Modelling of Lithium-Lead/Water Interactions in a Fusion Reactor Design

J.P. Herzog and M.L. Corradini

September 1983
(revised August 1984)

UWFDM-559

FUSION TECHNOLOGY INSTITUTE

UNIVERSITY OF WISCONSIN

MADISON WISCONSIN

Modelling of Lithium-Lead/Water Interactions in a Fusion Reactor Design

J.P. Herzog and M.L. Corradini

Fusion Technology Institute
University of Wisconsin
1500 Engineering Drive
Madison, WI 53706

http://fti.neep.wisc.edu

September 1983 (revised August 1984)

UWFDM-559

MODELING OF LITHIUM-LEAD/WATER INTERACTIONS IN A FUSION REACTOR DESIGN

J.P. Herzog

M.L. Corradini

Fusion Engineering Program
Nuclear Engineering Department
University of Wisconsin-Madison
Madison, Wisconsin 53706

September 1983

(Revised August 1984)

UWFDM-559

Prepared for EG&G Idaho Inc. and the Department of Energy Idaho Operations Office under DOE Contract No. DE-AC07-76ID01570.

MODELING OF LITHIUM-LEAD/WATER INTERACTIONS IN A FUSION REACTOR DESIGN

J.P. Herzog and M.L. Corradini

University of Wisconsin, Madison, WI 53706

Abstract

A parametric model was developed to predict the transient pressure and temperature behavior for a liquid-metal/water interaction in a steam generator following an assumed tube rupture. The model results suggest two preliminary conclusions. First, the maximum temperature for lithium-lead due to the reaction, although above normal limits, is below the thermodynamic maximum value rapidly falling to within operating limits. Second, the pressure history and hydrogen generated from water injection into lithium or lithium-lead are quite similar for a given value of the metal/water mixing parameter. This suggests that the pressure-flow characteristics govern the integral response given an assumed degree of chemical reaction. For a more accurate prediction of the accident response one must consider the reaction kinetics for lithium and lithium-lead interactions; e.g. lithium may be a "vapor phase combustion" process while lithium-lead would be governed by metal surface mass transfer phenomena. Under the contact mode considered complete reduction of water to hydrogen cannot be precluded.

Introduction

Lithium and its alloys, in particular lithium-lead alloys, have been considered recently as possible breeder-blanket materials in conceptual designs of fusion power reactors, due to their favorable neutronic, breeding, and heat transfer properties. These materials do represent some safety hazard, though, due to their chemically reactive nature with other reactor materials, e.g. air, water, and concrete.

Current evaluations of the hazard potential of lithium and lithium-alloy breeders in contact with other reactor materials has been based upon thermodynamic calculations of possible chemical reactions, and on dynamic parametric calculations for specific fusion reactor designs. These calculations have led to rough comparisons of the overall hazard potential of different lithium and lithium-alloy breeders with other potential reactor materials.[1,2] Also, scoping experiments were performed at Argonne National Laboratory by R. Clemmer et al.[3-5] and are now underway at HEDL by L. Muhlestein.[6] These tests indicated that qualitatively the reaction between lithium and lithium-alloy breeders with H_2O is quite different (see Table 1). Additional work by Jepson et al.[7] with lithium-alloys and the ternary oxides ($LiAlO_2$, $LiSiO_3$, Li_4SiO_4, and $LiTiO_3$) showed that these oxides present minimal safety related problems when used with H_2O; however, they do require neutron multipliers, such as lithium-lead for breeding and power needs. They go on to state that "...the combined favorable neutronics and minor safety compatibility concerns of lithium oxide and $Li_{17}Pb_{83}$ (a particular eutectic lithium-lead alloy; Li 17 a/o) make them prime candidates as blanket materials." Recently some European investigators[8,9] have initiated studies on the potential of certain breeder-

Table 1. Reactions of Li-Pb Alloys and Lithium With Water

Case	Composition	Sample State[a]	Temp/°K	Water Temp/°K	Reaction
1	Li_7Pb_2	s	773	298	Modest
2	Li_7Pb_2	s	773	369	Vigorous
3	Li_7Pb_2	s	873	368	Vigorous
4	Li_7Pb_2	ℓ	1103	368	Very Vigorous
5	$Li_{0.62}Pb_{0.38}$	ℓ	773	368	Vigorous
6	$Li_{0.17}Pb_{0.83}$	ℓ	773	368	Very Modest
7	Li	ℓ	773	368	H_2 Detonation
8	Li[b]	ℓ	773	368	Detonation

[a] s = solid, ℓ = liquid

[b] injected under water

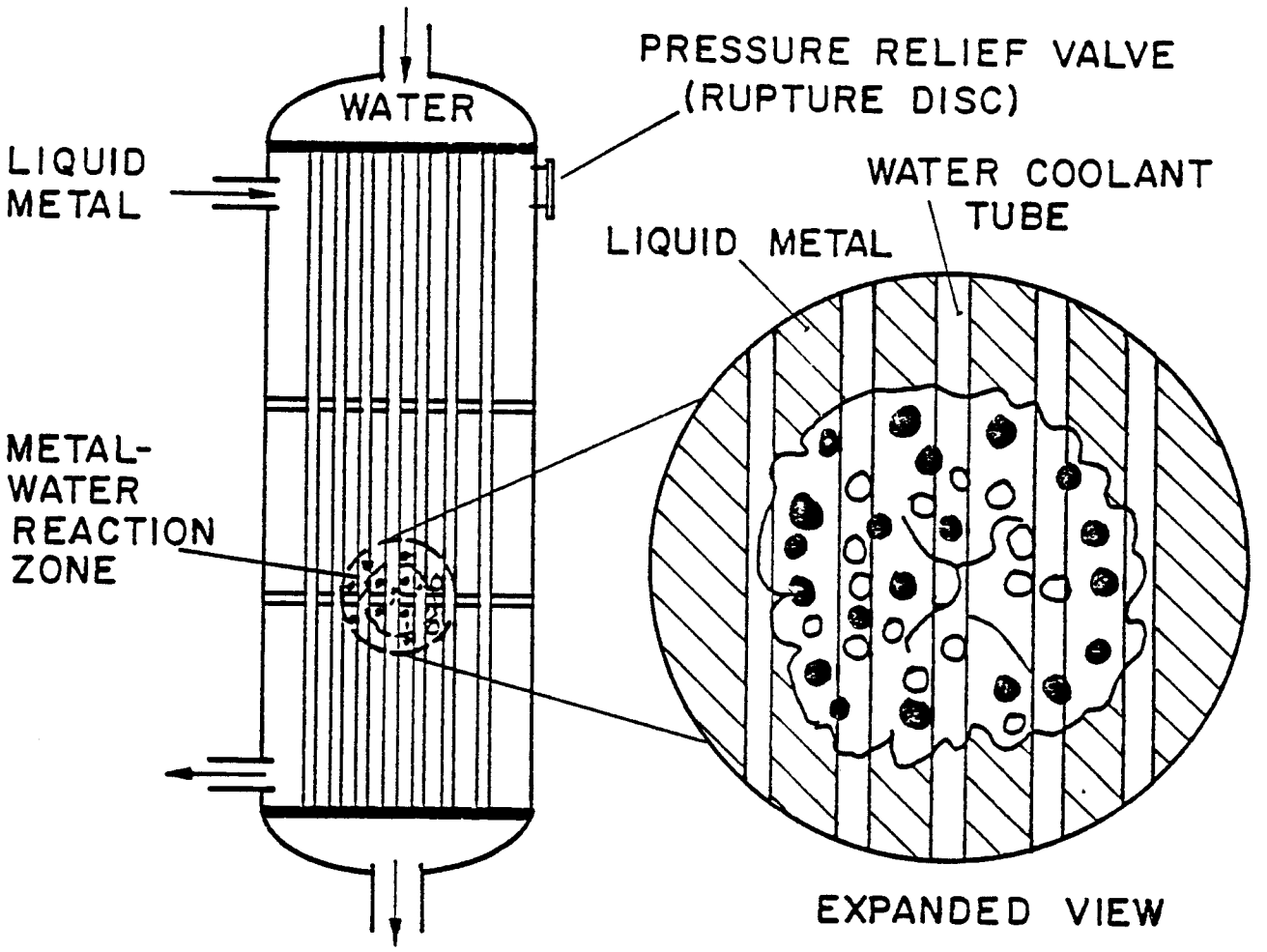
blanket designs and have provided specific design proposals to reduce the overall hazard potential of a $Li_{17}Pb_{83}$ breeder-blanket.

Our current work is being done in conjunction with the DOE Fusion Safety Program and previously with the Mirror Advanced Reactor Study (MARS).[10] The MARS conceptual fusion reactor design utilizes the lithium-lead alloy $Li_{17}Pb_{83}$ (hereon designated as "lithium-lead") as a liquid-metal breeder and primary coolant. Based upon a number of previously mentioned reasons,[3-7] "lithium-lead" was chosen as the breeder-coolant for the MARS design; e.g. high tritium breeding ratio, good neutron multiplication, acceptable corrosion rates, and relatively benign chemical reaction rates with water and air.

We limit our comments to the lithium-lead/water and the lithium/water interactions as applied to a MARS conceptual fusion reactor design. For various accident sequences one can identify four possible "contact modes" between the molten metal breeder and the water. These "contact modes" are important because they determine how the molten metal and water will hydrodynamically mix and the energy and mass transfer rates between the materials. The first contact mode might occur after a tube rupture in a liquid-metal steam generator. One could identify this contact mode as "coolant injection" due to the high pressure injection of the steam/water into the low pressure liquid-metal (Fig. 1). The second contact mode would be characterized by pouring of the liquid-metal from a ruptured blanket component into a pool of water, also present due to the accident. This contact mode is identified as a "pouring contact mode." A "Melt-Coolant" interaction is a generic class of heat transfer phenomena in which one hot liquid, "melt," interacts with a more volatile cold liquid, "coolant," producing vapor and perhaps oxidizing the melt. Historically, this contact mode has been considered in fission reactor safety,

Fig. 1

STEAM GENERATOR TUBE RUPTURE



- HIGH PRESSURE TWO-PHASE BLOWDOWN

- LIQUID METAL ENTRAINED IN EXPANDING MIXING ZONE

although the other modes of contact are just as plausible. This contact may occur, in a fusion reactor, after a severe accident in which molten metal is poured from a ruptured component into a stagnant pool of water in the containment (Fig. 2). The third contact mode could be characterized by a rupture of water and breeder-blanket tubes in the vacuum vessel (i.e. torus or central cell), resulting in a spray of these reactants into a common volume (Fig. 3). This contact mode is of special concern in a fusion design because the major radioactive inventory resides within the vacuum vessel. One may consider this contact mode to be a subset of the previous two, because it is the simultaneous injection of the liquid-metal breeder and water into a common volume. The fourth contact mode would occur if the liquid-metal and the water came into contact as stratified layers of materials with different densities (e.g. lithium pouring on water, water pouring on lithium-lead). We expect this to be the most benign of the possible contact modes because even though the two materials are liquid, density stratification would initially limit their surface area for mixing.

This paper will be concerned only with modeling the first contact mode, coolant injection. A model for the second, metal pouring, has been presented elsewhere.[11] This mode was originally developed for fission reactor safety concerns,[12,13] and can be easily modified for a fusion reactor case. We plan to investigate the third and fourth contact modes in future work.

Background

For the coolant injection we specifically consider a steam tube rupture accident in a Westinghouse liquid-metal/water steam generator,[14] the specifications of which are given in Fig. 4. The model being developed predicts the temperature and pressure history and the hydrogen generation rate due to

Fig. 2

LIQUID METAL SPILL IN CONTAINMENT

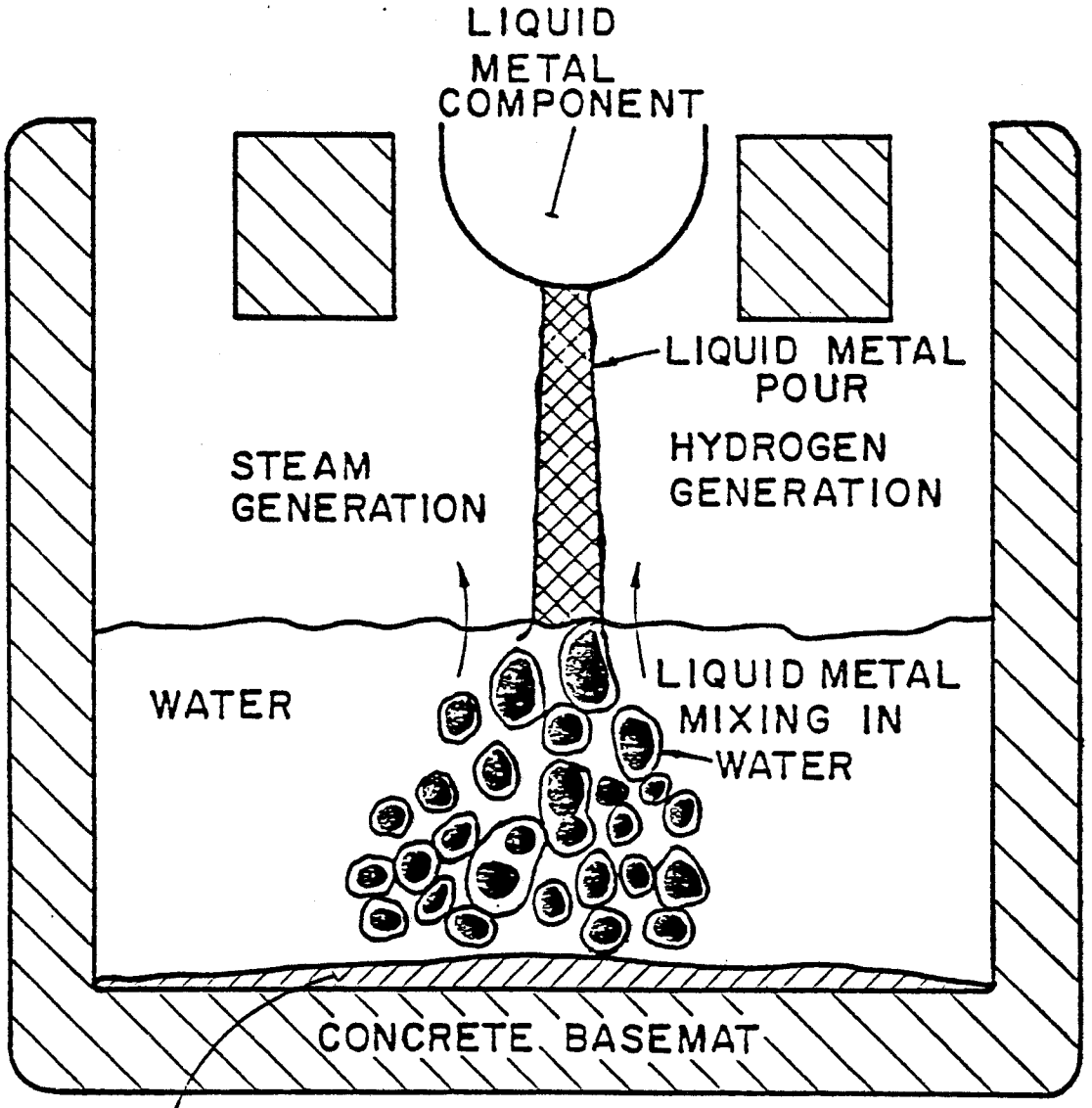
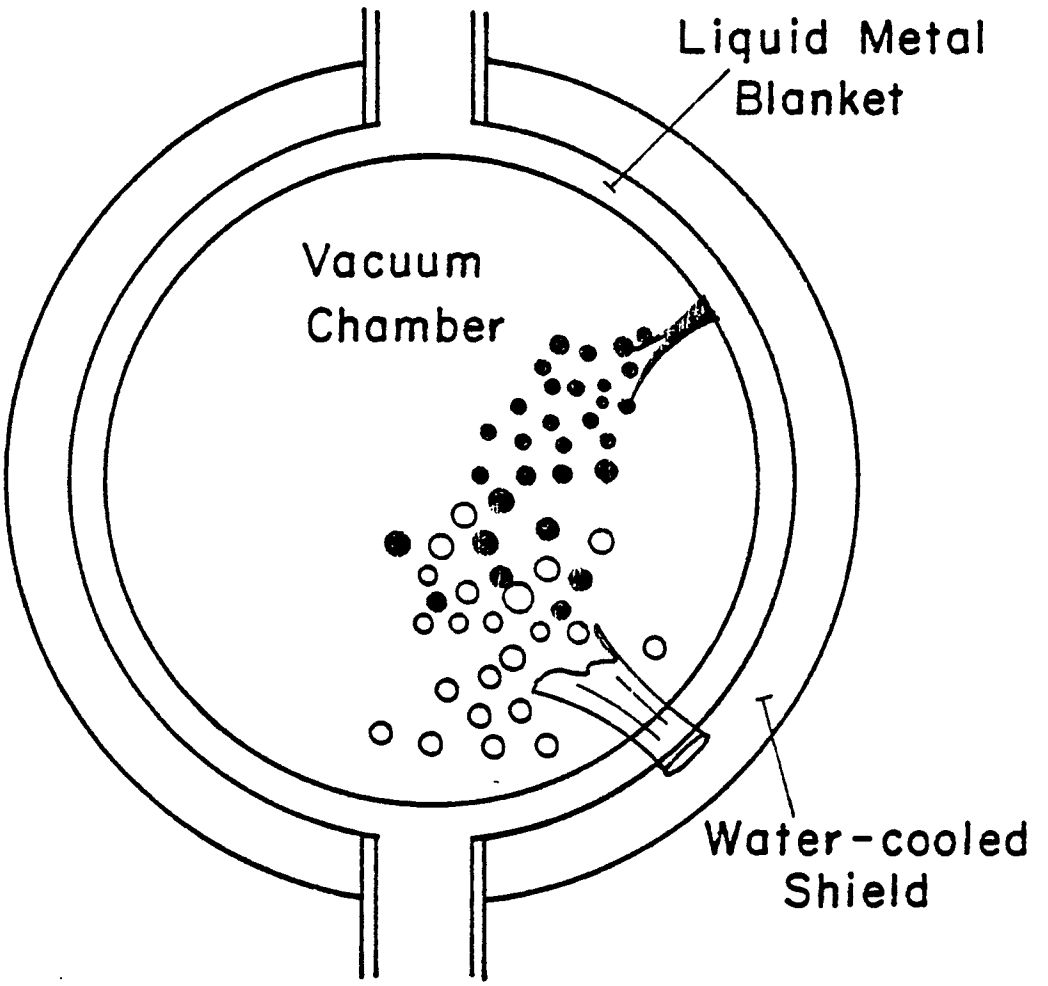


Fig. 3

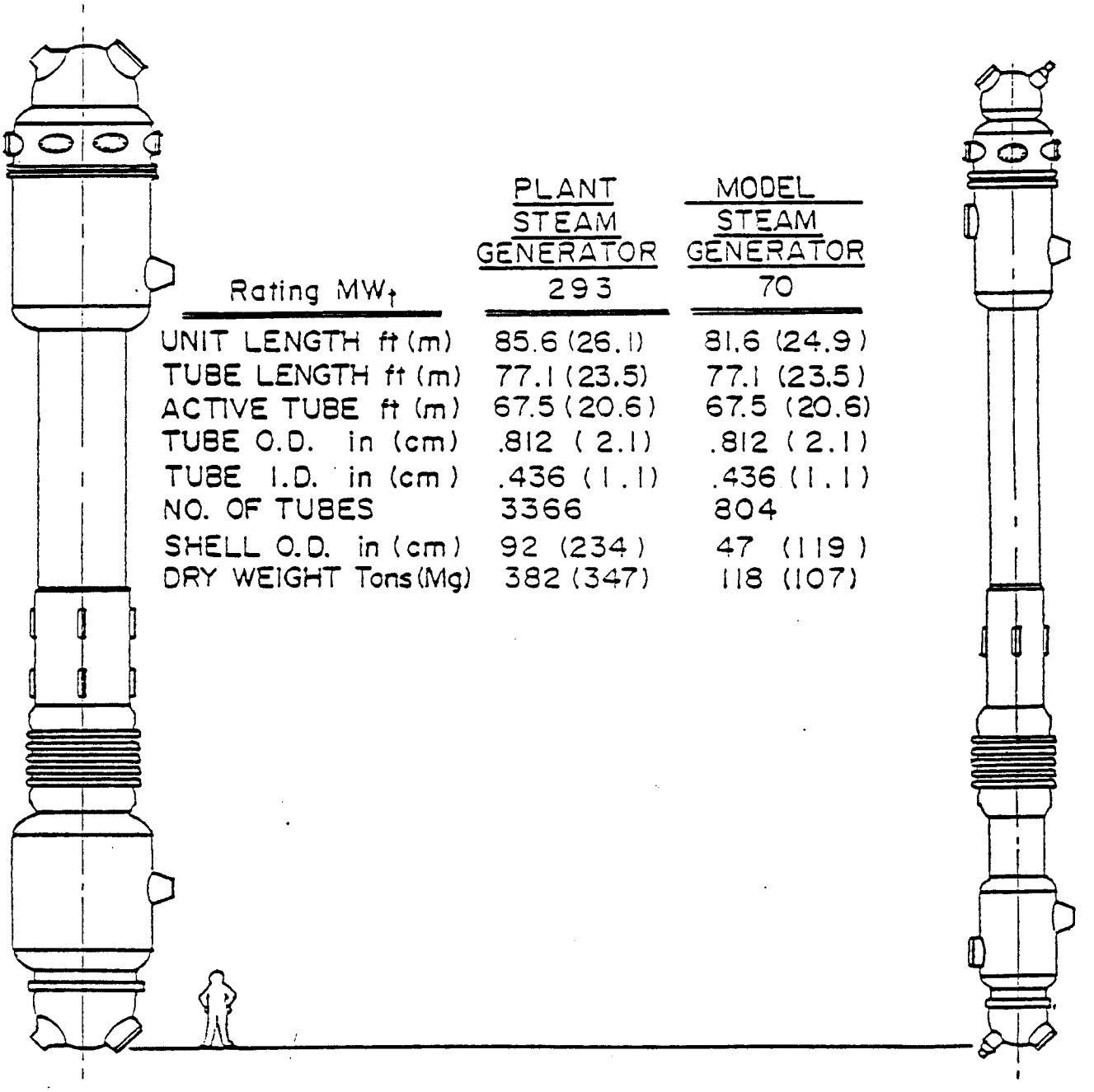
COOLANT LEAKAGE INTO VACUUM CHAMBER



- SIMULTANEOUS LEAKAGE OF TWO FLUIDS DUE TO A COMMON FAULT (e.g. SEISMIC EVENT)
- MIXING OF FLUIDS IS HIGHLY SITUATION DEPENDENT AND PROBABLY VERY LIMITED
- THIS CONTACT MODE CAN BE EXCLUDED FROM FURTHER CONSIDERATION

Fig. 4

WESTINGHOUSE STEAM GENERATOR



Rating MW_t	PLANT STEAM GENERATOR 293	MODEL STEAM GENERATOR 70
UNIT LENGTH ft (m)	85.6 (26.1)	81.6 (24.9)
TUBE LENGTH ft (m)	77.1 (23.5)	77.1 (23.5)
ACTIVE TUBE ft (m)	67.5 (20.6)	67.5 (20.6)
TUBE O.D. in (cm)	.812 (2.1)	.812 (2.1)
TUBE I.D. in (cm)	.436 (1.1)	.436 (1.1)
NO. OF TUBES	3366	804
SHELL O.D. in (cm)	92 (234)	47 (119)
DRY WEIGHT Tons (Mg)	382 (347)	118 (107)

an assumed guillotine break of a steam tube and the resulting liquid-metal/water chemical reaction. The model is applied to both a lithium and lithium-lead breeder in order to obtain a general comparison between these two candidate breeder-blanket materials. We also present a reliability and availability analysis for the steam generator in Appendix A.

