.64632,-360.93828,342.18431,-244.50
1042,155.18535,5.9728487,-5.1965860,7.7779182,-33.301902,-16.254622
2,-177.31074,127.48742,137.46153,155.97836,6.8335354,-26.149751,65.
3326396,-26.181978,0.,0.,0.,0.,-0.1564104,-0.72546108,-9.1734289,4.
43125840,0.,0.,0.,0.,-6.3972405,26.409282,-47.740374,56.313130,0.,0
5.,0.,0.,-3.9661401,15.453061,-29.142470,29.568796,0.,0.,0.,0.,-0.6
69048554,2.7407416,-5.102807,3.9636085,0.,0.,0.,0./
DATA BET/-410.30848,337.31180,-137.46618,6.7874983,136.87317,79.84
1797,13.041253/
DATA GAM/-416.05860,-209.88866,-733.96848,10.401717,645.8188,399.1
1757,71.531353/
OTK=1./TK
C DETERMINE PSI FUNCTIONS
TLOG=ALOG(TK)
F=ALP(1)+ALP(2)*TK+(ALP(7)+ALP(8)*TK)*TLOG
FT=ALP(2)+ALP(8)+ALP(7)*OTK+ALP(8)*TLOG
TP=TK
DO TO I=2,5
FT=FT+ALP(I+1)*TP*FLOAT(I)
TP=TP*TK
70 F=F+ALP(I+1)*TP
FTT=2.*(ALP(3)+TK*(3.*ALP(4)+TK*(6.*ALP(5)+10.*ALP(6)*TK)))+(ALP(8
1)-ALP(7)*OTK)*OTK
C DETERMINE H FUNCTIONS
RC=0.634
J=1
80 TP=R-RC
SUM=1.
DO 90 I=1,7
SUM=SUM*TP
90 DTAU(I)=SUM
100 HL(J)=A(1,J)+A(2,J)*DTAU(1)+A(3,J)*DTAU(2)+A(4,J)*DTAU(3)
HLP(J)=A(2,J)+2.*A(3,J)*DTAU(1)+3.*A(4,J)*DTAU(2)
HLPP(J)=2.*A(3,J)+6.*A(4,J)*DTAU(1)
IF (J-2) 110,110,140
110 DO 120 I=5,8
HL(J)=HL(J)+A(I,J)*DTAU(I-1)
HLP(J)=HLP(J)+A(I,J)*DTAU(I-2)*FLOAT(I-1)
120 HLPP(J)=HLPP(J)+A(I,J)*DTAU(I-3)*FLOAT((I-1)*(I-2))
J=J+1
IF (J-2) 130,130,100
130 RC=1.
GO TO 80
140 IF (J-7) 150,160,160
150 J=J+1
GO TO 100
160 CONTINUE
C DETERMINE L FUNCTIONS
ED=EXP(-DE*R)
DO 170 J=1,7
SUM=BET(J)+GAM(J)*R

```

```

HL(J)=HL(J)+ED*SUM
HLP(J)=HLP(J)-ED*(DE*SUM-GAM(J))
170 HLPP(J)=HLPP(J)+DE*ED*(DE*SUM-2.*GAM(J))
C DETERMINE Q FUNCTIONS
TAU=1000.*OTK
TP=TAU-2.5
DTAU(1)=TP
DO 180 J=2,5
180 DTAU(J)=TP*DTAU(J-1)
DTAUC=TAU-1.544912
Q=0.
QR=0.
QRR=0.
DO 190 J=3,7
Q=Q+DTAU(J-2)*HL(J)
QR=QR+DTAU(J-2)*HLP(J)
190 QRR=QRR+DTAU(J-2)*HLPP(J)
SUM=0.
TP=0.
DO 200 J=4,7
SUM=SUM+DTAU(J-3)*HL(J)*FLOAT(J-2)
200 TP=TP+DTAU(J-3)*HLP(J)*FLOAT(J-2)
QTT=0.
DO 210 J=5,7
210 QTT=QTT+DTAU(J-4)*HL(J)*FLOAT((J-2)*(J-3))
QT=HL(2)+Q+DTAUC*(HL(3)+SUM)
QRT=HLP(2)+QR+DTAUC*(HLP(3)+TP)
QTT=2.*(HL(3)+SUM)+DTAUC*(2.*HL(4)+QTT)
QRR=HLPP(1)+DTAUC*(HLPP(2)+QRR)
QR=HLP(1)+DTAUC*(HLP(2)+QR)
Q=HL(1)+DTAUC*(HL(2)+Q)
SUM=TAU*OTK
QTT=SUM*(2.*QT*OTK+SUM*QTT)
QRT=-SUM*QRT
QT=-SUM*QT
RT=GASC*TK
Q=R*Q
QR=R*QR*R
C DETERMINE THERMODYNAMIC FUNCTIONS
P=R*RT*(1.+Q+QR)
DPR=RT*(1.+2.*Q+4.*QR+QRR*R**3)
DPT=P*OTK+R*R*RT*(QT+R*QRT)
CV=-TK*(FTT+R*GASC*(2.*QT+TK*QTT))
E=F-TK*(FT+R*RT*QT)
S=-FT-GASC*(ALOG(R)+Q+R*TK*QT)
RETURN
END

```

APPENDIX C: INPUT INSTRUCTIONS

The International System of Units (SI) must be used. The standard WONDY IV input instructions apply;¹¹ however, the vapor explosion routine must be entered through the STAT5 subroutine. The equation of state constants for the CES array are defined as follows:

<u>CES Array Number</u>	<u>Mathematical Symbol</u>	<u>Remarks</u>
1*	$\bar{\rho}_{CO}$	Initial value of $\bar{\rho}_C$.