In 1981, Krane and Kazimi[1] compared lithium and lithium alloy/water reactions for a hypothetical coolant tube leak in the blanket of the University of Wisconsin NUWMAK conceptual fusion reactor. They first performed a thermodynamic calculation where the breeder and coolant were allowed to interact instantaneously and then determined the final equilibrium temperature of the blanket materials, based on a stoichiometric amount of water and breeder, with a variable degree of completion of the chemical reaction (0 to 100%). Next, a dynamic calculation was performed in which the LITFIRE computer program[1] was modified to predict the thermal response of the blanket materials. The calculation was based on a specified flow rate of water (0.2 kg/s) into a constant volume, spherically shaped reaction zone, in which the reaction occurred and the reaction products remained. They determined the temperature response of concentric shells of the undisturbed breeder material and used the resulting temperature profiles as the basis for their qualitative comparison of the hazard potential of different lithium-alloy based breeders. The analysis did not vary the leakage rate of coolant into the breeder and neglected the pressure transient within the breeder zone. This analysis was therefore most applicable for very slow leaks over the long time spans.

Our current investigation extends this preliminary work. We begin with a thermodynamic equilibrium calculation to determine the final temperature of a mixture of lithium, lithium-lead and water. We generalize this calculation so

that it only depends upon the initial molar ratio of water to lithium in the mixture and not on any absolute amount of water or liquid-metal. A dynamic calculation is then performed using a parametric model to predict the consequences of a steam tube rupture. Our parametric model allows for a number of effects:

1) a dynamic reaction zone volume,
2) variable liquid-metal/water mixture ratios,
3) a dynamic pressure calculation,
4) pressure relief valve flow out of the steam generator,
4) a critical flow model for the tube rupture break flow.

In the next section, we discuss the thermodynamic equilibrium model followed by a discussion of the model and the current results. Finally, some current thoughts on the mechanism for liquid-metal/water chemical reactions are presented.

Thermodynamic Equilibrium Model

The stoichiometric chemical reaction for lithium with water is

$$Li + H_2O \rightarrow LiOH + \frac{1}{2} H_2 - 49 \frac{kcal}{gmole\ of\ Li} \qquad (@\ 25^0C) \tag{1}$$

and for lithium-lead with water

$$Li_{17}Pb_{83} + 0.17\ H_2O + i_f \rightarrow 0.17\ LiOH + 0.085\ H_2 + 0.83\ Pb$$
$$- 8.33 \frac{kcal}{gmole\ of\ Li_{17}Pb_{83}} \qquad (@\ 25^0C) \tag{2}$$

where i_f is the heat of formation of $Li_{17}Pb_{83}$ (see nomenclature). The thermo-

dynamic equilibrium modeling determined, for various amounts of liquid-metal and water, the final equilibrium temperature of the products and any remaining reactants; assuming that the energy generated by the reaction does not leave the "fuel-coolant" system. The initial temperature of the reactants is given by the average temperature of the metal breeder and water in the steam generator (for the MARS fusion design, 400°C for the metal at 1.7 bars and 375°C for the water at 170 bars). To determine the final equilibrium temperature of the system, we simply balance the energy of the reactants and the products of the above reactions, for a given ratio of initial moles of lithium to moles of water (defined as the parameter $x \equiv n_{H_2O}/n_{Li}$). Given x, one can solve for the final equilibrium temperature regardless of the absolute amount of reactants. The energy balance has three forms depending on whether $x < 1$, $x = 1$, or $x > 1$. For the lithium breeder the three balances are

$$C_L[T_{B_0} - T_0] + xi_{wo} = [C_{LH} + C_H][T_f - T_0] + Q + [x - 1]i_{wf} \qquad \text{for } x > 1 \quad (3a)$$

$$C_L[T_{Bo} - T_0] + i_{wo} = [C_{LH} + C_H][T_f - T_0] + Q \qquad \text{for } x = 1 \quad (3b)$$

$$C_L[T_{Bo} - T_0] + xi_{wo} = x[C_{LH} + C_H][T_f - T_0] + xQ + [1 - x]C_L[T_f - T_0] \qquad \text{for } x < 1 \quad (3c)$$

The equations for lithium-lead are similar in form to these.

The results of this calculation are shown in Figs. 5 and 6, for the final equilibrium temperature (T_f) as a function of the parameter x for lithium and lithium-lead.

FIGURE 5

THERMODYNAMIC EQUILIBRIUM TEMPERATURE (T_f) vs. X FOR Li BREEDER

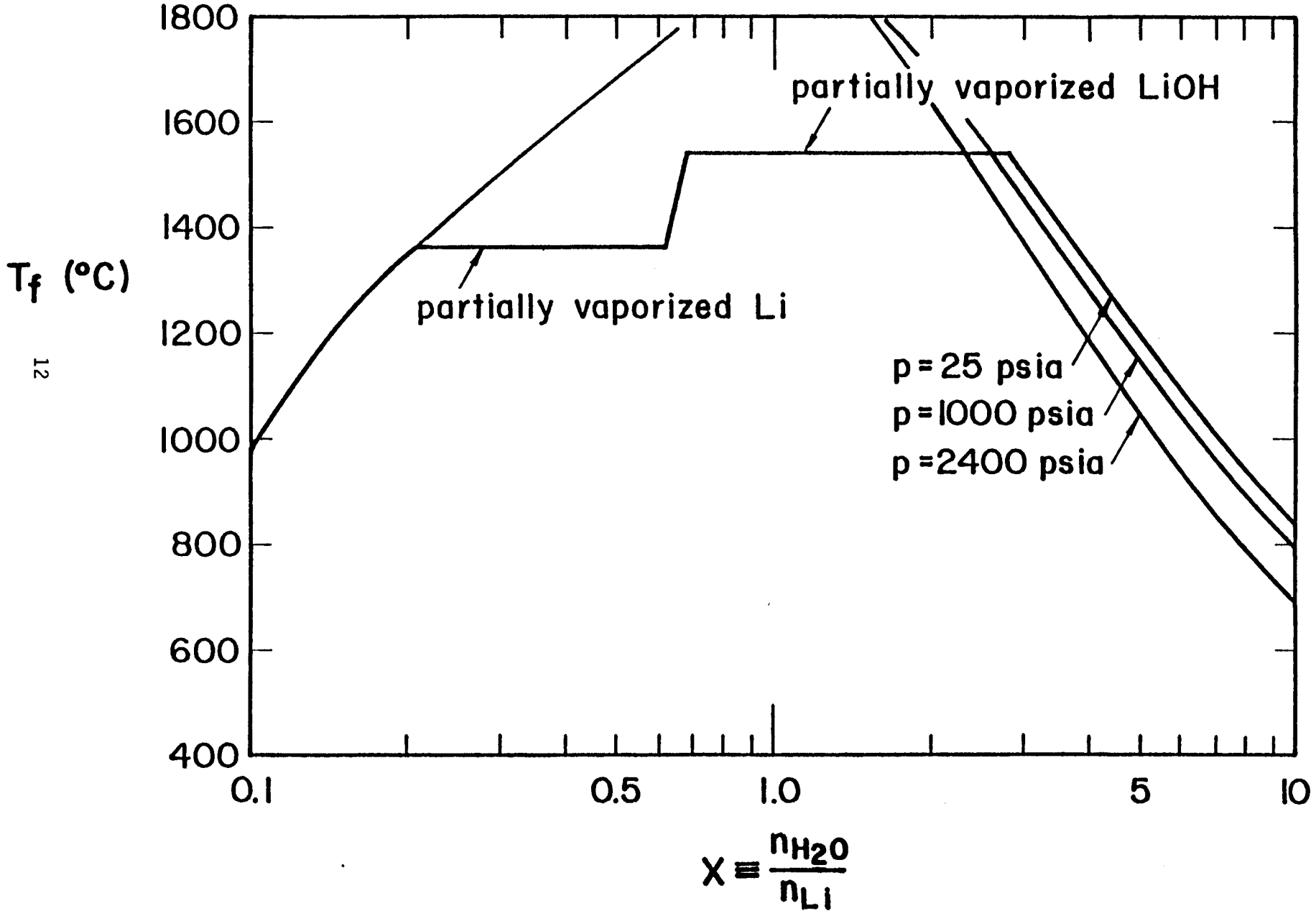
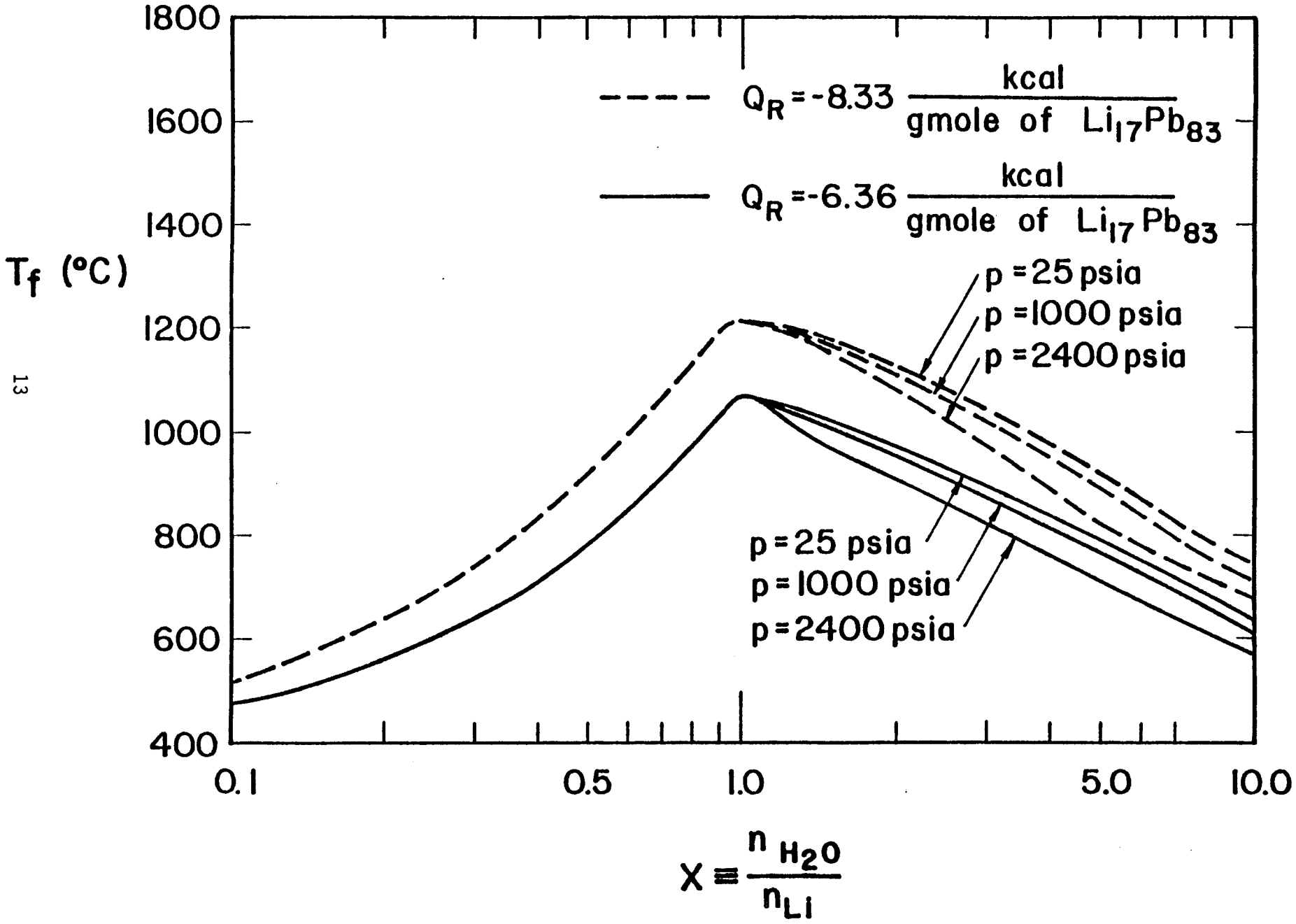


FIGURE 6

THERMODYNAMIC EQUILIBRIUM TEMPERATURE (T_f) vs. X FOR $Pb_{83}Li_{17}$ BREEDER



In Fig. 5 the constant equilibrium temperature indicates 1.7 bars where lithium and lithium hydroxide begin to vaporize (25 psia). This calculation would produce higher equilibrium temperatures as the pressure in the vicinity of the interaction increases; e.g. for a high pressure of 170 bars the peak equilibrium temperature would be 3800°C. The $Li_{17}Pb_{83}$ energy balance was carried out for two values of the heat of reaction (Q). One of the values of Q (-8.33 kcal/(gmole of $Li_{17}Pb_{83}$)) is arrived at by assuming that the heat of formation of $Li_{17}Pb_{83}$ (i_f) is negligible. The other value of Q (-6.36 kcal/(gmole of $Li_{17}Pb_{83}$)) is arrived at by including an estimate of the heat of formation, i_f. This estimate of the heat of formation of $Li_{17}Pb_{83}$ is given by

$$i_f = \Delta G + T\Delta S \tag{4}$$

where G is the Gibbs free energy and S is the entropy as calculated by E.M. Larsen.[15]

This thermodynamic calculation provides an upper bound on the mixture in the reaction zone of the steam generator, due to a steam tube rupture. Comparison of Figs. 5 and 6 shows that the lithium-lead may produce substantially lower temperatures than lithium, primarily due to the much larger thermal inertia of the lead. Also, the liquid lithium may produce substantial system pressure increases due to vaproization of the lithium or lithium-hydroxide for a constant volume situation. The possible vaporization of Li or LiOH from using a pure lithium breeder would pose additional safety hazards as lithium and associated radioactivity may take the form of mobile aerosols.

Dynamic Parametric Model

The model for the coolant injection contact mode is applied to a Westinghouse liquid-metal steam generator.[14] This design is the most logical choice, since Westinghouse is currently involved in the component development of a large prototype steam generator for LMFBR applications and fusion systems.

The Westinghouse "duplex tube" design (Fig. 4) utilizes double walled tubes with a helium gas at the interface of the two tubes, that can be used for detection of small leaks in either tube. The MARS design requires that 2840 MW of energy from the blanket be transferred across the steam generator with a temperature drop of 350° to 300°C. Since the design power rating of the Westinghouse steam generator is 293 MW, the MARS power station would require ten steam generators of this design. The large number of plant steam generators, although more expensive than a smaller number, would reduce the hazard of steam generator accidents, by confining the accident to a single generator and isolating the extent of damage and cleanup or replacement costs.

The steam generator accident modeled is one in which there is a sudden and complete rupture of a steam tube ("guillotine break"), essentially leaving two water flow paths into the liquid-metal. Since the water is at a much higher pressure than the metal breeder (170 versus 1.7 bars), the mode of contact between the liquid-metal breeder and the water is high pressure coolant injection. For our current calculations, our model contains these major assumptions:

1) We base our calculations on the MARS design parameters. The initial pressure of the reactants is 17. MPa for the water and 0.17 MPa for the

breeder. Also, the intial shell side, liquid-metal breeder volume and temperature are taken to be 2.78×10^7 cm^3 and 673 K, respectively.

2) There are two interaction zones. The first zone, designated the Reaction Zone, is assumed to be a spherically shaped region that forms around the break. This zone is a homogeneous mixture of reactants and products at thermal equilibrium, which can grow in time. The other zone, designated the Nonreaction Zone, consists of the rest of the shell side of the steam generator. This zone is assumed to be a homogeneous region of unreacted liquid-metal breeder at thermal equilibrium.

3) The flow rate of water into the reaction zone is modeled by the one-dimensional homogeneous equilibrium model (HEM) for critical flow, i.e.

$$S_{wo} = S_{wb} \tag{5}$$

$$V_{wb} = [2(i_{wo} - i_{wb})]^{1/2} \tag{6}$$

$$\dot{m}_w = A_b \rho_{wb} v_{wb} \tag{7}$$

where the enthalpy at the break location, i_{wb}, is found knowing S_{wb} and P_{wb}.

4) The flow of the liquid-metal breeder into the reaction zone is determined by a mixing parameter x. x is defined as the ratio of the molar flow rate of water to the molar flow rate of lithium into the reaction zone.

5) The reactants, including hydrogen, remain in the reaction zone.

6) The system pressure is maintained below 170 bars (the water back pressure) by a pressure relief valve. This is accomplished by allowing a portion of

the unreacted liquid-metal breeder to leave the nonreaction zone each timestep through the valve. The flow rate out through the valve is modeled by a quasi-steady mechanical energy balance (Bernoulli's equation)

$$\dot{m}_{bp} = \rho_b A_{prv} \left[\frac{2}{K\rho_b} (P - P_\infty)\right]^{1/2} \tag{8}$$

where K is the loss coefficient through the valve (isentropic would be K = 1).

7) We assume that the increase in pressure in the shell side of the steam generator suspends the normal flow of the metal through the steam generators.

8) There is no back flow through the broken steam tubes.

9) The thermodynamic and transport properties of the liquid-metal reactants and products are assumed to be simple functions of temperature. The liquids are incompressible. The gases are perfect. For $x > 1$, any unreacted water is assumed to be superheated steam.

This parametric model is the next logical step beyond a simple thermodynamic calculation. We employ two control volumes and a specified mixing parameter in order to keep the modeling of the dynamic process relatively simple and unambiguous; this seems justified because our current knowledge of the mechanisms of liquid-metal/water interactions is so limited. Consistent with this approach is the use of a 1-D HEM critical flow model for water inflow and a quasi-steady mechanical energy balance for liquid-metal outflow. Because the pressure transient within the shell side of the steam generator is expected to be large but less than the 170 bar in the water, assumptions 7 and 8 are quite reasonable. Because the transient caused by the tube rupture occurs over such

short times (1 s) the retention of H_2 in the reaction zone is reasonable (assumption 5). Finally, the simple equations of state for liquid-metal and water are known to be approximate; subsequent calculations will investigate the effect of using more complete equations of state.

Using the mixing parameter, x, and the relief valve area, A_{prv}, as variables and the above assumptions, we solve the following mass and energy balances:

Reaction zone mass balance

$$\frac{dm_R}{dt} = \dot{m}_{br} + \dot{m}_w \ . \tag{9}$$

Reaction zone energy balance

$$\frac{dE_R}{dt} = -Q_c - Q_r - p\frac{dV_r}{dt} + \dot{m}_{br} i_b + \dot{m}_w i_w \tag{10}$$

where the reaction zone forced convection heat transfer (Q_r) to the unbroken coolant tubes is given by

$$Q_r = h_t A_{t_r}(t)(T_r - T_w) \ . \tag{11}$$

The convective heat transfer coefficient, h_t, is calculated based on the shell and tube side flow and the heat transfer resistance across the steel tubes; the steel tube dominates the heat transfer resistance. The conductive heat transfer between the reaction zone and the nonreaction zone (Q_c) is given by

$$Q_c = 4\pi R^2 \frac{kn}{\lambda}(T_r - T_n) \ . \tag{12}$$

The penetration depth, λ, is the conduction length scale from boundary layer theory. The area, $4\pi R^2$, is based on the assumption of a spherical reaction zone.