2	C_O	Stability sound speed. A constant normally larger than the coolant sound speed.
3*	$\bar{\rho}_{VO}$	Initial value of $\bar{\rho}_V$.
4*	$\bar{\rho}_{fO}$	Initial value of $\bar{\rho}_f$.
5	ϕ_{CO}	Initial value of ϕ_C .
6*	ϕ_{VO}	Initial value of ϕ_V .
7	θ_{CO}	Initial value of θ_C .
8	θ_{VO}	Initial value of θ_V .
9	θ_{fO}	Initial value of θ_f .
10	R_{VO}	Initial value of R_V .
11	R_{fO}	Initial value of R_f .
12*	ρ_{CO}	$\phi_{CO}\bar{\rho}_{CO}$
13*	ρ_{fO}	$\phi_{fO}\bar{\rho}_{fO}$
14*	ρ_{VO}	$\phi_{VO}\bar{\rho}_{VO}$
15*	R_{CO}^3	Eqn. (10)
16	C_{pf}	Eqn. (33)

*Computed Internally

<u>CES Array Number</u>	<u>Mathematical Symbol</u>	<u>Remarks</u>
17	S_f	Eqn. (32)
18	$\bar{\rho}_{fr}$	Eqn. (32)
19	$(h_v - h_c)_{min}$	Minimum value of latent heat used in heat transfer calculations.
20	α	Eqn. (37)
21	γ	Eqn. (35)
22	σ	Eqn. (35)
23	M_v	Eqn. (37)
24	Q	Eqn. (32)
25	$(R_v - R_f)_{min}$	Minimum value of vapor film thickness used in Eqn. (42).
26	ERROR	Error parameter for STEP.12
27*	ρ_o	Initial value of ρ .
28	P_{co}	Initial value of P_c .
29	P_{vo}	Initial value of P_v .
30		Not used.
31	$(\theta_s)_{min}$	Minimum value of θ_s used in heat conduction calculations.
32		Not used.
33		Not used.
34		Not used.
35		Not used.

*Computed internally.

APPENDIX D: LIST OF INPUT VALUES FOR EXAMPLE PROBLEM

The following list conforms to the standard WONDY IV notation¹¹ and uses the International System of Units:

Card Number 1:

TITLE. TOM MIX - EXAMPLE PROBLEM

Card Number 2:

LPHA	1
NOP	1
NVAR	21
LHBT	4
RHBT	1
LACT	-
NJOB	-
NIL	0
NOL	1
NUL	30
MORE	0
JTAPE	0
NSTART	0
W4020	0

Card Number 3:

TMAX	1.
DELT(4)	2.0E-6
SIGSEP	-1.0E100

SIGACT	1.0E3
XZERO	0.0
LBCN	-
RBCN	-

Card Number 4:

KT1	0.95
KT2	1.05
B1	0.5
B2	0.03
SIGMAX	-
EMAX	1.0E100
HMAX	-

Card Number 5:

S1	2.8E-5
Δ 1	0.05E-4
S2	1.0

Card Number 6:

S1	0.0
Δ 1	1.0E-6
S2	1.0

Card Number 9:

I	8
ADDDATA(8)	2.1E6
ADDDATA(9)	1.0E5
ADDDATA(10)	30.0E-6

Card Number 10:

PLATE	1.
STATE	5.0
NOMESH	120.0
THKNS	0.6
DELTA	0.0025
DELTA1	0.0025
XRATIO	-
XGAP	-

Card Number 15:

1.	958.3
2.	5000.0
3.	0.1578
4.	-
5.	0.80
6.	-
7.	303.2

Card Number 16:

8.	1373.2
9.	2443.2
10.	0.0102
11.	0.0100
12.	-
13.	-
14.	-

Card Number 17:

15. -
16. 900.0
17. 1.0E11
18. 7850.0
19. 1.0E5
20. 0.2
21. 0.0

Card Number 18:

22. 0.4
23. 18.0
24. 25.42
25. 1.0E-6
26. 1.0E-6
27. -
28. 1.0E5

Card Number 19:

29. 1.0E5
30. -
31. 100.0
32. -
33. -
34. -
35. -

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