The nonreaction zone mass balance is

$$\frac{dm_n}{dt} = -\dot{m}_{br} - \dot{m}_{bp} , \tag{13}$$

and the nonreaction zone energy balance is

$$\frac{dE_n}{dt} = Q_c - Q_n - p\frac{dV_n}{dt} - \dot{m}_{br} i_b - \dot{m}_{bp} i_b \tag{14}$$

where the nonreaction zone forced convection heat transfer, Q_n, to the unbroken coolant tubes is given by

$$Q_n = h_t A_{t_n}(t)(T_n - T_w) . \tag{15}$$

The areas A_{t_r} and A_{t_n} in Eqs. (11) and (15) sum up to the total tube surface area. One should note that the energy balances include the heat of formation of each constituent and therefore automatically include the heat of reaction from the oxidation of lithium.

Approximating the differentials by finite difference techniques, we have written a computer program that explicitly calculates shell side pressure, reaction and nonreaction zone temperature, and the hydrogen mass generated, all as functions of time from the accident initiation. For information concerning the use and structure of the computer program, the reader is referred to Appendix B.

In Fig. 7, we have plotted the system pressure as a function of time for three different values of the pressure relief valve area, A_{prv}. This parameter is used to determine the flow rate of unreacted liquid-metal breeder out of the system by Eq. (8). A comparatively small value of A_{prv} would mean a comparatively small flow rate of unreacted liquid-metal breeder out of the system, and little pressure relief. This is illustrated in Fig. 7 by comparing the top curve (A_{prv} = 0.005 m^2) with the other two curves (A_{prv} = 0.01 m^2 and A_{prv} = 0.05 m^2). One notes that the system pressure quickly approaches the limiting pressure of the high pressure water (17 MPa), for smaller values of A_{prv}. Another trend illustrated in this, and which is exhibited in the results of every calculation, is that the system pressure quickly (< 1 x 10^{-4} s) reaches a maximum pressure (P_{max}), and levels off near P_{max} for the early part of the calculation. In Fig. 8, we have plotted the maximum system pressure as a function of A_{prv} for both lithium and lithium-lead liquid-metal breeders. The similar shape of the two curves in this figure indicates a relationship between the lithium and lithium-lead. From Eq. (8), the flow rate of unreacted liquid-metal breeder out of the system ($\dot{m}_{bp}$) is proportional to A_{prv} and the square root of the liquid-metal breeder density (ρ_b)

$$\dot{m} \propto A_{prv}(\rho_b)^{1/2} \quad . \tag{16}$$

If the abscissa of Fig. 8 was $\rho_b^{(-1/2)}A_{prv}$ instead of A_{prv}, the two curves would be coincident. This similarity in behavior for the two liquid-metal breeders is demonstrated in Fig. 9.

The liquid-metal/water interaction with a fixed value of x is governed by the pressure response. This is because the flow rate of water into the re-

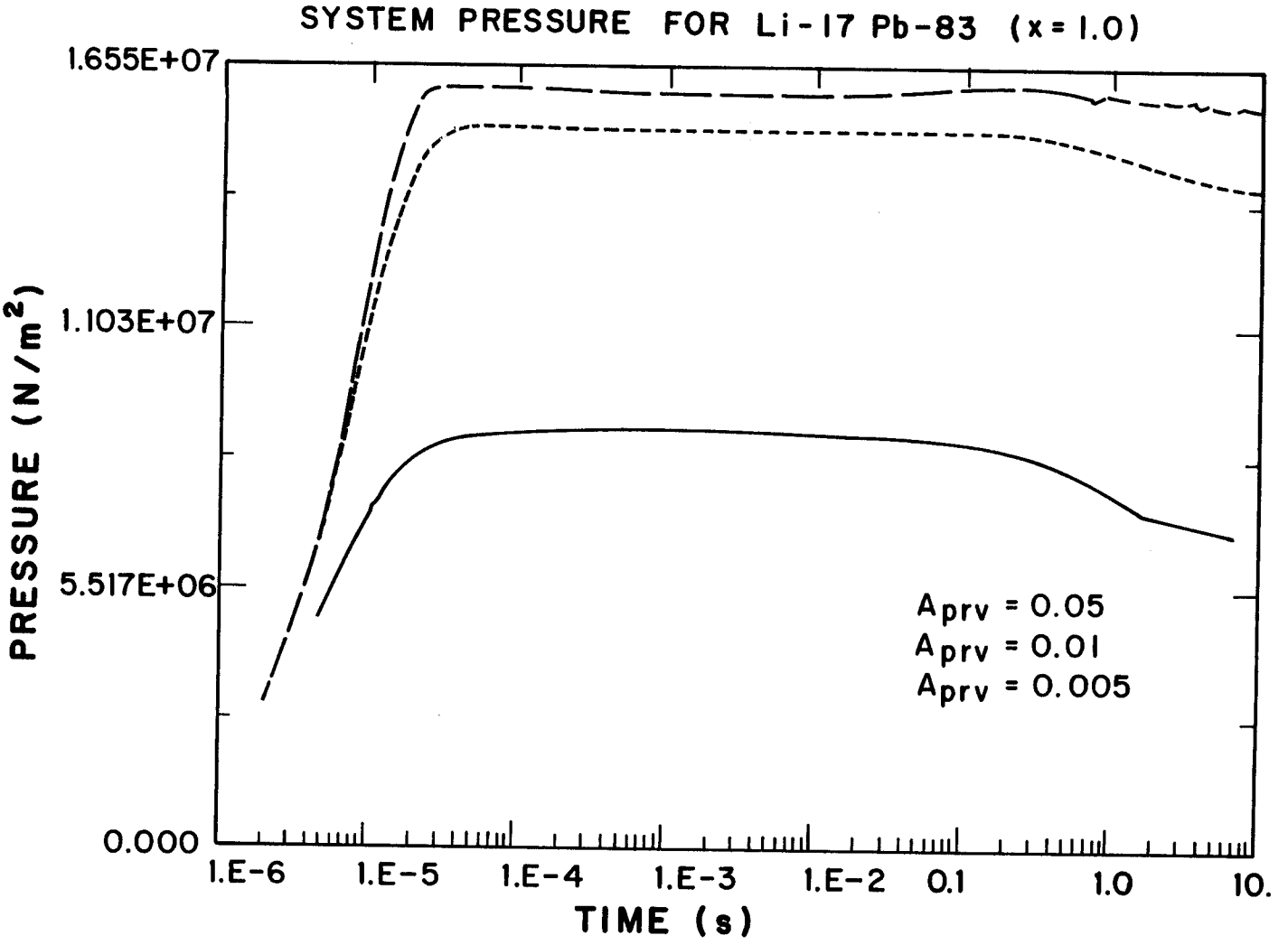

SYSTEM PRESSURE FOR Li-17 Pb-83 (x = 1.0)
1.655E+07
1.103E+07
5.517E+06
0.000
PRESSURE (N/m²)
1.E-6
1.E-5
1.E-4
1.E-3
1.E-2
0.1
1.0
10.
TIME (s)
Aprv = 0.05
Aprv = 0.01
Aprv = 0.005

Figure 7

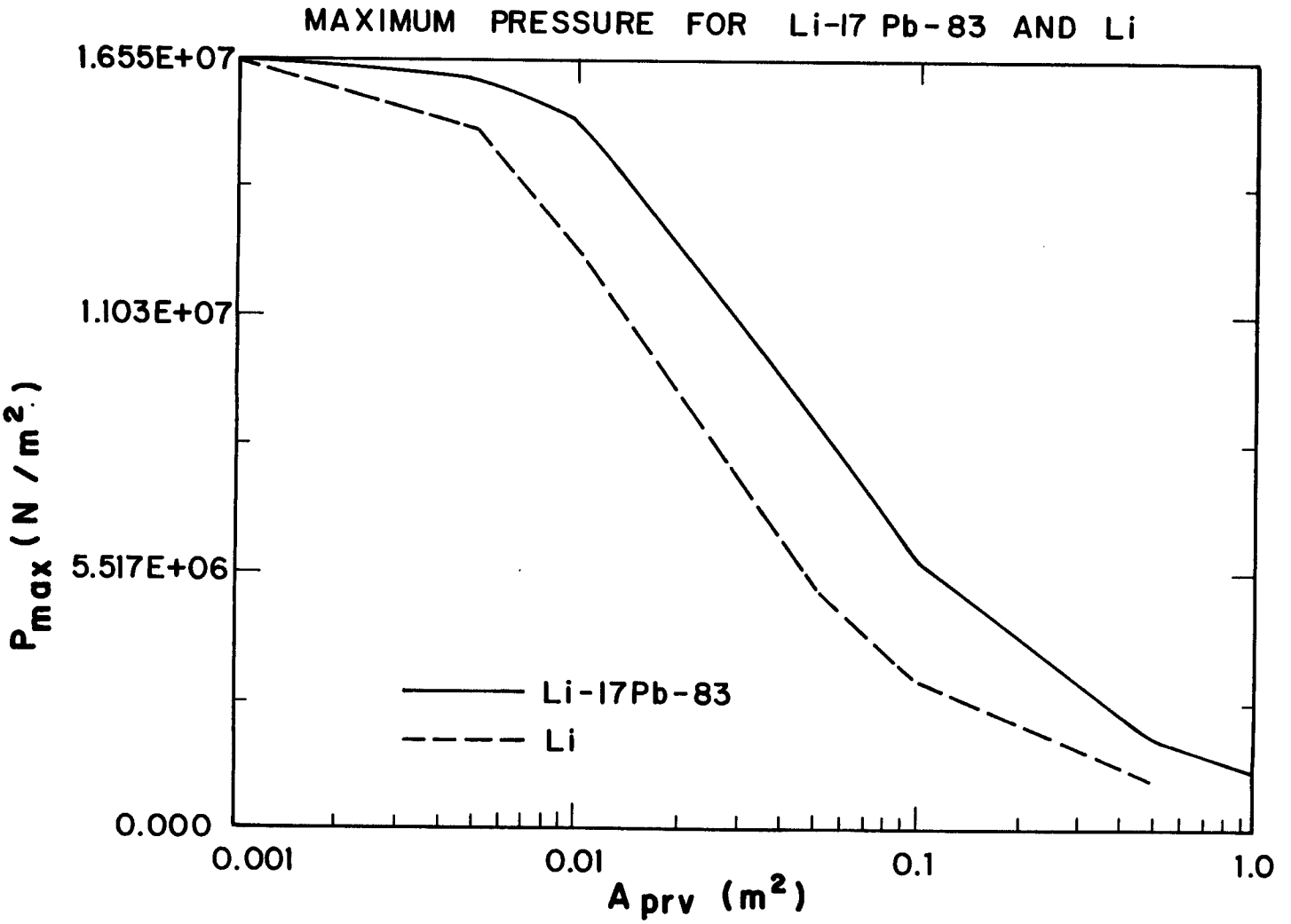

MAXIMUM PRESSURE FOR Li-17 Pb-83 AND Li
1.655E+07
1.103E+07
5.517E+06
0.000
P max (N / m²)
Li-17Pb-83
Li
0.001
0.01
0.1
1.0
A prv (m²)

Figure 8

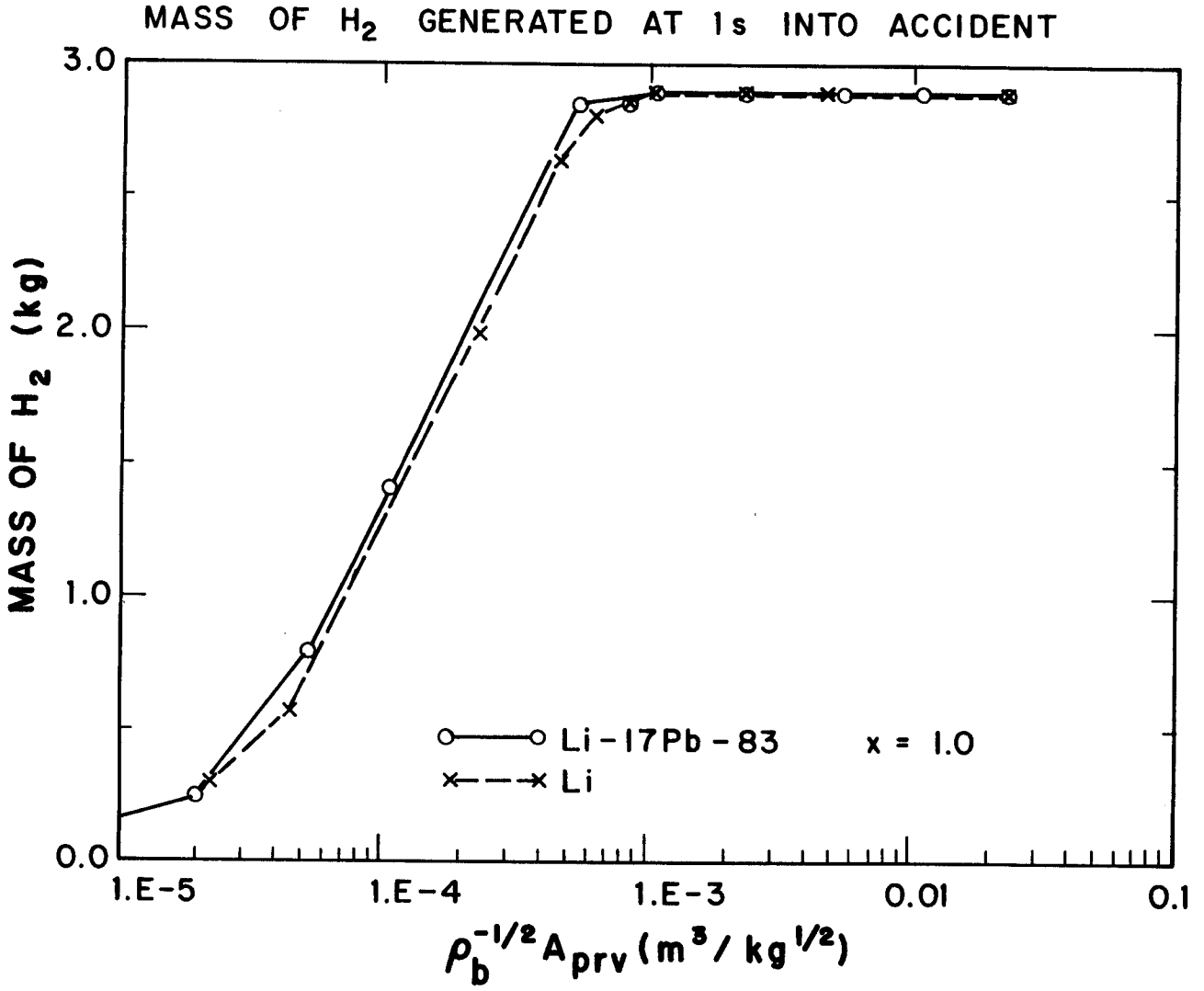

MASS OF H_2 GENERATED AT 1s INTO ACCIDENT
MASS OF H_2 (kg)
3.0
2.0
1.0
0.0
1.E-5
1.E-4
1.E-3
0.01
0.1
$\rho_b^{-1/2} A_{prv}$ (m^3 / $kg^{1/2}$)
Li-17Pb-83
x = 1.0
Li

Figure 9

action zone (and thus the flow rate of liquid-metal breeder through x) is a function of the system pressure. The flow rate of unreacted liquid-metal out of the system is also a function of the system pressure. Thus, the flow rates into and out of the system are coupled together through the pressure history. For a constant mixing parameter (e.g., x = 1) the integral pressure behavior and hydrogen generated into lithium or lithium-lead is very similar. If we attempt to determine the mechanistic amount of hydrogen generated this preliminary conclusion might be altered. However, at this point in our modeling of the melt-water interaction we do not feel there would be a large difference in the amount of lithium reacted with water for Li or LiPb. The reason is that the water is injected into an almost infinite sea of liquid metal and probably has enough time to completely chemically react. A variance in the mixing parameter to more realistic values may alter the peak temperatures and pressures calculated in the reaction zone, but not the degree of chemical reaction; i.e. all the water is reduced to hydrogen.

One would not expect the temperature response of the two liquid-metal/water pairs to be similar because of the lower thermal inertia of lithium.

In Fig. 10, we have plotted the temperature of the reaction zone (T_r) and the temperature of the nonreaction zone (T_n) as functions of time, for a typical calculation. This figure illustrates representative trends in the two temperatures, regardless of the values of the parameters X and A_{prv} or the choice of the liquid-metal breeder. The trend in the reaction zone teperature is that it reaches its maximum temperature ($T_{r_{max}}$) very early in the calculation, and then steadily decreases to an asymptotic temperature (648 K). The trend in the nonreaction zone temperature is that it steadily decreases from its initial temperature (673 K) to an asymptotic temperature (648 K). This

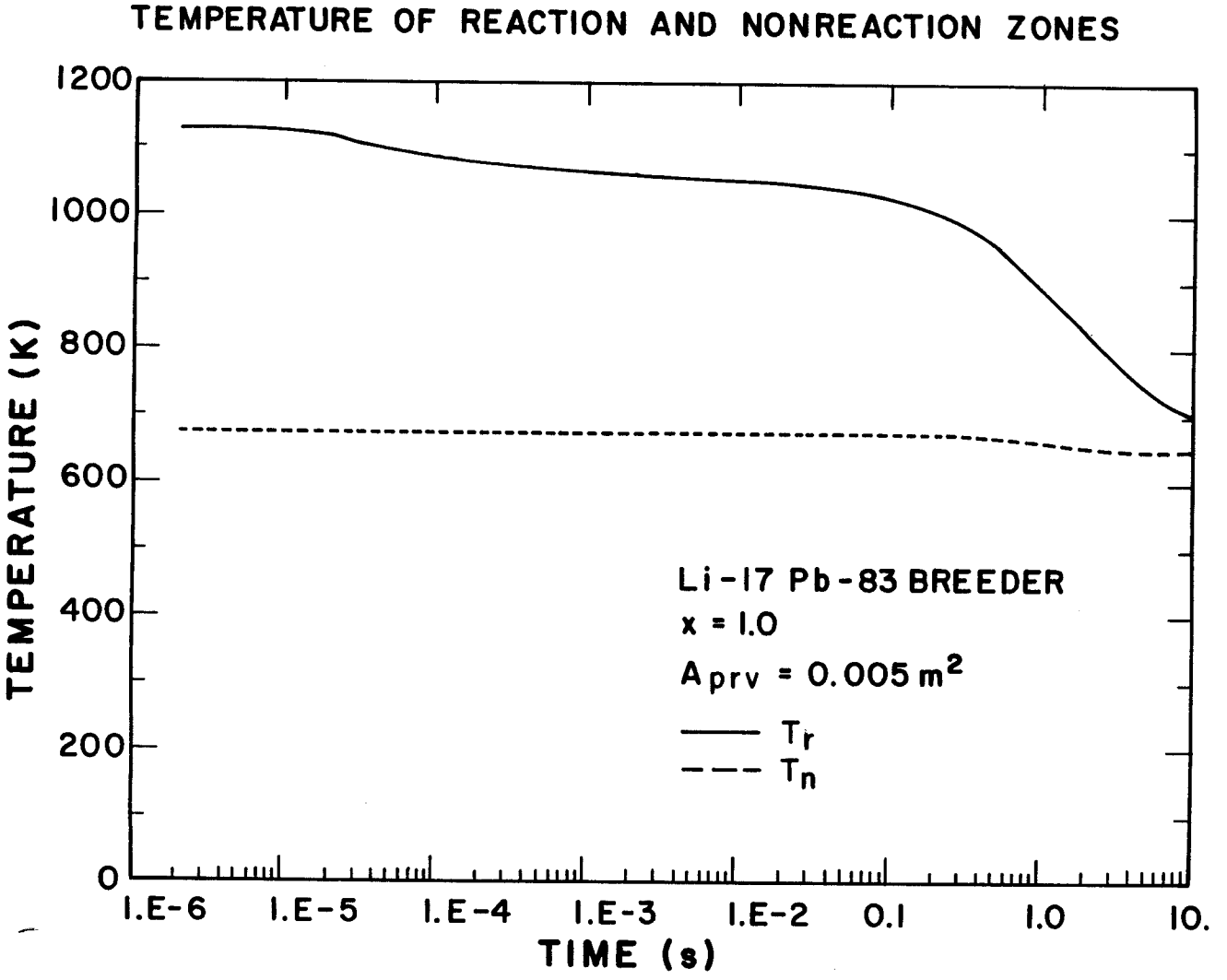

TEMPERATURE OF REACTION AND NONREACTION ZONES
1200
1000
800
600
400
200
0
TEMPERATURE (K)
Li-17 Pb-83 BREEDER
x = 1.0
A prv = 0.005 m2
Tr
Tn
1.E-6
1.E-5
1.E-4
1.E-3
1.E-2
0.1
1.0
10.
TIME (s)

Figure 10

asymptotic temperature is the ambient temperature of the water in the unbroken steam temperature. This shows that the energy from the exothermic reaction is quickly and effectively removed from the system by forced convection through the unbroken steam tubes. This occurs because the accident suspends the normal flow of liquid-metal breeder through the steam generator due to the rapid pressure buildup. The normal function of the steam generator, which is the transfer of the energy of the liquid-metal breeder, is thus diverted to transfer of the chemical heat of the reaction. The reason that the maximum reaction zone temperature is reached early is because the amount of the reaction products in the reaction zone is at a minimum. Therefore, the amount of heat absorbed by the reaction products is also at a minimum.

Figure 11 presents the temperature history of the reaction zone, T_r, for lithium and lithium-lead liquid-metal breeders, for the same values of X and A_{prv}. The peak lithium temperature is significantly higher than the peak lithium-lead temperature. The major reason is again the large thermal storage capacity of lithium-lead compared to lithium. This peak temperature for lithium is above the melting point of the stainless steel (~ 1800 K). When the reaction zone temperature decreases to 1800 K (in roughly 10 ms), the reaction zone volume is approximately 0.01 m^3. Assuming a spherical reaction zone, this corresponds to a reaction zone radius of 0.13 m. Because the steam tube pitch is 0.037 m, the high reaction zone temperature may cause failure of surrounding tubes causing the tube rupture to propagate to surrounding steam tubes. This would not be the case for lithium-lead, because the reaction zone temperature is far below the steel melting point.

In Fig. 12, we have plotted the maximum reaction zone temperature as a function of the mixing parameter x, for lithium-lead. Comparing Fig. 12 to

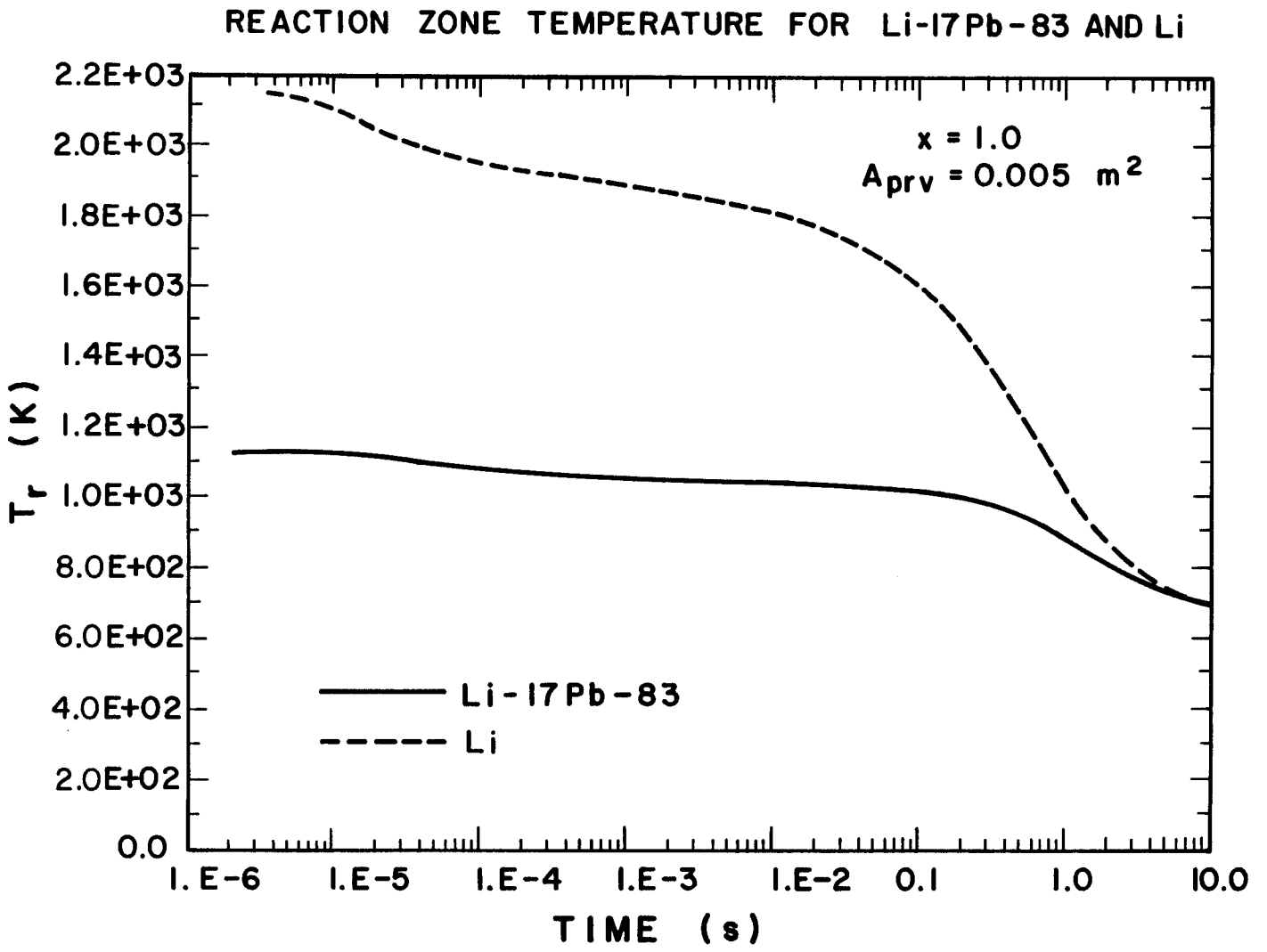

REACTION ZONE TEMPERATURE FOR Li-17Pb-83 AND Li
2.2E+03
2.0E+03
1.8E+03
1.6E+03
1.4E+03
1.2E+03
1.0E+03
8.0E+02
6.0E+02
4.0E+02
2.0E+02
0.0
T_r (K)
x = 1.0
A_{prv} = 0.005 m^2
Li-17Pb-83
Li
1.E-6
1.E-5
1.E-4
1.E-3
1.E-2
0.1
1.0
10.0
TIME (s)

Figure 11

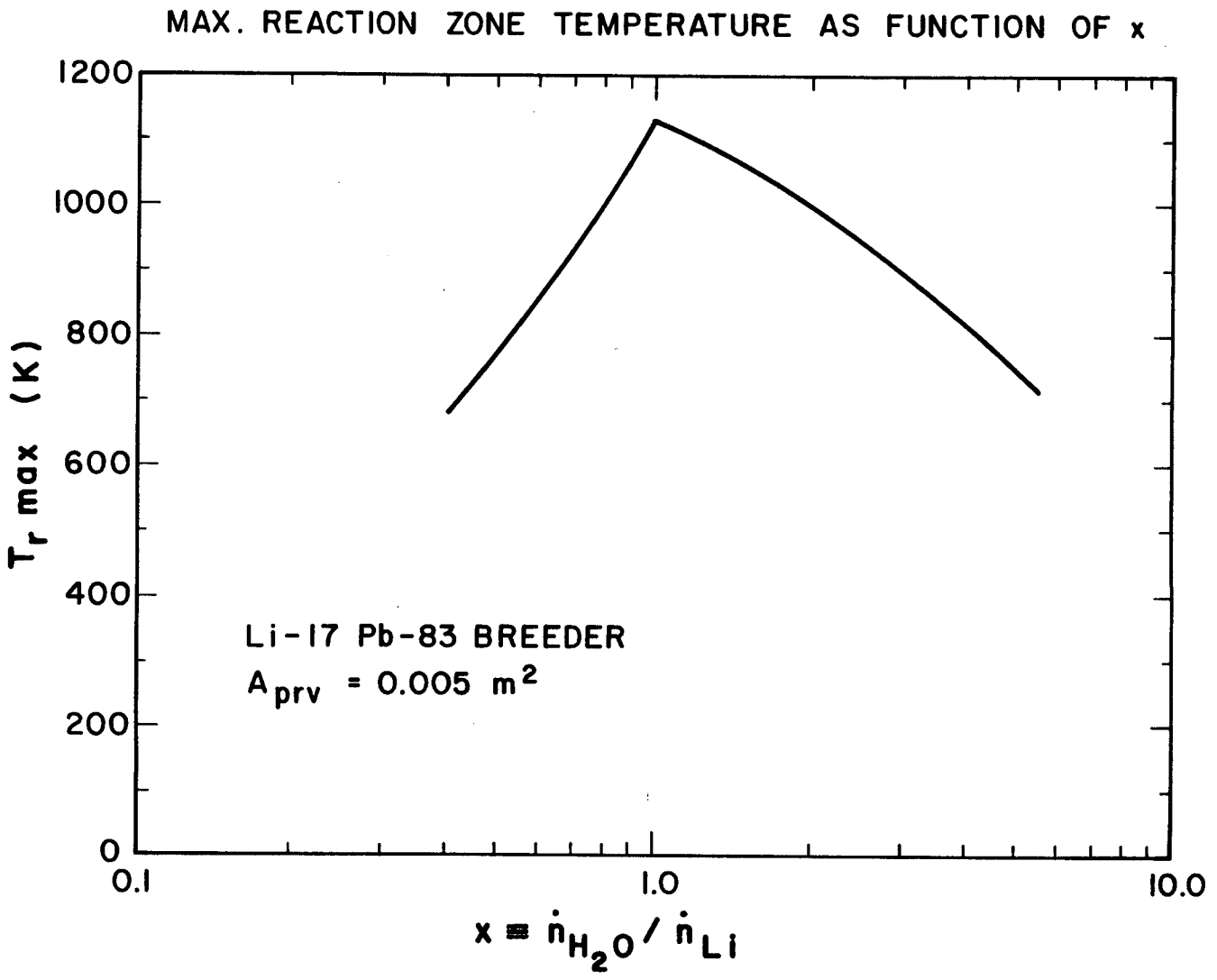

MAX. REACTION ZONE TEMPERATURE AS FUNCTION OF x
1200
1000
800
600
400
200
0
T_r max (K)
Li-17 Pb-83 BREEDER
A_{prv} = 0.005 m^2
0.1
1.0
10.0
$x \equiv \dot{n}_{H_2O} / \dot{n}_{Li}$

Figure 12

Fig. 6 (Q_R = -6.36 kcal/(gmole of $Li_{17}Pb_{83}$)), one sees that both the parametric model and thermodynamic equilibrium model exhibit the same variation in temperature as a function of x. The main difference, as exhibited in these two figures, is that the parametric model predicts lower temperatures than the thermodynamic equilibrium model. The reason for this is that the parametric model allows energy to flow out of the system through the pressure relief valve and through convection to unbroken steam tubes, while the thermodynamic equilibrium model has no provision for energy transfer from the system. The reason that the curves in Fig. 12 and Fig. 6 exhibit the same temperature response as x varies, is that because if x is greater than 1, some of the water entering the reaction zone does not react but absorbs energy from the reaction; and likewise, if x is less than 1, some of the lithium or lithium-lead entering the reaction zone does not react but absorbs energy from the reaction.

Considerations for Liquid-Metal/Water Reactions

Given a mixing ratio between the liquid metal (Li or $Li_{17}Pb_{83}$) and water, the parametric model indicated that the pressure history and hydrogen generated are quite similar. The temperature history of each is different, although both are below the thermodynamic limits. The next step in our work is to relax the assumption of a constant mixing parameter ratio, X, and investigate the fundamental rate mechanisms for liquid metal oxidation. In this way we can improve our chemical reaction modeling and more accurately determine if the amount of hydrogen generated is different for different lithium alloys under different contact modes. This may be an important consideration in determining the hydrogen inventory after an accident.

The amount of hydrogen generated during a liquid-metal/water interaction is the product of two physical processes; the first is the kinetic rate of reaction per unit surface area, and the second is the available metal surface area that evolves during the "fuel-coolant" interaction. Metal oxidation is practically limited by mass transfer in the gas and liquid (or solid oxide) phases near the metal surface.[17,18] In the gas phase, steam must diffuse through the evolved hydrogen to the liquid metal surface. If the chemical reaction is exothermic and the heat of reaction is large, the liquid metal surface will heat up substantially as it oxidizes until the liquid metal vapor pressure becomes significant causing substantial liquid metal vapor evaporation, oxidizing as it diffuses into the steam vapor. This vapor-phase oxidation of the liquid metal is the dominant mechanism of normal combustion processes; it has a very rapid oxidation rate. Liquid sodium oxidation is thought to be governed by this mechanism.[19]

Because of the low thermal inertia of lithium, it is quite possible that under certain circumstances lithium metal can overheat sufficiently and undergo "vapor-phase combustion."[19]

On the other hand, if the liquid metal vapor pressure is negligible at comparable temperatures as in the case of lithium-lead (the lithium chemical activity is 0.1% that in pure lithium), then steam vapor must diffuse to the metal surface through evolved hydrogen for liquid metal oxidation. Following past work,[17] the governing mass transfer equation for this process can be written in a general form for equimolar counterdiffusion of perfect gases (steam and hydrogen) as

$$\frac{dN_H}{dt} = A \frac{D_H}{R_0 T_V} \frac{dP_H}{dn} \qquad (15)$$

where: dN_H/dt is the molar rate of hydrogen diffusion in steam (mole/s)

D_H is the diffusion coefficient for steam and hydrogen

R_0 is the universal gas constant

P_H is the hydrogen partial pressure

T_V is the gas-vapor temperature

n is the outward directed normal

A is the surface area.

One can integrate this equation for a certain geometry, assuming a constant D_H for a pressure and a mean gas temperature.

The second mass transfer resistance, in the absence of "vapor-phase combustion," is the diffusion of oxygen atoms through the metal oxide (liquid or solid) to the unreacted metal. This diffusional process is quite complex; for example, for solid oxide being formed on the metal surface, the hydrogen generation rates are usually correlated from test data[18] under the boundary conditions that an excess of steam is present and the solid metal oxide resists further mass transfer. For zirconium,[18] the rate of reaction is given by a parabolic kinetic rate expression

$$\frac{d}{dt}(W^2) = 3.8(10^3)\exp\left(\frac{-84300}{R_0 T_V}\right) \tag{16}$$

where W is the cumulative mass of hydrogen in kg/m^2 and R_0 is given here in cal/gmole °K. Now for a liquid oxide the process is even more complex because the oxide may be miscible in the metal or the molten metal and oxide components could become mechanically mixed by internal convection currents. In this case, very little data exists for liquid metals.

At the present time there have been no controlled experiments that measure the kinetic rate of reaction for lithium or lithium based alloys' oxidation. Therefore, it is not yet clear what the reason is for the qualitatively less reactive behavior observed for lithium-lead as compared to lithium in scoping tests.[3-5] Our intention is to perform simple experiments to determine the rate of chemical reaction for these liquid metals.

The second physical process to consider is the available surface area for reaction that is evolved during liquid-metal/water contact. For this coolant injection mode of contact the water is depressurized as it flows out the break and begins to flash into steam as it reacts with the liquid metal. In the current model we consider the reaction zone to be spherical and to remain intact during the reaction. In reality though the water-steam mixture will break apart into individual bubbles and rise in the liquid metal. The available surface area then will be dictated by the breakup of the two-phase jet issuing forth from the break, and the rise time of the steam and water to the liquid metal surface at the top of the steam generator. In the current contact mode with a "large" inventory of liquid metal we would expect complete chemical reaction to be quite possible. We are now considering the modeling of the jet breakup and bubble transport to determine the limits of complete chemical reaction.

Conclusions

A parametric model was developed to predict the transient pressure and temperature behavior for a liquid-metal/water interaction in a steam generator following a steam tube rupture. The model results suggest two preliminary conclusions. First, the maximum temperature for lithium-lead during the reaction is not a safety concern for the steam generator, because it is below

the thermodynamic maximum value and the melting point of the steel tube and quickly falls to within operating limits. Second, the pressure history and hydrogen generated from water injection into lithium or lithium-lead are quite similar for a given value of the metal/water mixing parameter. This suggests that the pressure-flow characteristics govern the integral response given an assumed degree of chemical reaction. For a more accurate analysis, one must consider reaction kinetics for lithium and lithium-lead interactions; it is expected that lithium may be a "vapor phase combustion" process while lithium-lead is governed by metal surface mass transfer phenomena.

Acknowledgement

Support for this work has been provided by the U.S. Department of Energy through the EG&G Fusion Safety Program. Special thanks are extended to S. Piet for helpful suggestions and encouragement.

APPENDIX A

AVAILABILITY/RELIABILITY ASSESSMENT OF A LIQUID METAL STEAM GENERATOR

An important part of the design of any large component of a nuclear power plant system is the evaluation of the qualitative and quantitative reliability and availability of that component. The reliability of the component is expressed by the probability that it will perform properly under stated conditions for a stated time. The availability of the component is defined as the fraction of time the system is operational.

The assessment of the reliability and availability of a component generally encompasses three procedures. First a qualitative analysis is performed that provides the designer with an identification of the various failure modes that contribute to the system unreliability. Next, a quantitative analysis is performed which provides the designer with a numerical value for the reliability and availability of the component. The final step is to provide an extensive test on parts of the component, or a scaled down version of the component to verify the qualitative and quantitative analysis.[21]

Besides conducting an extensive project into the design and development of a liquid metal steam generator, Westinghouse conducted a qualitative and quantitative analysis of the reliability and availability of a number of liquid metal steam generator designs.[14] Given the present limited operating experience with liquid metal heat exchangers, available data from PWR steam generators and engineering judgement have been used liberally in the quantitative analysis. Therefore, the reliability and availability estimates predicted by the quantitative analysis are most useful in comparing the relative merit of alternative designs. We have used the Westinghouse quantitative

analysis to evaluate the relative merit of the duplex tube with leak detection design and the single tube design, with both designs satisfying the MARS heat transfer requirements. Although the Westinghouse analysis is applied to a liquid sodium steam generator, we assume the analysis can be applied to a liquid lithium-lead steam generator, because of the similarity in physical and transport properties between liquid sodium and liquid lithium-lead alloys.

The Westinghouse qualitative analysis was based on limited failure data from the operation of liquid sodium heat exchangers.

The analysis leads to the following conclusions. Because two-thirds of the failures are located at welds, associated with welded joints, or are suspected of occurring in weld areas, these weld areas require special design quality assurance and development attention. Corrosion related failures are also prominent. Another important observation is that no failure has occurred while operating at rated power. Leaks are most likely to occur during start-up, shutdown, or power level changes.

The quantitative analysis conducted by Westinghouse was begun by constructing a fault tree based on observations from the qualitative analysis. The fault tree analysis begins by selecting the top failure event and then determining the probability of this event occurring. In this analysis, the top failure event is the forced shutdown of the steam generator. Based on the probability of subordinate events occurring, the probability of the top failure event occurring can then be determined. This analysis can be cast into algebraic equations, with the probability of subordinate events and the number of tubes in the steam generator as independent variables.

For the duplex tube design with leak detection, the analysis identified three scenarios that lead to the shutdown of the steam generator. The first

scenario identified is the detection of a water leak but no reaction. This would mean that either the tube has failed but the other tube still holds. The second scenario identified is characterized by a small leak with a relatively small, localized reaction. The third scenario is characterized by a large leak with a large reaction; this is the type of accident scenario on which the models in the paper are based. For the single tube design, the first accident scenario, as described above, could not occur, since any tube failure would lead to the water and liquid metal coming into contact.

The weakness of the Westinghouse analysis is that they have very little data on which to base the probabilities of the subordinate events occurring. For the duplex tube design, the subordinate events can be broken down into four event groups. The first event group consists of the failure of the inner tube. Westinghouse assumes that the probability that the inner tube will fail is equal to the probability that a steam tube, of equal thickness, will fail in a PWR steam generator:

$$\lambda_i = \lambda_{PWR} \cdot \qquad (A.1)$$

This is a conservative probability, since in the PWR, the tube contacts relatively caustic water on both sides of the tube; while in the duplex tube design, the tube contacts water on the inside and relatively inert helium on the outside. The second group consists of the failure of the outer tube. One would expect that the probability that the outer tube fails would be less than the probability that the inner tube fails, because the outer tube contacts the liquid-metal, which is less caustic than water, on the outside and relatively inert helium on the inside. Westinghouse assumes that the probability that

the outer tube fails is equal to the probability that the inner tube fails multiplied by a factor (C_1), which is less than 1:

$$\lambda_o = C_1 \lambda_i \ . \qquad (A.2)$$

For their analysis, Westinghouse assumes C_1 equals 1/10. The third group consists of interdependent failures. An interdependent failure occurs when one tube fails due to the failure of the other tube. Given the failure of the outer tube, the probability that the inner tube will fail will be small because the liquid-metal must migrate across the helium gap, and the helium is at a higher pressure than the liquid-metal. In the Westinghouse analysis, the probability that the inner tube will fail, given the failure of the outer tube, is determined by a factor (C_2) that equals 1/20. Given a failure of the inner tube, the probability that the outer tube fails will be larger than the other interdependent failure because of the higher pressure and the more caustic nature of the water. Again, the probability that the outer tube fails, given the failure of the inner tube, is determined by a factor (C_3) that equals 3/4. The fourth event group consists of the probability that an originally small break will deteriorate into a large break, leading to the accident scenario, on which the bulk of this paper is based. In the Westinghouse analysis, the probability of a large break occurring, given a small break, is determined by a factor (C_4), which arbitrarily equals 1/10. This means that 1 in every 10 small breaks will deteriorate into a large break.

For the single tube design, of the four factors described above, only the fourth (C_4) comes into play. Also, the probability that the steam tube will fail is equal to the probability that a PWR steam tube will fail.

With the equations based on the fault tree analysis, and with the probabilities and factors described above, the overall probability that a forced shutdown of the steam generator will occur (λ_{SG}) can be approximated. This probability is a measure of the unreliability of the steam generator. A more significant measure of the relative merit of a design is the unavailability of the component. It is a measure of the fraction of operating time that the component can be expected not to be operating due to an accident, which causes the forced shutdown of the component, and the time it takes to repair the component. The unavailability can be expressed as

$$E_U = \frac{\lambda}{\mu + \lambda} \tag{A.3}$$

where μ is the reciprocal of the time needed to repair the component after an accident, and λ is the probability that the accident occurs. For each of the three accident scenarios described earlier in this section, Westinghouse has determined the probable amount of time needed to repair the steam generator. For the detected leak but no reaction scenario, the repair time is 10 days. For the small leak and localized reaction scenario, the repair time is 7 weeks. For the large leak and extensive reaction scenario, the repair time is 13 months.

In our analysis, we have taken the Westinghouse equations based on their fault tree analysis and applied them to the duplex tube with leak detection and the single tube steam generator designs. Both designs fulfill the MARS

heat transfer requirements. For the duplex tube design, this translates into a steam generator with 3286 duplex tubes. For the single tube design, if we assume the thickness of the single tube is equal to the total thickness of the duplex tube, the steam generator would require 2450 single tubes. Even though both the duplex tube steam generator and the single tube steam generator have the same power rating, the duplex tube steam generator requires more tubes than the single tube steam generator because of the greater heat transfer resistance of the duplex tube, which is due to the presence of the helium gap. One should note that the MARS power station requires either 10 duplex tube steam generators or 10 single tube steam generators. The unavailability analysis below is applied only to one, isolated steam generator.

In the first part of our analysis we determined the overall unavailability of the two designs. The overall unavailability is the sum of the unavailability calculated for each of the three accident scenarios. Using the values of the four probability factors as used in the Westinghouse analysis (C_1 = 1/10, C_2 = 1/20, C_3 = 3/4, C_4 = 1/10), the overall probability that a forced shutdown of the steam generator will occur (λ_{SG}) and the overall unavailability of the steam generator, in percent (E_{tot}), for the two steam generator designs is as follows. For the duplex tube design:

$$\lambda_{SG} = 2.78 \times 10^{-5} \text{ hr}^{-1}$$

and

$$E_{tot} = 0.70\% \ .$$

For the single tube design:

$$\lambda_{SG} = 2.3 \times 10^{-5} \text{ hr}^{-1}$$

$$E_{tot} = 4.2\% \ .$$

What this means is that although both designs show roughly the same overall probability that a forced shutdown will occur, the overall percentage of time that the steam generator can be expected to be inoperable due to a forced shutdown is significantly smaller for the duplex tube design. This is because the overall probability that a forced shutdown will occur is due mainly to a detected leak but no reaction accident scenario ($\lambda = 2.75 \times 10^{-5}$ hr^{-1}), for the duplex tube design. The probability of a small leak, small reaction is 2.7×10^{-7} hr^{-1}, and the probability of a large leak, large reaction is 1.6×10^{-8} hr^{-1}. Because the largest portion of the probability of forced shutdown is due to the detected leak but no reaction scenario, which has a relatively short repair time, the overall unavailability of the duplex tube design will be due mainly to the detected leak but no reaction scenario. Thus, this analysis demonstrates the effectiveness of the leak detection component of the duplex tube design.

In the second part of our analysis, we determined the sensitivity of the calculated unavailability of the two designs, to the variation of the four probability factors used in the Westinghouse analysis. Specifically, we calculated the unavailability of the two designs when one of the four probability factors is varied, while the other three factors are held constant at the values used in the Westinghouse analysis.

The first factor varied is the factor that determines the probability that the outer tube, of the duplex tube, fails. The value used by Westinghouse for this factor is 1/10. This means that the probability that the outer tube will fail is 1/10 of the probability that the inner tube will

fail. As this factor is increased from 0.1 to 1.0, the total unavailability of the duplex tube design increases from 0.7% to 1.7%, which is still significantly less than the unavailability of the single tube design (4.2%). Thus, even if the outer tube fails with the same probability of the inner tube, the duplex tube design is far superior than the single tube design.

The second factor varied is the factor that determines the probability that the inner tube will fail, due to the failure of the outer tube. As this factor is increased from the value used in the Westinghouse analysis (C_2 = 0.05) to 1.0, the unavailability of the duplex tube design increases from 0.7% to 1.3%. The third factor varied is the factor that determines the probability that the outer tube will fail, due to the failure of the inner tube (C_3). In this case, as the factor is varied from 0 to 1.0, the unavailability of the duplex tube design does not vary appreciably from 0.7%. Thus the overall unavailability of the duplex tube steam generator is not very sensitive to interdependent failures.

The last factor varied is the factor that determines the probability that a small break will deteriorate into a large break (C_4). For the duplex tube design, as the value of C_4 varies from 0 to 1.0, the overall unavailability varies, roughly linearly with C_4, from 0.69% to 1.0%. For the single tube design, as the value of C_4 varies from 0 to 1.0, the overall unavailability varies, roughly linearly with C_4, from 2.3% to 18.4%. Again, this demonstrates the effectiveness of the duplex tube with leak detection design, because even if every small break and localized reaction deteriorates into a large break and extensive reaction, the overall unavailability of the duplex tube steam generator is still only 1.0%. This is because the bulk of this unavailability is due to the detection of the leak but no reaction scenario.

Thus, if a leak is detected, more often than not, the steam generator will be shut down before the leak deteriorates into a break and a subsequent reaction.

In conclusion, although the duplex tube design produces no advantage over the single tube design, in lowering the probability of a forced shutdown due to a tube failure, the effect of a tube failure on the overall unavailability of the duplex tube design is significantly lower than the effect of a tube failure on the overall unavailability of the single tube design. The effect of the leak detection capability of the duplex tube design is to significantly reduce the overall unavailability of the duplex tube steam generator design by stopping most tube failures before they can deteriorate into a tube break and subsequent reaction, which could severely damage the steam generator.

The final step in the assessment of the reliability and availability of the steam generator will be to provide an extensive test of the steam generator to verify the conclusions of this analysis. Westinghouse is currently building a 70 MW full scale liquid-metal steam generator to verify their quantitative analysis. Their current program schedule states that they will complete the 70 MW steam generator at the end of this year, and begin testing early next year. Therefore the verification of their quantitative analysis should come within the next two years.

APPENDIX B

MARSBURN USER GUIDE

This appendix is intended as a manual describing the structure and formula derivation of the MARSBURN computer program for the interested reader, and as a guide for the program user. This appendix is divided into three sections. The first section contains a handbook describing the structure and formula derivation of the main subroutines in the program. The second section, the user guide, contains a printout of the terminal display from a typical run through the program along with an analysis of this display. The last section is a program listing.

B.1 Program Description

This section is designed to give the reader an overview of the program structure and of the interrelation of the program subroutines. To obtain the best understanding of the program structure, the reader is referred to Section 3 of this appendix, the program listing. This first section should only be used to elucidate the comment lines in the program listing. This section is divided into subsections, headed by subroutine names, each of which refer to that subroutine.

The program is written in FORTRAN. The definition and unit designation of program variables is given in a list at the beginning of the program. The program variables are in MKS units, except for mass which is often expressed in moles instead of kilograms.

B.1.1 Subroutine DRIVE

This subroutine controls the action of the mass balance subroutine (MDRIVE) and the energy balance subroutines (ENERRZ and ENERNZ). It keeps

track of the time from accident initiation and uses this to determine whether or not the calculation should proceed, by the action of a DO WHILE loop. During each pass through the loop, the mass and energy balances are iterated upon until the end of timestep pressure and temperature satisfy six conditions. The first of these conditions is that the end of timestep pressure cannot be greater than the average of the beginning of timestep pressure and the steam tube ambient pressure. This keeps the flow rate of water from the broken steam tube, which is a function of the difference between the steam tube ambient and the system pressure, from changing too rapidly during the timestep. The second condition is that the system pressure does not exceed the steam tube ambient pressure, in accordance with the assumption of no backflow through the broken steam tube. The third condition is that the system pressure as calculated by the mass balance subroutine is close to the system pressure as calculated with the end of timestep reaction zone temperature. The fourth condition is that the reaction zone temperature cannot fall below the nonreaction zone temperature. The fifth condition is that neither the reaction nor the nonreaction zone temperature can fall below 648 K, which is the ambient water temperature in the unbroken steam tubes. This condition makes sure that the unbroken steam tubes will transfer energy out of the system by forced convection. The sixth and final condition is that if the timestep decreases to below 1×10^{-12} s, the program execution halts, and a message that this condition has been invoked is sent to the user's terminal. This condition is invoked when the reaction and nonreaction zone temperatures converge to the same temperature which causes either the fourth or fifth conditions to be invoked repeatedly. Each time the fourth or fifth condition

is invoked, the timestep is halved and the loop is reiterated. Thus, this last condition is meant to avoid the possibility of an endless loop.

B.1.2 Subroutine MDRIVE

Each time a call is made to MDRIVE, the reaction and nonreaction zone mass balances are carried out over ten equal time intervals for the current timestep. This is done because the reaction rate, and hence system pressure, depend upon the flow rate of water into the system and the flow of unreacted liquid-metal breeder out of the system, which in turn both depend upon the system pressure. This interrelation of the mass balances and reaction rate, through the system pressure, deems necessary the increased accuracy gained by carrying out the mass balances 10 times for each time the energy balances are carried out.

The mass balance is divded between two subroutines, FLOWRT and MASS.

B.1.3 Subroutine FLOWRT

This subroutine calculates the flow rate and specific energy of water from the broken steam tube by use of the homogeneous equilibrium model. The flow rate of steam and liquid H_2O was determined at 14 different pressures. Linear interpolation formulas were then derived for pressures between these 14 points.

B.1.4. Subroutine MASS

This subroutine calculates the reaction and nonreaction zone mass balances given the flow rate of H_2O into the reaction zone. The amount of liquid-metal breeder flowing into the reaction zone and reacting is determined by the amount of H_2O flowing into the reaction zone through the mixing parameter x. From the system pressure, the flow rate of unreacted liquid-metal breeder through the pressure relief valve can be determined, and thus the

nonreaction zone mass balance can be carried out. On the basis of these balances, the new reaction and nonreaction zone volume and system pressure is then determined. This new pressure can then be used during the next time the mass balances are calculated. Thus for each call made to MDRIVE, the mass balances are calculated 10 times, each time based on the pressure determined from the previous time the mass balances were calculated.

B.1.5 Subroutine ENERRZ

This subroutine solves the reaction zone energy balance:

$$\frac{dE_R}{dt} = -Q_c - Q_r - p\frac{dV_r}{dt} + \dot{m}_{br}i_b + \dot{m}_w i_w \ . \tag{10}$$

First, the energy flow terms on the right hand side of this equation over the timestep interval Δt are determined. Then, with the beginning of timestep reaction zone energy (E_{Ri}), the end of timestep reaction zone energy (E_{Rf}) can be determined:

$$E_{Rf} = E_{Ri} + \Delta t(-Q_c - Q_r - p\frac{dV_r}{dt} + \dot{m}_{br}i_b + \dot{m}_w i_w) \ . \tag{11}$$

Using the temperature derivative of the above equation, the end of timestep temperature of the reaction zone (T_{rf}) is then determined with Newton's method for determining the roots of an equation. This process is carried out by the subroutine ROOT.

The nonreaction zone energy balance is solved by the subroutine ENERNZ in the same manner as outlined above.

B.2 User Guide

This section contains a printout of the interactive terminal display from a typical run through the program, along with a printout containing a portion of the output from the run. The following page contains the terminal display. The arrows in the right hand margin point to the inputs provided by the user corresponding to program prompts. The letter (I) implies that the input must be an integer, and the letter (D) implies that the input must be double precision. The page after that contains the output from the run.

When the program is run interactively, the program first sends to the terminal the default values of the main program variables (X, APRV, PPRV, TIMEND, NPIPES, VRO) and then prompts the user to decide if he wants to change the default values of these variables. As shown in the printout of the terminal display, during this run, the value of TIMEND was the only variable changed, by entering a 1 after the prompt. Entering any other integer after the prompt implies that the user is satisfied with the default value of the variable. These variables are defined as:

X - the mixing parameter, the program will run properly for any value of x between 0.4 and 5.4.

APRV - the area of the pressure relief value (m^2).

PPRV - the set point pressure at which the pressure relief valve opens (N/m^2).

TIMEND - the time length of the accident(s).

NPIPES - the number of broken pipes.

VRO - the initial volume of the reaction zone; this variable must be nonzero for the program to run properly (m^3).

The next program prompt asks the user to choose the type of breeder for the program run. If this prompt is answered with a 1, the program then

```
THE DEFAULT VALUE OF X =    1.000
THE DEFAULT VALUE OF APRV =  5.0000E-03 M2
THE DEFAULT VALUE OF PPRV =  1.7240E+05 PA
THE DEFAULT VALUE OF TIMEND =    10.00      SEC
THE DEFAULT VALUE OF NPIPES =    1
THE DEFAULT VALUE OF VR0 =  1.0000E-05 M3
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF X
2                                                                          I
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF APRV
2                                                                          I
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF PPRV
2                                                                          I
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF TIMEND
1                                                                          I
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF NPIPES
2                                                                          I
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF VR0
2                                                                          I
ENTER THE NEW VALUE OF TIMEND
1.                                                                         D
THE DEFAULT LIQUID METAL BREEDER IS LI-17 PB-83
 IF YOU WANT TO ENTER THE PROPERTIES OF A DIFFERENT TYPE OF BREEDER
 ENTER A 1
1                                                                          I
ENTER THE NEW BREEDER DENSITY - KG3
510.                                                                       D
ENTER THE NEW BREEDER HEAT OF FORMATION - J/MOLE
0.                                                                         D
ENTER THE NEW BREEDER THERMAL CONDUCTIVITY- W/M-K
50.                                                                        D
ENTER THE NEW BREEDER THERMAL DIFFUSIVITY - M2/SEC
2.32D-5                                                                    D
ENTER THE NEW BREEDER ATOMIC FRACTION OF LI
     I. E.    ENTERING   1.   IMPLIES A PURE LI BREEDER.
    ENTERING   .5   IMPLIES LI-50 PB-50 .
1.                                                                         D
ENTER A 1 IF YOU WANT GENERAL OUTPUT
1                                                                          I
ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE  MOLAR COMPONENTS
OF  THE REACTION ZONE AND THE FLOWRATES INTO AND OUT OF THE SYSTEM
1                                                                          I
ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE THE ENERGY STATUS OF THE TWO ZONES
1                                                                          I
ENTER A 1 IF YOU WANT DEBUG OUTPUT
2                                                                          I
 PROGRAM EXECUTION NOW BEGINS
THERE ARE     22 LINES IN THESE OUTPUT FILES
 TIME vs. TEMP OF R.Z. AND N.Z. IS IN LOGICAL UNIT NO. 11
  TIME vs. PRESSURE IS IN LOGICAL UNIT NO. 12
 TIME vs. MASS Rx IS IN LOGICAL UNIT NO. 13
 TIME vs. H2O AND BREEDER FLOW RATES IS IN LOGICAL UNIT NO. 14
  THE GENERAL OUTPUT FILE IS IN LOGICAL UNIT NO.30
   THE DEBUG OUTPUT IS IN LOGICAL UNIT NO. 15

          THE MAXIMUM PRESSURE =  1.4786E+07 N/M2
          THE MAXIMUM REACTION ZONE TEMPERATURE =    2103.      K
          FOR X =    1.000        AND APRV =  5.0000E-03 M2
FORTRAN STOP
```

```
 THE PROGRAM VARIABLES ARE :
              THE MIXING PARAMETER ---------    1.000
              PRESSURE RELIEF VALVE AREA -   5.0000E-03 M2
              PRV PRESSURE SET POINT -------   1.7240E+05 N/M2
              CALCULATION END TIME ---------    1.000      SEC
              NUMBER OF BROKEN STEAM TUBES    1
              THE INITIAL REACTION ZONE VOL 1.0000E-05 M3
              THE BREEDER IS COMPOSED OF    100.0      % LI   AND   0.0000E+00 % PD
```

```
**********************************************************
      END OF TIMESTEP TIME ----------   4.0052E-07 SEC


      REACTION ZONE TEMPERATURE - -     2163.       K
      NONREACTION ZONE TEMPERATURE       673.0      K

      SYSTEM PRESSURE ---------------   1.8031E+06 PA

      REACTION ZONE VOLUME ----------   1.0090E-05 M3
      GAS VOLUME ---------------------  1.0085E-05 M3


      MOLAR FLOWRATE - H2O ----------     722.1      MOLES/SEC
      MOLAR FLOWRATE TO R.Z. - LMD       722.1      MOLES/SEC
      MOLAR FLOWRATE OUT OF PRV --    1.2992E+05 MOLES/SEC

      MASS OF H2 IN R.Z. ------------   6.9398E-04 MOLES
      MASS OF PD IN R.Z. ------------   0.0000E+00 MOLES
      MASS OF UNREACTED LI IN R.Z.   0.0000E+00 MOLES
      MASS OF UNREACTED H2O IN R.Z.  0.0000E+00 MOLES
      MASS OF LIOH IN R.Z. ----------   3.4699E-04 MOLES

      R.Z. EXPANSION VELOCITY -------     82.65      M/SEC


      CONDUCTION ENERGY -------------   1.4257E+07 J/SEC
      FLUID EXPANSION WORK ----------   2.4068E+05 J/SEC
      ENERGY FLOW INTO R.Z. ---------  -1.4457E+08 J/SEC
      ENERGY FLOW OUT OF N.Z. -------   1.9764E+09 J/SEC
      CONVECTION ENERGY OUT OF R.Z.      60.30      J/SEC
      CONVECTION ENERGY OUT OF N.Z.  5.9663E+09 J/SEC

      FINAL ENERGY OF R.Z. ----------    -74.42      J
      FINAL ENERGY OF N.Z. ----------   2.9293E+10 J

      INITIAL ENERGY OF R.Z. --------   0.0000E+00 J
      INITIAL ENERGY OF N.Z. --------   2.9290E+10 J

      SUM OF ENERGY CHANGE TOTAL -      -1258.      J
      TOTAL INTERNAL ENERGY ---------   -1258.      J
```

prompts the user to enter the properties of the new breeder. The printout of the terminal display shows that the breeder chosen during this run was pure lithium.

Next, the program prompts the user to choose the type and composition of the output. If the user wants debug output, the program will then prompt the user to choose for which of the subroutines he wants debug output.

After the program is executed, the program alerts the user to the location of the standard output files, the general output file, and the debug output file. The program then tells the user the maximum system pressure and reaction zone temperature reached during the run.

The standard output files are composed of lists of numbers without comment. Each line of output in logical unit number 11 consists of the time (s), temperature of the reaction zone (K), and temperature of the nonreaction zone (K). Each line of output in logical unit number 12 consists of the time (s) and the system pressure (N/m^2). Each line of output in logical unit number 13 consists of the time (s) and the mass of H_2 in the reaction zone (mole). Each line of output in logical unit 14 consists of the time (s), the molar flow rate of H_2O into the system (mole/s), and the molar flow rate of unreacted liquid-metal breeder out of the system (mole/s). All quantities in the standard output files are end of timestep quantities. A line is sent to each of these files every time a pass is made through the controlling DO-loop.

The composition of the general output file is shown on the second page of printout. This page shows the general output generated for the first pass through the controlling DO-loop. At the top of the general output file, the program variables chosen for the execution of the program are given. The first portion of the output generated for each pass through the controlling

DO-loop is self-explanatory. The R.Z. expansion velocity is simply a measure of how quickly the boundary between the reaction zone and nonreaction zone is expanding through the system. It equals the difference between the end of timestep reaction zone radius and the beginning of timestep reaction zone radius divided by the timestep. The next 10 lines refer to quantities in the reaction zone energy balance

$$E_{Rf} = E_{Ri} + \Delta t(-Q_c - Q_r - p\frac{dV_r}{dt} + \dot{m}_{br}i_b + \dot{m}_w i_w) \qquad (B.1)$$

and the nonreaction zone energy balance

$$E_{Nf} = E_{Nf} + \Delta t(Q_c - Q_n - p\frac{dV_r}{dt} - \dot{m}_{br}i_b - \dot{m}_{bp}i_b) \qquad (B.2)$$

where Q_c = conduction energy

$p\frac{dV_r}{dt}$ = fluid expansion work

$\dot{m}_{br}i_b + \dot{m}_w i_w$ = energy flow into R.Z.

$\dot{m}_{br}i_b + \dot{m}_{bp}i_b$ = energy flow out of N.Z.

Q_r = convection energy out of R.Z.

Q_n = convection energy out of N.Z.

E_{Rf} = final energy of R.Z.

E_{Nf} = final energy of N.Z.

E_{Ri} = initial energy of R.Z.

E_{Ni} = initial energy of N.Z.

The last two lines in the output are an internal check to show that energy is being conserved. If Eqs. (B.1) and (B.2) are added together, the resulting equation is

$$E_{Rf} - E_{Ri} + E_{Nf} - E_{Ni} = \Delta t(-Q_r - Q_n + \dot{m}_w i_w - \dot{m}_{bp} i_{bp}) \ . \qquad (B.3)$$

If both sides of this equation are summed for each timestep j, then the equation becomes

$$\sum_j (E_{Rfj} - E_{Rij} + E_{Nfj} - E_{Nij}) = \sum_i \Delta t_j(-Q_{rj} - Q_{nj} + \dot{m}_{wj} i_{wj} - \dot{m}_{bpj} i_{bpj}) \ . \qquad (B.4)$$

If one notes that the initial energy of one timestep equals the final energy of the previous timestep, i.e.

$$E_{Rij} = E_{Rf(j-1)} \qquad (B.5)$$

and

$$E_{Nij} = E_{Ni(j-1)} \ , \qquad (B.6)$$

then the left hand side of Eq. (B.4) becomes

$$\sum_j (E_{Rfj} - E_{Rf(j-1)} + E_{Nfj} - E_{Nf(j-1)}) = E_{Rfj} - E_{Rf0} + E_{Nfj} - E_{Nf0} \ . \qquad (B.7)$$

If one notes that the initial energy of the reaction zone, at the start of the calculation, is 0, then Eq. (B.4) can be written as

$$E_{Rfj} - E_{Nfj} - E_{Nf0} = \sum_{j} \Delta t_j(-Q_{rj} - Q_{nj} + \dot{m}_{wj} i_{wj} - \dot{m}_{bj} i_{bj}) \ . \qquad (B.8)$$

The last two output lines correspond to the right hand side of Eq. (B.8) and the left hand side of Eq. (B.8), respectively. If energy is to be conserved by the program, the last two output lines must always be equal.

```
0001    C
0002    C*****************************************************************
0003    C *      *    **    ****    ****  ****   *    *  ****   *       *
0004    C **   **   *  *   *   *  *      *   *  *    *  *   *  **      *
0005    C * * * *  *    *  *   *  *      *   *  *    *  *   *  * *     *
0006    C *  *  *  ******  ****    ***   ****   *    *  ****   *  *    *
0007    C *     *  *    *  **         *  *   *  *    *  **     *   *   *
0008    C *     *  *    *  * *        *  *   *  *    *  * *    *    * *
0009    C *     *  *    *  *  *       *  *   *  *   **  *  *   *     **
0010    C *     *  *    *  *   *  ****   ****    *** *  *   *  *      *
0011    C
0012    C*****************************************************************
0013    C*****************************************************************
0014    C
0015    C
0016    C     First we provide a list containing descriptions of the major
0017    C  program variables.
0018    C     The variables followed by an asterick (*) appear written in
0019    C  various similar forms in various subroutines, as subroutine dummy
0020    C  variables ( i.e., in the subroutine MDRIVE, the variable MH2O
0021    C  appears as MH2OA ).
0022    C     B. o. t. is defined as beginning of timestep.
0023    C     E. o. t. is defined as end of timestep.
0024    C     LMB is defined as liquid metal breeder.
0025    C     R. Z. is defined as reaction zone.
0026    C     N. Z. is defined as nonreaction zone.
0027    C
0028    C
0029    C       APLI - atom percent of LI in the LMB.
0030    C
0031    C       APRV - area of the pressure relief valve. ( M2 )
0032    C
0033    C       DELTAT (*) - the length of the timestep. ( SEC )
0034    C
0035    C       DLI - density of the liquid LI. ( KG/M3 )
0036    C
0037    C       DLIOH - density of the liquid LIOH. ( KG/M3 )
0038    C
0039    C       DLMB - density of the LMB. ( KG/M3 )
0040    C
0041    C       DPB - density of the liquid PB. ( KG/M3 )
0042    C
0043    C       DRDT - the time derivative of the radius; it is a measure
0044    C              of how fast the R. Z. is expanding. ( M/SEC )
0045    C
0046    C       DSEH2 - temperature derivative of the specific energy of
0047    C               the H2 gas. ( J/MOLE-K )
0048    C
0049    C       DSEH2O - temperature derivative of the specific energy of
0050    C                water vapor. ( J/MOLE-K )
0051    C
0052    C       DSELI - temperature derivative of the specific energy of
0053    C               the liquid LI. ( J/MOLE-K )
0054    C
0055    C       DSEPB - temperature derivative of the specific energy of
0056    C               the liquid PB. ( J/MOLE-K )
0057    C
```

```
0058  C       DSLIOH - temperature derivative of the specific energy of
0059  C                the LIOH. ( J/MOLE-K )
0060  C
0061  C       ENGIN - the internal energy of the H2O and LMB flowing into
0062  C               the reaction zone. ( J/SEC )
0063  C
0064  C       ENGOUT - the internal energy of the LMB flowing out of the
0065  C                nonreaction zone. ( J/SEC )
0066  C
0067  C       FRH2O (*) - the flow rate of the water from the broken steam
0068  C               tube(s). ( KG/SEC )
0069  C
0070  C       FRPRV (*) - the flow rate of unreacted LMB flowing through
0071  C               the pressure relief valve. ( KG/SEC )
0072  C
0073  C       FRSTM (*) - the flow rate of steam from the broken steam
0074  C               tube(s). ( KG/SEC )
0075  C
0076  C       HVAP - this is the saturated vapor enthalpy of H2O.
0077  C               ( J/MOLE )
0078  C
0079  C       IPRV - this is a flag that describes the condition of the
0080  C              pressure relief valve.
0081  C
0082  C       MASLMB - mass of the LMB flowing into the R. Z. ( KG )
0083  C
0084  C       MASPRV - mass of the LMB flowing through the pressure
0085  C                relief valve. ( KG )
0086  C
0087  C       MH2I (*), MH2F (*) - moles of H2 gas in the R. Z. at the
0088  C                            b. o. t. and e. o. t. ( MOLE )
0089  C
0090  C       MH2O (*) - moles of H2O flowing into the R. Z. during the
0091  C                  timestep. ( MOLE )
0092  C
0093  C       MH2OL - moles of liquid H2O flowing into the R.Z. during
0094  C               the timestep. ( MOLE )
0095  C
0096  C       MH2OFR - molar flowrate of H2O into the R. Z. during the
0097  C                timestep. ( MOLE/SEC )
0098  C
0099  C       MLI - moles of LI flowing into the R.Z. during the timestep
0100  C             ( MOLE )
0101  C
0102  C       MLIOHI (*), MLIOHF (*) - moles of LIOH in the R. Z. at the
0103  C                                b. o. t. and e. o. t. ( MOLE )
0104  C
0105  C       MLMB (*) - moles of LMB flowing into the R.Z. during the
0106  C                  timestep. ( MOLE )
0107  C
0108  C       MLMBFR - molar flowrate of LMB into the R. Z. during the
0109  C                timestep. ( MOLE/SEC )
0110  C
0111  C       MLMBNF - moles of LMB in the N. Z. at the e. o. t. ( MOLE )
0112  C
0113  C       MNZO - moles of LMB in the system at the beginning of the
0114  C              program ( MOLE )
```

```
0115    C
0116    C       MPBI (*), MPBF (*) - moles of PB in the R. Z. at the b. o. t.
0117    C                            and e. o. t. ( MOLE )
0118    C
0119    C       MPRVFR - molar flowrate of LMB out of the pressure relief
0120    C                valve during the timestep. ( MOLE/SEC )
0121    C
0122    C       MSTM (*) - moles of steam flowing into the R. Z. during the
0123    C                  timestep ( MOLE )
0124    C
0125    C       NOUT - an internal count of the number of runs through the
0126    C              driving DO loop.
0127    C
0128    C       NPIPES - the number of broken steam tubes.
0129    C
0130    C       PBREAK - the pressure at the steam tube break. ( N/M2 )
0131    C
0132    C       PEND - penetration depth; a conduction length scale ( M )
0133    C
0134    C       PEPS - the pressure epsilon; a convergence measure. ( N/M2 )
0135    C
0136    C       PI (*), PF (*) - the b. o. t. and e. o. t. system pressure
0137    C                        ( N/M2 )
0138    C
0139    C       PPRV - the set point pressure at which the pressure relief
0140    C              valve ruptures. ( N/M2 )
0141    C
0142    C       PVDOT - the product of the pressure and the time derivative
0143    C               of the R. Z. volume. ( J/SEC )
0144    C
0145    C       QCOND - the conductive heat transfer between the reaction
0146    C               and nonreaction zones. ( J/SEC )
0147    C
0148    C       QFCNZ - the convective heat transfer from the N. Z. to
0149    C               unbroken steam tubes. ( J/SEC )
0150    C
0151    C       QFCRZ - the convective heat transfer from the R. Z. to
0152    C               unbroken steam tubes. ( J/SEC )
0153    C
0154    C       RADRZI, RADRZF, RADAVG - the b. o. t., e. o. t., and average
0155    C                                R. Z. radius ( M )
0156    C
0157    C       SEH2OL - the specific energy of the liquid H2O. ( J/MOLE )
0158    C
0159    C       SEH2 - the specific energy of the H2 gas. ( J/MOLE )
0160    C
0161    C       SELI - the specific energy of the liquid LI. ( J/MOLE )
0162    C
0163    C       SELIOH - the specific energy of the LIOH. ( J/MOLE )
0164    C
0165    C       SEPB - the specific energy of the liquid PB. ( J/MOLE )
0166    C
0167    C       SESTM - the specific energy of the steam ( J/MOLE )
0168    C
0169    C       SUMQ - the time integral of the time rate of change of
0170    C              system energy. ( J )
0171    C
```

```
0172    C       SUMU - the total system energy. ( J )
0173    C
0174    C       TCLMB - the themal conductivity of the LMB ( W/M-K )
0175    C
0176    C       TDLMB - the themal diffusivity of the LMB ( M2/SEC )
0177    C
0178    C       TEMPNI (*), TEMPNF (*) - the b. o. t. and e. o. t. temper-
0179    C                                ature of the N. Z. ( K )
0180    C
0181    C       TEMPRI (*), TEMPRF (*) - the b. o. t. and e. o. t. temper-
0182    C                                ature of the R. Z. ( K )
0183    C
0184    C       TEPS - the temperature epsilon; a convergence measure. ( K )
0185    C
0186    C       TIMEND - the length of the accident scenerio. ( SEC )
0187    C
0188    C       TVAP - the vaporization temperature of the superheated steam.
0189    C              ( K )
0190    C
0191    C       UMH2OI (*), UMH2OF (*) - the unreacted amount of H2O in the
0192    C                                R. Z. at the b. o. t. and e. o. t.
0193    C                                ( MOLE )
0194    C
0195    C       UMLII (*), UMLIF (*) - the unreacted amount of LI in the R. Z.
0196    C                              at the b. o. t. and e. o. t. ( MOLE )
0197    C
0198    C       UNZI, UNZF - the b. o. t. and e. o. t. internal energy of
0199    C                    the N. Z. ( J )
0200    C
0201    C       UNZO - the internal energy of the system at the beginning
0202    C              of the program ( J )
0203    C
0204    C       URZI, URZF - the b. o. t. and e. o. t. internal energy of
0205    C                    the R. Z. ( J )
0206    C
0207    C       VGASF - the volume of the gas in the R. Z. at the e. o. t.
0208    C               ( M3 )
0209    C
0210    C       VNRI (*), VNRF (*) - the b. o. t. and e. o. t. volume of
0211    C                            the N. Z. ( M3 )
0212    C
0213    C       VRI (*), VRF (*) - the b. o. t. and e. o. t. volume of the
0214    C                          R. Z. ( M3 )
0215    C
0216    C       VTOT - total volume of the system. ( M3 )
0217    C
0218    C       X - the mixing ratio; it is the ratio of the flow rate of
0219    C           H2O to flow rate of LI that enters the R. Z. during
0220    C           a timestep.
0221    C
0222    C       XH2OHF - the heat of formation of the H2O. ( J/MOLE )
0223    C
0224    C       XLCPRV - the loss coefficient of the pressure relief valve.
0225    C
0226    C       XLMBHF - the heat of formation of the LMB. ( J/MOLE )
0227    C
0228    C
```

```
0229    C*****************************************************************
0230    C     This is the main driving routine of the MARSBURN program.
0231    C
0232          IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0233          IMPLICIT INTEGER ( I-L,N )
0234          PARAMETER ( IWRITE = 6 )
0235          PARAMETER ( IOUT = 20, ITEMP = 11, IPRES = 12, IMH2 = 13,
0236         1            IFLOW = 14 )
0237          LOGICAL DEBUG(7)
0238          COMMON /DEB/ DEBUG, IDBOUT
0239          COMMON /INPUT/
0240         1  X, APRV,
0241         2  PPRV, XLCPRV,
0242         3  DELTAI, TIMEND, NPIPES, VTOT,
0243         4  TEPS, PEPS, VRO
0244          COMMON /PROP/
0245         1  DLMB, DLIOH, DLI, DPB,
0246         2  XLMBHF,
0247         3  TCLMB, TDLMB,
0248         4  APLI
0249    C
0250    C
0251    C     First we set the default values for the common block
0252    C  variables.
0253    C
0254    C  Beginning with INPUT.
0255          X = 1.
0256          APRV = .005
0257          PPRV = 1.724D5
0258          XLCPRV = 2.69
0259    C     This is equivalent to the constant in the equation for the
0260    C  critical velocity for flow through an orifice.
0261    C
0262          DELTAI = 1.D-4
0263          TIMEND = 10.
0264          NPIPES = 1
0265          VTOT = 27.75
0266          TEPS = 1.
0267          PEPS = 1.D5
0268          VRO = 1.D-5
0269    C  We must provide a volume at the beginning of the calculation for
0270    C  the first timestep water flow.  This volume is equivalent to a
0271    C  spherical volume around the break with an effective radius of
0272    C  1.34 cm.  This radius is less than the tube pitch ( 1.84 cm ).
0273    C  Therefore the original break volume is confined to the region
0274    C  of one tube.
0275    C
0276    C     Now we set the default values for the PROP common block.
0277    C  The default liquid metal breeder is LI-17 PB-83.
0278          DLMB = 8.976D3
0279          DLIOH = 1.63D3
0280          DLI = 510.
0281          DPB = 1.071D4
0282          XLMBHF = -1.422D4
0283          TCLMB = 35.
0284          TDLMB = 2.27D-5
0285          APLI = .17
```

```
0286    C
0287    C     The final default is the debug output logical unit number.
0288            IDBOUT = 15
0289    C
0290    C     Now we call the INCHNG (input change) subroutine which prompts
0291    C  the user to set the rest of the common block variables and
0292    C  allows the user to change the default value of some of the
0293    C  common block variables.
0294            CALL INCHNG
0295    C
0296    C    Now we set the initial values of program variables for the
0297    C  first timestep.
0298            TEMPRI = 673.
0299            TEMPNI = 673.
0300            PI = 1.724D5
0301            VNRI = VTOT - VR0
0302            VRI = VR0
0303            MPBI = 0.
0304            UMLII = 0.
0305            UMH2OI = 0.
0306            MLIOHI = 0.
0307            MINERT = PI * VR0 /  ( TEMPRI * 8.314 )
0308    C     This is the initial gas in the reaction zone since the
0309    C  initial reaction zone volume must be nonzero.  The gas is inert
0310    C  and is only present to keep the pressure calculations consistent.
0311            MH2I = 0.
0312            DELTAT = DELTAI
0313            NOUT = 0
0314            NFLAG = 0
0315    C
0316            WRITE ( IWRITE,110 )
0317     110      FORMAT ( '  PROGRAM EXECUTION NOW BEGINS ' )
0318    C     We are now ready to call the driving subroutine.
0319            CALL DRIVE (
0320           1  TEMPRI, TEMPNI, PI, VNRI, VRI,
0321           1  MPBI, UMLII, UMH2OI, MLIOHI, MH2I, MINERT,
0322           2  DELTAT, NOUT, NFLAG,
0323           3  PMAX, TMAX  )
0324    C
0325            WRITE ( IWRITE,100 ) NOUT, ITEMP, IPRES, IMH2, IFLOW
0326     100      FORMAT ( ' THERE ARE ',I5,' LINES IN THESE OUTPUT FILES'/
0327           1 '  TIME vs. TEMP OF R.Z. AND N.Z. IS IN LOGICAL UNIT NO. ',
0328           2 I2/ '   TIME vs. PRESSURE IS IN LOGICAL UNIT NO. ',I2/
0329           3    '  TIME vs. MASS H2 IS IN LOGICAL UNIT NO. ', I2 /
0330           4    '  TIME vs. H2O AND BREEDER FLOW RATES IS IN LOGICAL ',
0331           5    'UNIT NO. ', I2 )
0332    C
0333            WRITE ( IWRITE,101 ) IOUT, IDBOUT
0334     101      FORMAT ( '   THE GENERAL OUTPUT FILE IS IN LOGICAL UNIT',
0335           1    ' NO.', I2 / '    THE DEBUG OUTPUT IS IN LOGICAL UNIT',
0336           2    ' NO. ', I2 )
0337            WRITE ( IWRITE,102 ) PMAX, TMAX, X, APRV
0338     102      FORMAT ( 5X/10X, 'THE MAXIMUM PRESSURE = ',1P1G11.4,
0339           1             ' N/M2 ' / 10X, 'THE MAXIMUM REACTION ZONE',
0340           2             ' TEMPERATURE = ',1P1G11.4,' K' / 10X, 'FOR X = ',
0341           3             1P1G11.4, '   AND APRV = ',1P1G11.4, ' M2 ' )
0342    C
```

```
0343     C      That's all folks!
0344              STOP
0345              END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	557	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	577	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	188	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	1502	

ENTRY POINTS

Address	Type	Name
0-00000000		MARSPRG$MAIN

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
5-00000038	R*8	APLI	4-00000008	R*8	APRV	4-00000020	R*8	DELTAI	2-00000058	R*8	DELTAT
5-00000010	R*8	DLI	5-00000008	R*8	DLIOH	5-00000000	R*8	DLMB	5-00000018	R*8	DPB
3-0000001C	I*4	IDBOUT	2-00000050	R*8	MH2I	2-00000048	R*8	MINERT	2-00000040	R*8	MLIOHI
2-00000028	R*8	MPBI	2-00000074	I*4	NFLAG	2-00000070	I*4	NOUT	4-00000030	I*4	NPIPES
4-00000044	R*8	PEPS	2-00000010	R*8	PI	2-00000060	R*8	PMAX	4-00000010	R*8	PPRV
5-00000028	R*8	TCLMB	5-00000030	R*8	TDLMB	2-00000008	R*8	TEMPNI	2-00000000	R*8	TEMPRI
4-0000003C	R*8	TEPS	4-00000028	R*8	TIMEND	2-00000068	R*8	TMAX	2-00000038	R*8	UMH2OI
2-00000030	R*8	UMLII	2-00000018	R*8	VNRI	4-0000004C	R*8	VRO	2-00000020	R*8	VRI
4-00000034	R*8	VTOT	4-00000000	R*8	X	4-00000018	R*8	XLCPRV	5-00000020	R*8	XLMBHF

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label
1-00000036	100'	1-00000145	101'	1-000001B0	102'	1-00000014	110'

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name
	DRIVE		INCHNG

```
0001    C
0002    C
0003    C*******************************************************
0004    C
0005    C
0006            SUBROUTINE INCHNG
0007    C
0008    C     This subroutine sets the values of the logical vector
0009    C  DEBUG, the common block OUT, and allows the user to change
0010    C  the default values of X, APRV, PPRV, TIMEND, NPIPES, VRO,
0011    C  DLMB, XLMBHF, TCLMB, TDLMB, and APLI.
0012            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0013            IMPLICIT INTEGER ( I-L,N )
0014            INTEGER IDEBUG(7), IINPUT(7)
0015            CHARACTER*6  CINPUT(6)
0016            CHARACTER*6  NAME(7)
0017            LOGICAL DEBUG(7)
0018            COMMON /DEB/ DEBUG, IDBOUT
0019            COMMON /OUT/ JOUT1, JOUT2, JOUT3
0020            COMMON /INPUT/
0021           1  X, APRV,
0022           2  PPRV, XLCPRV,
0023           3  DELTAI, TIMEND, NPIPES, VTOT,
0024           4  TEPS, PEPS, VRO
0025              COMMON /PROP/
0026           1  DLMB, DLIOH, DLI, DPB,
0027           2  XLMBHF,
0028           3  TCLMB, TDLMB,
0029           4  APLI
0030              PARAMETER ( IREAD = 5, IWRITE = 6 )
0031    C
0032    C     First we set the character arrays NAME and CINPUT.
0033              NAME(1) = 'DRIVE '
0034              NAME(2) = 'MDRIVE'
0035              NAME(3) = 'MASS  '
0036              NAME(4) = 'ENERRZ'
0037              NAME(5) = 'ROOT  '
0038              NAME(6) = 'PCONTL'
0039              NAME(7) = 'ENERNZ'
0040    C
0041              CINPUT(1) = 'X      '
0042              CINPUT(2) = 'APRV   '
0043              CINPUT(3) = 'PPRV   '
0044              CINPUT(4) = 'TIMEND'
0045              CINPUT(5) = 'NPIPES'
0046              CINPUT(6) = 'VRO    '
0047    C
0048    C     Now we see if the user wants to change any default values.
0049              WRITE ( IWRITE,100 ) X, APRV, PPRV, TIMEND, NPIPES, VRO
0050     100        FORMAT ( 10X/
0051           1     ' THE DEFAULT VALUE OF X = ',1P1G11.4/
0052           2     ' THE DEFAULT VALUE OF APRV = ',1P1G11.4,' M2 '/
0053           3     ' THE DEFAULT VALUE OF PPRV = ',1P1G11.4,' PA '/
0054           4     ' THE DEFAULT VALUE OF TIMEND = ',1P1G11.4,' SEC '/
0055           5     ' THE DEFAULT VALUE OF NPIPES = ',I3 /
0056           6     ' THE DEFAULT VALUE OF VRO = ',1P1G11.4,' M3 ' )
0057    C
```

```
0058            DO  10  I = 1,6
0059              WRITE ( IWRITE,101 )  CINPUT(I)
0060     101        FORMAT(' ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT',
0061          1       ' VALUE OF ', 6A )
0062              READ ( IREAD,* ) IINPUT(I)
0063      C
0064       10     CONTINUE
0065      C
0066            IF ( IINPUT(1) .EQ. 1 )  THEN
0067              WRITE ( IWRITE,102 )
0068     102        FORMAT ( ' ENTER THE NEW VALUE OF X' )
0069              READ ( IREAD,* ) X
0070            END IF
0071      C
0072            IF  ( IINPUT(2) .EQ. 1 )  THEN
0073              WRITE ( IWRITE,103 )
0074     103        FORMAT ( ' ENTER THE NEW VALUE OF APRV' )
0075              READ ( IREAD,* ) APRV
0076            END IF
0077      C
0078            IF  ( IINPUT(3) .EQ. 1 )  THEN
0079              WRITE ( IWRITE,104 )
0080     104        FORMAT ( ' ENTER THE NEW VALUE OF PPRV' )
0081              READ ( IREAD,* ) PPRV
0082            END IF
0083      C
0084            IF  ( IINPUT(4) .EQ. 1 )  THEN
0085              WRITE ( IWRITE,105 )
0086     105        FORMAT ( ' ENTER THE NEW VALUE OF TIMEND ' )
0087              READ ( IREAD,* ) TIMEND
0088            END IF
0089      C
0090            IF  ( IINPUT(5) .EQ. 1 )  THEN
0091              WRITE ( IWRITE,106 )
0092     106        FORMAT ( ' ENTER THE NEW VALUE OF NPIPES' )
0093              READ ( IREAD,* ) NPIPES
0094            END IF
0095      C
0096            IF  ( IINPUT(6) .EQ. 1 )  THEN
0097              WRITE ( IWRITE,107 )
0098     107        FORMAT ( ' ENTER THE NEW VALUE OF VR0' )
0099              READ ( IREAD,* ) VR0
0100            END IF
0101      C
0102      C     Now for the choice of the liquid metal breeder.
0103              WRITE ( IWRITE,110 )
0104     110        FORMAT ( ' THE DEFAULT LIQUID METAL BREEDER IS LI-17',
0105          1     ' PB-83' / '  IF YOU WANT TO ENTER THE PROPERTIES OF',
0106          2     ' A DIFFERENT TYPE OF BREEDER ',/
0107          3     '  ENTER A 1 ' )
0108              READ ( IREAD,* ) IINPUT(7)
0109      C
0110            IF  ( IINPUT(7) .EQ. 1 )  THEN
0111              WRITE ( IWRITE,111 )
0112     111        FORMAT ( ' ENTER THE NEW BREEDER DENSITY - KG3 ' )
0113              READ ( IREAD,* ) DLMB
0114      C
```

```
0115              WRITE ( IWRITE,112 )
0116       112      FORMAT ( ' ENTER THE NEW BREEDER HEAT OF FORMATION ',
0117           1      '- J/MOLE ' )
0118              READ ( IREAD,* ) XLMBHF
0119       C
0120              WRITE ( IWRITE,113 )
0121       113      FORMAT (' ENTER THE NEW BREEDER THERMAL CONDUCTIVITY',
0122           1      '- W/M-K ' )
0123              READ ( IREAD,* ) TCLMB
0124       C
0125              WRITE ( IWRITE,114 )
0126       114      FORMAT (' ENTER THE NEW BREEDER THERMAL DIFFUSIVITY ',
0127           1      '- M2/SEC ' )
0128              READ ( IREAD,* ) TDLMB
0129            WRITE ( IWRITE,115 )
0130       115      FORMAT ( ' ENTER THE NEW BREEDER ATOMIC FRACTION OF LI'
0131           1            / 5X, 'I. E.   ENTERING  1.  IMPLIES A PURE LI',
0132           2            ' BREEDER.'/ 5X, 'ENTERING  .5  IMPLIES LI-50',
0133           3            ' PB-50 . ' )
0134              READ ( IREAD,* ) APLI
0135       C
0136            END IF
0137       C
0138       C     Now we set the type of output wanted for this run.
0139            WRITE ( IWRITE,200 )
0140       200    FORMAT ( ' ENTER A 1 IF YOU WANT GENERAL OUTPUT' )
0141            READ ( IREAD,* )  JOUT1
0142       C
0143            IF  ( JOUT1 .NE. 1 ) GO TO 55
0144              WRITE ( IWRITE,201 )
0145       201      FORMAT(' ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE ',
0146           1      ' MOLAR COMPONENTS' / ' OF THE REACTION ZONE AND THE',
0147           2      ' FLOWRATES INTO AND OUT OF THE SYSTEM' )
0148              READ ( IREAD,* ) JOUT2
0149       C
0150              WRITE ( IWRITE,202 )
0151       202      FORMAT(' ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE',
0152           1      ' THE ENERGY STATIS OF THE TWO ZONES.' )
0153              READ ( IREAD,* ) JOUT3
0154       55     CONTINUE
0155       C
0156       C
0157       C     Finally we set the debug switches.
0158              WRITE ( IWRITE,300 )
0159       300      FORMAT ( ' ENTER A 1 IF YOU WANT DEBUG OUTPUT ' )
0160            READ ( IREAD,* ) JOUT4
0161       C
0162       C
0163            IF  ( JOUT4 .EQ. 1 )  THEN
0164              DO  20  I = 1,7
0165                WRITE ( IWRITE,301 ) NAME(I)
0166       301        FORMAT ( ' ENTER A 1 IF YOU WANT DEBUG OUTPUT',
0167           1        ' FOR SUBROUTINE ', 6A )
0168                READ ( IREAD,* ) IDEBUG(I)
0169       C
0170                IF  ( IDEBUG(I) .EQ. 1 )  THEN
0171                  DEBUG(I) = .TRUE.
```

```
0172                ELSE
0173                  DEBUG(I) = .FALSE.
0174                END IF
0175     20       CONTINUE
0176           END IF
0177     C
0178     C     That's all folks!
0179           RETURN
0180           END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	1246	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	1434	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	152	PIC CON REL LCL NOSHR NOEXE RD WRT LONG
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	OUT	12	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
6	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	3024	

65

ENTRY POINTS

Address	Type	Name
0-00000000		INCHNG

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
6-00000038	R*8	APLI	5-00000008	R*8	APRV	5-00000020	R*8	DELTAI	6-00000010	R*8	DLI
6-00000008	R*8	DLIOH	6-00000000	R*8	DLMB	6-00000018	R*8	DPB	2-00000088	I*4	I
3-0000001C	I*4	IDBOUT	4-00000000	I*4	JOUT1	4-00000004	I*4	JOUT2	4-00000008	I*4	JOUT3
2-0000008C	I*4	JOUT4	5-00000030	I*4	NPIPES	5-00000044	R*8	PEPS	5-00000010	R*8	PPRV
6-00000028	R*8	TCLMB	6-00000030	R*8	TDLMB	5-0000003C	R*8	TEPS	5-00000028	R*8	TIMEND
5-0000004C	R*8	VRO	5-00000034	R*8	VTOT	5-00000000	R*8	X	5-00000018	R*8	XLCPRV
6-00000020	R*8	XLMBHF									

ARRAYS

Address	Type	Name	Bytes	Dimensions
2-00000038	CHAR	CINPUT	36	(6)
3-00000000	L*4	DEBUG	28	(7)
2-00000000	I*4	IDEBUG	28	(7)
2-0000001C	I*4	IINPUT	28	(7)
2-0000005C	CHAR	NAME	42	(7)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
**	10	**	20	0-0000043A	55	1-00000000	100'	1-000000F7	101'	1-00000135	102'
1-00000151	103'	1-00000170	104'	1-0000018F	105'	1-000001B1	106'	1-000001D2	107'	1-000001F0	110'
1-0000027E	111'	1-000002A6	112'	1-000002DD	113'	1-00000315	114'	1-0000034E	115'	1-000003DF	200'
1-00000407	201'	1-00000493	202'	1-000004EA	300'	1-00000511	301'				

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE DRIVE (
0007          1 TEMPRI, TEMPNI, PI, VNRI, VRI,
0008          1 MPBI,  UMLII, UMH2OI, MLIOHI, MH2I, MINERT,
0009          2 DELTAT, NOUT, NFLAG,
0010          3 PMAX, TMAX  )
0011    C
0012    C     This subroutine contains the driving do loop.  It also calls
0013    C  the mass balance subroutine (MDRIVE),
0014    C  the reaction zone energy balance (ENERRZ), and the nonreaction zone
0015    C  energy balance (ENERNZ).  It also contains statements that adjust
0016    C  the length of the timestep (DELTAT) depending upon the size of the
0017    C  pressure change over the timestep.  Finally,  it calls the sub-
0018    C  routine OUTPUT.
0019            IMPLICIT DOUBLE PRECISION  ( A-H,M,O-Z )
0020            IMPLICIT INTEGER  ( I-L,N )
0021            DOUBLE PRECISION  P(10), VRF(10)
0022            LOGICAL  DEBUG(7)
0023            PARAMETER ( IWRITE = 6 )
0024            COMMON /DEB/ DEBUG, IDBOUT
0025            COMMON /INPUT/
0026          1 X, APRV,
0027          2 PPRV, XLCPRV,
0028          3 DELTAI, TIMEND, NPIPES, VTOT,
0029          4 TEPS, PEPS, VRO
0030            COMMON /PROP/
0031          1 DLMB, DLIOH, DLI, DPB,
0032          2 XLMBHF,
0033          3 TCLMB, TDLMB,
0034          4 APLI
0035    C
0036    C     To begin we set up the do loop.
0037            IPRV = 0
0038            TIME = 0.
0039    C
0040            SUMQ = 0.
0041            MNZO = VNRI * DLMB / ( ( 1 - APLI ) * .20721 +
0042          1         APLI * 6.94D-3 )
0043            PDUM = 0.
0044    C     The above PDUM is a dummy variable, used to tell SENER not
0045    C  to carry out the equations to determine the specific energy of
0046    C  the water, since that information will not be needed here.
0047            CALL SENER (
0048          1 TEMPNI, PDUM,
0049          2
0050          3 SEH2,  SELIOH, SEH2O,  SEPB, SELI,
0051          3 DSEH2, DSLIOH, DSEH2O, DSEPB, DSELI )
0052            UNZO = MNZO * ( ( 1 - APLI ) * SEPB + APLI *
0053          1         SELI + XLMBHF )
0054    C
0055            URZI = 0.
0056            UNZI = UNZO
0057    C
```

```
0058    C
0059    C
0060            DO  100  WHILE  ( TIME .LE. TIMEND )
0061              TEMPAV = TEMPRI
0062     200      CONTINUE
0063    C
0064    C     First a call to the mass balance subroutine.
0065              CALL MDRIVE (
0066           1  TEMPAV, MPBI, UMLII, UMH2OI, MLIOHI, MH2I, VNRI, PI, IPRV,
0067           1  VRI,  MINERT,
0068           2  DELTAT,
0069           3  MH2O, MSTM, MLMB, MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,
0070           3  FRPRV, VNRF, VRF, VGASF, P, ICONTL, SESTM, SEH2OL )
0071              IF ( ICONTL .EQ. 1 )  GO TO 200
0072    C     This condition checks to see if DELTAT was adjusted during the
0073    C  execution of MDRIVE.  If it has, MDRIVE is reexecuted until
0074    C  DELTAT is not adjusted during execution of MDRIVE.
0075    C
0076    C     Now the call to the reaction zone energy balance.
0077              CALL ENERRZ (
0078           1  TEMPRI, TEMPNI, DELTAT, PI, P, VRF, MPBI, UMLII,
0079           1  UMH2OI, MLIOHI, MH2I, MH2O, MSTM, MLMB, MPBF, UMLIF, UMH2OF,
0080           1  MLIOHF, MH2F, VRI, URZI, SESTM, SEH2OL,
0081           2
0082           3  QCOND, PVDOT, URZF, ENGIN, QFCRZ, TEMPRF, DRDT )
0083    C
0084    C     Now for the pressure control statements.
0085    C
0086    C     First we determine the end of timestep pressure.
0087              PF = 8.314 * ( MH2F + MINERT + UMH2OF ) * TEMPRF / VGASF
0088              PCHECK = ( PI + 1.6543D7 ) * .5
0089              IF  ( PF .GT. PCHECK )  THEN
0090    C
0091    C     If this condition is true, it means that the pressure has
0092    C  increased more than half of the way to 1.6543D7 psia, which is the
0093    C  water tube back pressure.  This means that the system maybe
0094    C  changing too rapidly over the timestep. To be prudent then, the
0095    C  timestep is decreased by a call to PCONTL.  And the balances are
0096    C  recalculated.
0097              CALL PCONTL (
0098           1  PI, PF,
0099           2  DELTAT
0100           3  )
0101              IF  ( DEBUG(1) )  THEN
0102                WRITE ( IDBOUT,1000 )
0103     1000         FORMAT ( '***** PF is greater than PCHECK ' )
0104                WRITE ( IDBOUT,1001 )  PF, PCHECK
0105     1001         FORMAT ( ' PF PCHECK ' / 1P2G11.4 )
0106              END IF
0107              GO TO 200
0108              END IF
0109    C
0110              IF  ( DABS( PF - P(10) ) .GT. PEPS )  THEN
0111    C
0112    C     If this condition is true, then calculating the mass balance
0113    C  isothermally may not be good assumption.  To correct this, we
0114    C  recalculate the mass balance with a different temperature, which
```

```
0115     C  is the final reaction zone temperature over this last iteration.
0116     C
0117               TEMPAV = TEMPRF
0118     C
0119               IF  ( DEBUG(1) )  THEN
0120                 WRITE ( IDBOUT,1003 ) PF, P(10)
0121      1003         FORMAT ( ' PF P(10) ' / 1P2G11.4 )
0122                 WRITE ( IDBOUT,1002 )
0123      1002         FORMAT ( '     ***** nonisothermal pressure ' )
0124               END IF
0125               GO TO 200
0126             END IF
0127     C
0128     C      The pressure control statements are now completed.
0129     C
0130     C      Now for the nonreaction zone energy balance.
0131     C
0132             IF  ( NFLAG .EQ. 1 )  GO TO 300
0133     C      If this condition is true, then the nonreaction zone temper-
0134     C  ture has converged to the steam tube ambient temperature ( 648K ).
0135     C  In this case, the nonreaction zone temperature will remain
0136     C  at 648K, and it is not necessary to carry out the nonreaction
0137     C  zone energy balance.
0138           CALL ENERNZ (
0139          1  VNRI, VNRF, TEMPNI, DELTAT, PVDOT, QCOND, FRPRV, MLMB,
0140          1  UNZI,
0141          2
0142          3  UNZF, TEMPNF, ENGOUT, QFCNZ )
0143     C
0144     C
0145     C      Now for the temperature control statements.
0146     C
0147     C      The first temperature control case is when TEMPRF and TEMPNF
0148     C  converge to one temperature and remain at this temperature.
0149     C  This is caused by either the value of X being too large or too
0150     C  small.  This causes the reaction rate to be too small, so that
0151     C  the system reaches an equilibrium condition.  This will cause
0152     C   the program to not work properly because the timestep decreases
0153     C  significantly.  If this happens, we halt the program.
0154           IF  ( DELTAT .LT. 1.D-12 )  THEN
0155             WRITE ( IWRITE,1004 ) TIME, TEMPRF, TEMPNF, PF
0156      1004     FORMAT ( ' PROGRAM EXECUTION HALTED ',1P1G11.4,
0157          1          ' SECONDS INTO THE ACCIDENT'/5X, 'BECAUSE EQUILI',
0158          2          'BRIUM WAS REACHED BETWEEN THE TWO ZONES - WITH:'/
0159          3          5X,'REACTION ZONE TEMPERATURE = ', 1P1G11.4 /
0160          4          5X,'NONREACTION ZONE TEMPERATURE = ', 1P1G11.4/
0161          5          5X,'SYSTEM PRESSURE = ',1P1G11.4 )
0162               GO TO 101
0163             END IF
0164     C
0165     C
0166             IF  ( ( TEMPNF - 648. ) .LE. .01 )  THEN
0167               NFLAG = 1
0168               TEMPNF = 648.
0169             END IF
0170     C      This alerts the program that the nonreaction zone temperature
0171     C  has converged to the steam tube ambient temperature.
```

```
0172     300    CONTINUE
0173     C
0174     C      If the reaction temperature has fallen below the nonreaction
0175     C   zone temperature, the timestep is too large.
0176           IF  ( TEMPNF .GE. TEMPRF )  THEN
0177             DELTAT = DELTAT * .5
0178             GO TO 200
0179           END IF
0180     C      To correct this, we must readjust the timestep size and
0181     C   return to the beginning of the loop.
0182     C
0183     C
0184           SUMU = UNZF + URZF - UNZO
0185           SUMQ = DELTAT * ( ENGIN - ENGOUT - QFCRZ - QFCNZ )
0186          1          + SUMQ
0187     C      These are the sum of the energy changes in the reaction
0188     C   zone and nonreaction zone.  If energy is conserved these will
0189     C   be equal .
0190     C
0191     C
0192           MH2OFR = MH2O / DELTAT
0193           MLMBFR = MLMB / DELTAT
0194           MPRVFR = FRPRV / ( ( 1 - APLI ) * .20721 + APLI * 6.94D-3 )
0195     C      These are the molar flowrates of H2O and LMB into the reaction
0196     C   zone, and LMB out of the pressure relief valve, respectively.
0197     C
0198     C      Now for the output routine.
0199     C   First we update TIME.
0200           TIME = TIME + DELTAT
0201           CALL OUTPUT (
0202          1  TIME, TEMPRF, TEMPNF, PF, VRF(10), VGASF, MH2OFR, MLMBFR,
0203          1  MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, MLIOHF,
0204          1  QCOND, PVDOT, ENGOUT, ENGIN, URZF, UNZF, QFCRZ, QFCNZ,
0205          1  DRDT, SUMQ, SUMU, URZI, UNZI,
0206          2  NOUT, NFLAG, PMAX, TMAX
0207          3  )
0208     C
0209     C      Finally, we reset the loop.
0210     C   First we increase DELTAT.  This is done so that the timestep
0211     C   does not remain smaller than it needs to be.
0212           DELTAT = 2. * DELTAT
0213           PI = PF
0214           VRI = VRF(10)
0215           VNRI = VNRF
0216           TEMPRI = TEMPRF
0217           TEMPNI = TEMPNF
0218           UMLII = UMLIF
0219           UMH2OI = UMH2OF
0220           MPBI = MPBF
0221           MLIOHI = MLIOHF
0222           MH2I = MH2F
0223           URZI = URZF
0224           UNZI = UNZF
0225           IF  ( PI .GT. PPRV )  IPRV = 1
0226     C
0227     C      This condition checks to see if the rupture disk has opened
0228     C   during this pass through the do loop.  If it has, IPRV is set
```

```
0229     C  to 1, and remains set to 1 through the rest of the program
0230     C  execusion.  This alerts the subroutine MASS that the disk has
0231     C  ruptured.
0232       100     CONTINUE
0233       101     CONTINUE
0234     C      That's all folks!
0235             RETURN
0236             END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	966	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	352	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	1044	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	2542	

ENTRY POINTS

Address	Type	Name
0-00000000		DRIVE

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
5-00000038	R*8	APLI	4-00000008	R*8	APRV	4-00000020	R*8	DELTAI	AP-00000030@	R*8	DELTAT
5-00000010	R*8	DLI	5-00000008	R*8	DLIOH	5-00000000	R*8	DLMB	5-00000018	R*8	DPB
2-000001C8	R*8	DRDT	2-000000E8	R*8	DSEH2	2-000000F8	R*8	DSEH2O	2-00000108	R*8	DSELI
2-00000100	R*8	DSEPB	2-000000F0	R*8	DSLIOH	2-000001B0	R*8	ENGIN	2-000001F0	R*8	ENGOUT
2-00000170	R*8	FRPRV	2-00000224	I*4	ICONTL	3-0000001C	I*4	IDBOUT	2-00000220	I*4	IPRV
2-00000168	R*8	MH2F	AP-00000028@	R*8	MH2I	2-00000130	R*8	MH2O	2-00000208	R*8	MH2OFR
AP-0000002C@	R*8	MINERT	2-00000160	R*8	MLIOHF	AP-00000024@	R*8	MLIOHI	2-00000140	R*8	MLMB
2-00000210	R*8	MLMBFR	2-000000B0	R*8	MNZO	2-00000148	R*8	MPBF	AP-00000018@	R*8	MPBI
2-00000218	R*8	MPRVFR	2-00000138	R*8	MSTM	AP-00000038@	I*4	NFLAG	AP-00000034@	I*4	NOUT
4-00000030	I*4	NPIPES	2-000001D8	R*8	PCHECK	2-000000B8	R*8	PDUM	4-00000044	R*8	PEPS
2-000001D0	R*8	PF	AP-0000000C@	R*8	PI	AP-0000003C@	R*8	PMAX	4-00000010	R*8	PPRV
2-000001A0	R*8	PVDOT	2-00000198	R*8	QCOND	2-000001F8	R*8	QFCNZ	2-000001B8	R*8	QFCRZ
2-000000C0	R*8	SEH2	2-000000D0	R*8	SEH2O	2-00000190	R*8	SEH2OL	2-000000E0	R*8	SELI
2-000000C8	R*8	SELIOH	2-000000D8	R*8	SEPB	2-00000188	R*8	SESTM	2-000000A8	R*8	SUMQ
2-00000200	R*8	SUMU	5-00000028	R*8	TCLMB	5-00000030	R*8	TDLMB	2-00000128	R*8	TEMPAV
2-000001E8	R*8	TEMPNF	AP-00000008@	R*8	TEMPNI	2-000001C0	R*8	TEMPRF	AP-00000004@	R*8	TEMPRI
4-0000003C	R*8	TEPS	2-000000A0	R*8	TIME	4-00000028	R*8	TIMEND	AP-00000040@	R*8	TMAX
2-00000158	R*8	UMH2OF	AP-00000020@	R*8	UMH2OI	2-00000150	R*8	UMLIF	AP-0000001C@	R*8	UMLII
2-00000110	R*8	UNZO	2-000001E0	R*8	UNZF	2-00000120	R*8	UNZI	2-000001A8	R*8	URZF
2-00000118	R*8	URZI	2-00000180	R*8	VGASF	2-00000178	R*8	VNRF	AP-00000010@	R*8	VNRI

```
  4-0000004C  R*8  VR0            AP-00000014@ R*8  VRI            4-00000034  R*8  VTOT           4-00000000  R*8  X
  4-00000018  R*8  XLCPRV          5-00000020  R*8  XLMBHF
```

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)
2-00000000	R*8	P	80	(10)
2-00000050	R*8	VRF	80	(10)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
**	100	0-000003C5	101	0-0000008C	200	0-000002C9	300	1-00000000	1000'	1-00000023	1001'
1-0000004E	1002'	1-00000039	1003'	1-00000073	1004'						

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name	Type	Name	Type	Name	Type	Name	Type	Name
	ENERNZ		ENERRZ		MDRIVE		OUTPUT		PCONTL		SENER

```
0001    C
0002    C
0003    C*********************************************************
0004    C
0005    C
0006              SUBROUTINE MDRIVE (
0007           1  TEMPR, MPBI, UMLII, UMH2OI, MLIOHI, MH2I, VNRI, PI, IPRV,
0008           1  VRI, MINERT,
0009           2  DELTAT,
0010           3  MH2OA, MSTMA, MLMBA, MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,
0011           3  FRPRVA, VNRF, VRF, VGASF, P, ICONTL, SESTMA, SEH2OL )
0012    C
0013    C      This subroutine contains a do loop that drives the reaction
0014    C   and nonreaction zones mass balance.
0015    C
0016    C      Since the reaction rate is determined by the interaction of the
0017    C   pressure and the inlet and outlet flows, the mass balances, which
0018    C   are dependant upon these flows, are the most important balances
0019    C   in the overall process.  To mirror this, the mass balances are
0020    C   carried out 10 times for each time the energy balances are
0021    C   calculated.
0022              IMPLICIT DOUBLE PRECISION  ( A-H,M,O-Z )
0023              IMPLICIT INTEGER ( I-L,N )
0024              DOUBLE PRECISION  P(10), VRF(10), MSTM(10), MH2O(10),
0025             1                  MLMB(10), FRPRV(10), SESTM(10)
0026              LOGICAL DEBUG(7)
0027              COMMON /DEB/ DEBUG, IDBOUT
0028              IF  ( DEBUG(2) ) THEN
0029                WRITE ( IDBOUT,1010 )
0030     1010         FORMAT ( '      ENTERING MDRIVE ' )
0031              END IF
0032              DELT = DELTAT * .1
0033              MPBB = MPBI
0034              UMLIB = UMLII
0035              UMH2OB = UMH2OI
0036              MLIOHB = MLIOHI
0037              MH2B = MH2I
0038              VNRB = VNRI
0039              PB = PI
0040              VRB = VRI
0041              DO 100  I = 1,10
0042    C
0043    C      First we determine the flowrate of H2O into the reaction zone.
0044                 CALL FLOWRT (
0045           1  PB,
0046           2
0047           3  FRH2O, FRSTM, SESTM(I), SEH2OL )
0048    C
0049    C      Now we calculate the mass balance.
0050                 CALL MASS (
0051           1  FRH2O, FRSTM, TEMPR, MPBB, UMLIB, UMH2OB, MLIOHB,
0052           1  MH2B, VNRB, PB, IPRV, VRB, MINERT,
0053           2  DELT,
0054           3  MH2O(I), MSTM(I), MLMB(I), MPBF, UMLIF, UMH2OF, MLIOHF,
0055           3  MH2F, FRPRV(I), VNRF, VRF(I), VGASF, P(I), ICONTL )
0056                 IF  ( ICONTL .EQ. 1 )  THEN
0057                   DELTAT = DELT * 10.
```

```
0058                GO TO 200
0059              END IF
0060        C     This condition checks to see if DELT  was adjusted during the
0061        C  execusion of MASS.  If it has, control is returned to DRIVE.
0062              MPBB = MPBF
0063              UMLIB = UMLIF
0064              UMH2OB = UMH2OF
0065              MLIOHB = MLIOHF
0066              MH2B = MH2F
0067              VNRB = VNRF
0068              PB = P(I)
0069              VRB = VRF(I)
0070         100  CONTINUE
0071        C
0072        C     Now we must determine the average flowrates over the total
0073        C  timestep.
0074              FRPRVA = 0.
0075              MSTMA = 0.
0076              MH2OA = 0.
0077              MLMBA = 0.
0078              SESTMA = 0.
0079              DO 300  I = 1,10
0080                MSTMA = MSTM(I) + MSTMA
0081                MH2OA = MH2O(I) + MH2OA
0082                MLMBA = MLMB(I) + MLMBA
0083                FRPRVA = FRPRV(I) + FRPRVA
0084                SESTMA = SESTM(I) + SESTMA
0085         300  CONTINUE
0086              SESTMA = SESTMA * .1
0087        C     SESTMA is an average value over the whole timestep.  And there-
0088        C  fore must be divided by 10 because it is evaluated over each of
0089        C  the 10 subintervals.  The other 4 quantities above are not aver-
0090        C  ages.  They are the flow of breeder and water for each of the
0091        C  subintervals, and therefore they must be summed over the whole
0092        C  timestep.
0093        C
0094        C     That's all folks!
0095              IF  ( DEBUG(2) )  THEN
0096                WRITE ( IDBOUT,1000)  MH2OA, MSTMA, MLMBA, FRPRVA
0097         1000     FORMAT ( ' MH2OA MSTMA MLMBA FRPRVA ' / 1P4G11.4 )
0098                WRITE ( IDBOUT,1001)  MPBF, UMLIF, UMH2OF, MLIOHF
0099         1001     FORMAT ( ' MPBF UMLIF UMH2OF MLIOHF ' / 1P4G11.4 )
0100                WRITE ( IDBOUT,1002 )  MH2F, VNRF, VGASF, SEH2OL
0101         1002     FORMAT ( ' MH2F VNRF VGASF SEH2OL ' / 1P4G11.4 )
0102                WRITE ( IDBOUT,1003 )  ( P(I), I = 1,10 )
0103         1003     FORMAT ( ' P ' / 1P4G11.4 / 1P4G11.4 / 1P2G11.4 )
0104                WRITE ( IDBOUT,1004 )  ( VRF(I), I = 1,10 )
0105         1004     FORMAT ( ' VRF ' / 1P4G11.4/ 1P4G11.4/ 1P2G11.4 )
0106                WRITE ( IDBOUT,1006 )  ( SESTM(I), I=1,10 )
0107         1006     FORMAT ( ' SESTM ' / 1P4G11.4 / 1P4G11.4/ 1P2G11.4 )
0108                WRITE ( IDBOUT,1005 )
0109         1005     FORMAT ( '     EXITING MDRIVE ' )
0110              END IF
0111         200  CONTINUE
0112              RETURN
0113              END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	779	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	252	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	672	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	1735	

ENTRY POINTS

Address	Type	Name
0-00000000		MDRIVE

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
2-00000190	R*8	DELT	AP-00000030@	R*8	DELTAT	2-000001D8	R*8	FRH2O	AP-00000054@	R*8	FRPRVA
2-000001E0	R*8	FRSTM	2-000001E8	I*4	I	AP-00000068@	I*4	ICONTL	3-0000001C	I*4	IDBOUT
AP-00000024@	I*4	IPRV	2-000001B8	R*8	MH2B	AP-00000050@	R*8	MH2F	AP-00000018@	R*8	MH2I
AP-00000034@	R*8	MH2OA	AP-0000002C@	R*8	MINERT	2-000001B0	R*8	MLIOHB	AP-0000004C@	R*8	MLIOHF
AP-00000014@	R*8	MLIOHI	AP-0000003C@	R*8	MLMBA	2-00000198	R*8	MPBB	AP-00000040@	R*8	MPBF
AP-00000008@	R*8	MPBI	AP-00000038@	R*8	MSTMA	2-000001C8	R*8	PB	AP-00000020@	R*8	PI
AP-00000070@	R*8	SEH2OL	AP-0000006C@	R*8	SESTMA	AP-00000004@	R*8	TEMPR	2-000001A8	R*8	UMH2OB
AP-00000048@	R*8	UMH2OF	AP-00000010@	R*8	UMH2OI	2-000001A0	R*8	UMLIB	AP-00000044@	R*8	UMLIF
AP-0000000C@	R*8	UMLII	AP-00000060@	R*8	VGASF	2-000001C0	R*8	VNRB	AP-00000058@	R*8	VNRF
AP-0000001C@	R*8	VNRI	2-000001D0	R*8	VRB	AP-00000028@	R*8	VRI			

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)
2-000000F0	R*8	FRPRV	80	(10)
2-00000050	R*8	MH2O	80	(10)
2-000000A0	R*8	MLMB	80	(10)
2-00000000	R*8	MSTM	80	(10)
AP-00000064@	R*8	P	80	(10)
2-00000140	R*8	SESTM	80	(10)
AP-0000005C@	R*8	VRF	80	(10)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
**	100	0-0000030A	200	**	300	1-00000018	1000'	1-0000003D	1001'	1-00000062	1002'
1-00000085	1003'	1-000000A3	1004'	1-000000E5	1005'	1-000000C3	1006'	1-00000000	1010'		

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name
	FLOWRT		MASS

```
0001    C
0002    C
0003    C*******************************************************
0004    C
0005    C
0006            SUBROUTINE FLOWRT (
0007          1 P,
0008          2
0009          3 FRH2O, FRSTM, SESTM, SEH2OL )
0010    C
0011    C     This subroutine calcuclates the flowrate of all the H2O and the
0012    C   steam from the broken tube(s) by the homogeneous equilibrium model.
0013    C   FRH2O and FRSTM are evaluated as functions of pressure.  These
0014    C   flows are from two seperate flow paths, one path connected
0015    C   to the upper plenum and one to the lower plenum.  The H2O from
0016    C   the upper plenum is superheated over the whole range of pressures,
0017    C   with the critical pressure at 8.9976D6 Pa.  The H2O from the lower
0018    C   plenum is subcooled.  This subroutine also determines the specific
0019    C   internal energy of the steam and liquid ( SESTM and SEH2OL ).
0020            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0021            IMPLICIT INTEGER ( I-L,N )
0022            COMMON /INPUT/
0023          1 X, APRV,
0024          2 PPRV, XLCPRV,
0025          3 DELTAI, TIMEND, NPIPES, VTOT,
0026          4 TEPS, PEPS, VR0
0027    C
0028            IF  ( P .LE. 7.54533D6 )  THEN
0029              FRSTM = 1.947
0030              FRH2O = 11.064
0031            ELSE IF (( P .LE. 8.2736D6 ) .AND. ( P .GT. 7.54533D6 )) THEN
0032              FRSTM = 1.947
0033              FRH2O = -5.91814D-7 * P + 15.5294
0034            ELSE IF (( P .LE. 8.9976D6 ) .AND. ( P .GT. 8.2736D6 )) THEN
0035              FRSTM = 1.947
0036              FRH2O = -6.326D-7 * P  + 15.8669
0037            ELSE IF (( P .LE. 9.6526D6 ) .AND. ( P .GT. 8.9976D6 )) THEN
0038              FRH2O = -6.2305D-7 * P + 15.781
0039              FRSTM = -6.56489D-9 * P + 2.00607
0040            ELSE IF (( P .LE. 1.0342D7 ) .AND. ( P .GT. 9.6526D6 )) THEN
0041              FRSTM = -3.04613D-8 * P + 2.23673
0042              FRH2O = -7.67044D-7 * P + 17.1709
0043            ELSE IF (( P .LE. 1.1032D7 ) .AND. ( P .GT. 1.0342D7 )) THEN
0044              FRSTM = -5.82609D-8 * P + 2.52423
0045              FRH2O = -6.85942D-7 * P + 16.3321
0046            ELSE IF (( P .LE. 1.1721D7 ) .AND. ( P .GT. 1.1032D7 )) THEN
0047              FRSTM = -7.73585D-8 * P + 2.73492
0048              FRH2O = -9.00871D-7 * P + 18.7032
0049            ELSE IF (( P .LE. 1.241D7 ) .AND. ( P .GT. 1.1721D7 )) THEN
0050              FRSTM = -1.16691D-7 * P + 3.19593
0051              FRH2O = -8.22642D-7 * P + 17.7863
0052            ELSE IF (( P .LE. 1.31D7 ) .AND. ( P .GT. 1.241D7 )) THEN
0053              FRSTM = -1.45073D-7 * P + 3.54815
0054              FRH2O = -8.69565D-7 * P + 18.3686
0055            ELSE IF (( P .LE. 1.3789D7 ) .AND. ( P .GT. 1.31D7 )) THEN
0056              FRSTM = -1.89695D-7 * P + 4.13271
0057              FRH2O = -1.02496D-6 * P + 20.4043
```

```
0058            ELSE IF (( P .LE. 1.4479D7 ) .AND. ( P .GT. 1.3789D7 )) THEN
0059              FRSTM = -2.33623D-7 * P + 4.73843
0060              FRH2O = -1.14391D-6 * P + 22.0445
0061            ELSE IF (( P .LE. 1.5168D7 ) .AND. ( P .GT. 1.4479D7 )) THEN
0062              FRSTM = -3.2656D-7 * P + 6.08407
0063              FRH2O = -1.43585D-6 * P + 26.2715
0064            ELSE IF (( P .LE. 1.5858D7 ) .AND. ( P .GT. 1.5168D7 )) THEN
0065              FRSTM = -4.50783D-7 * P + 7.96827
0066              FRH2O = -1.81478D-6 * P + 32.0191
0067            ELSE IF (( P .LE. 1.6547D7 ) .AND. ( P.GT. 1.5858D7 )) THEN
0068              FRSTM = -1.18978D-6 * P + 19.6873
0069              FRH2O = -4.7029D-6 * P + 77.8189
0070            ELSE
0071              FRH2O = 0.
0072              FRSTM = 0.
0073            END IF
0074      C     Now the total flowrates are determined by multiplying FRH2O
0075      C   and FRSTM by the number of broken pipes.
0076            FRH2O = FRH2O * NPIPES
0077            FRSTM = FRSTM * NPIPES
0078      C
0079      C     Now to determine the specific energy of the H2O as it leaves
0080      C   the break and enters the reaction zone.  The energy for the steam
0081      C   has been curve fitted to a parabolic form, with the independant
0082      C   variable being the pressure at the break.  If the system pressure
0083      C   is less than the critical pressure (8.9976D6 Pa ), then the
0084      C   energy of the steam is determined at the critical pressure.
0085      C   The specific energy is determined from the 1st law as:
0086      C    U = Ib - P * V -  1 / 2 * ( VEL ) ** 2  +  XH2OHF
0087      C    where, U is the specific energy, Ib is the back enthalpy,
0088      C   P * V is the pressure at the break times the specific volume
0089      C   at the break,  1/2 * ( VEL ) **2 is the kinetic energy of
0090      C   the water with VEL as the water velocity at the break, and
0091      C   XH2OHF is the heat of formation of the water.  For the subcooled
0092      C   water from the lower plenum, the second and third terms of the
0093      C   above equation are negligable.  Therefore SEH2OL is not a function
0094      C   of the break pressure.
0095            XH2OHF = -2.4185D5
0096            IF  ( P .LE. 8.9976D6 )  THEN
0097              PBREAK = 8.9976D6
0098            ELSE
0099              PBREAK = P
0100            END IF
0101            SESTM = 4.6404165D4 + 5.853535D-4 * PBREAK - 1.0704336D-11
0102           1          * ( PBREAK ** 2. ) + XH2OHF
0103      C
0104            SEH2OL = 2.315D4 + XH2OHF
0105      C
0106      C     That's all folks!
0107            RETURN
0108            END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	1237	PIC CON REL LCL SHR EXE RD NOWRT LONG
2	$LOCAL	16	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	1337	

ENTRY POINTS

Address	Type	Name
0-00000000		FLOWRT

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
3-00000008	R*8	APRV	3-00000020	R*8	DELTAI	AP-00000008@	R*8	FRH2O	AP-0000000C@	R*8	FRSTM
3-00000030	I*4	NPIPES	AP-00000004@	R*8	P	2-00000008	R*8	PBREAK	3-00000044	R*8	PEPS
3-00000010	R*8	PPRV	AP-00000014@	R*8	SEH2OL	AP-00000010@	R*8	SESTM	3-0000003C	R*8	TEPS
3-00000028	R*8	TIMEND	3-0000004C	R*8	VRO	3-00000034	R*8	VTOT	3-00000000	R*8	X
2-00000000	R*8	XH2OHF	3-00000018	R*8	XLCPRV						

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE MASS (
0007         1  FRH2O, FRSTM, TEMPR, MPBI, UMLII, UMH2OI, MLIOHI, MH2I,
0008         1  VNRI, PI, IPRV, VRI, MINERT,
0009         2  DELTAT,
0010         3  MH2O, MSTM, MLMB, MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,
0011         3  FRPRV, VNRF, VRF, VGASF, P, ICONTL )
0012    C
0013    C     This subroutine evaluates the end of timestep masses of the
0014    C  reaction products in the two zones, given the intial masses of
0015    C  the constituents of the zones and the inlet flowrate of water.
0016    C  On the basis of the end of timestep reaction zone composition
0017    C  and the beginning of timestep pressure, the volumes of the
0018    C  reaction and nonreaction zones and the flowrate out of the
0019    C  pressure relief valve are determined.
0020            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0021            IMPLICIT INTEGER ( I-L,N )
0022            LOGICAL DEBUG(7)
0023            COMMON /DEB/ DEBUG, IDBOUT
0024            COMMON /INPUT/
0025         1  X, APRV,
0026         2  PPRV, XLCPRV,
0027         3  DELTAI, TIMEND, NPIPES, VTOT,
0028         4  TEPS, PEPS, VR0
0029            COMMON /PROP/
0030         1  DLMB, DLIOH, DLI, DPB,
0031         2  XLMBHF,
0032         3  TCLMB, TDLMB,
0033         4  APLI
0034            IF  ( DEBUG(3) )  THEN
0035              WRITE ( IDBOUT,1000 )
0036     1000       FORMAT ( ' ENTERING MASS ' )
0037            END IF
0038    C
0039    C     REACTION ZONE MASS BALANCE :
0040    C
0041    C     First, from a mass balance on the reaction zone we can
0042    C  determine the molar composition of the reaction zone at the
0043    C  end of the timestep.
0044            MH2OL = 55.5 * FRH2O * DELTAT
0045            MSTM = 55.5 * FRSTM * DELTAT
0046            MH2O = MH2OL + MSTM
0047            MLI = MH2O / X
0048            MLMB = MLI / APLI
0049            MPBF = ( 1. - APLI ) * MLMB  +  MPBI
0050            IF  ( X .LE. 1. )  THEN
0051              UMLIF = MLI - MH2O  +  UMLII
0052              UMH2OF = 0.
0053              MLIOHF = MH2O  +  MLIOHI
0054              MH2F = 2. * MH2O  +  MH2I
0055            ELSE
0056              UMLIF = 0.
0057              UMH2OF = MH2O - MLI  +  UMH2OI
```

```
0058            MLIOHF = MLI   +  MLIOHI
0059            MH2F = 2. * MLI   +  MH2I
0060          END IF
0061    C
0062    C     NONREACTION ZONE MASS BALANCE :
0063    C
0064    C     From a mass balance on the nonreaction zone, the time rate
0065    C   of change of the nonreaction zone mass is found to be due to
0066    C   the flow of breeder into the reaction zone and the flow of
0067    C   breeder out of the pressure relief valve.
0068    C
0069    C     The flow of breeder into the reaction zone during the
0070    C   timestep is simply MLMB.
0071          MASLMB = ( ( 1 - APLI ) * .20721 + APLI * 6.94D-3 ) * MLMB
0072    C
0073    C     The flow of breeder out of the pressure relief valve is
0074    C   determined from Bernoulli's equation.  When the pressure first
0075    C   becomes greater than PPRV, the rupture disk opens.  The condition
0076    C   of the rupture disk is set by IPRV, 0 = intact disk , 1 =
0077    C   ruptured disk.  IPRV is not set to 1 during execusion of this
0078    C   subroutine, since
0079    C   MASS maybe iterated upon many times during the execusion of
0080    C   DRIVE and MDRIVE.
0081          FRPRV = 0.
0082          IF  ( IPRV .EQ. 1 )  GO TO 100
0083          IF  ( PI .GT. PPRV )  THEN
0084     100    CONTINUE
0085            IF  ( PI .LT. 1.0135D5 )  GO TO 300
0086              FRPRV = APRV * DSQRT ( 2. * DLMB * ( PI - 1.0135D5 )
0087         1            / XLCPRV )
0088     300    CONTINUE
0089          END IF
0090    C
0091          MASPRV = FRPRV * DELTAT
0092    C
0093    C     REACTION AND NONREACTION ZONE VOLUMES :
0094    C
0095    C     The nonreaction zone volume is simply the initial nonreaction
0096    C   zone volume - loss of volume due to the flow of breeder out
0097    C   of the zone.
0098          VNRF = VNRI   -  ( MASPRV + MASLMB ) / DLMB
0099    C
0100    C     The volume of the reaction zone is the total breeder volume
0101    C   -  the nonreaction zone volume.
0102          VRF = VRI   +  ( MASPRV + MASLMB ) / DLMB
0103    C
0104    C     We can now determine the volume of the gas ( H2 and H20g )
0105    C   in the reaction zone.
0106          VGASF = VRF   -  6.94D-3 * UMLIF / DLI   -  2.31D-2 * MLIOHF
0107         1          / DLIOH   -  .20721 * MPBF / DPB
0108    C
0109    C     ISOTHERMAL PRESSURE :
0110    C     Now that the end of timestep gas volume and mass has been
0111    C   determined, we can determine the end of timestep isothermal
0112    C   pressure.  That is, the end of timestep pressure is determined
0113    C   from the ideal gas law using the beginning of timestep reaction
0114    C   zone temperature TRI.
```

```
0115            P = 8.314 * ( MH2F + MINERT + UMH2OF ) * TEMPR / VGASF
0116            IF  ( P .GT. 1.6547D7 )  THEN
0117      C
0118      C       If this condition is true, it means that the shell side
0119      C     pressure has exceeded the water back pressure.  This condition
0120      C     is corrected by a call to PCONTL, which decreases the timestep.
0121              CALL PCONTL (
0122           1  PI, P,
0123           2  DELTAT
0124           3  )
0125                ICONTL = 1
0126                GO TO 200
0127      C
0128      C       This variable alerts the calling routines MDRIVE and DRIVE
0129      C     that DELTAT has been adjusted.
0130            ELSE
0131              ICONTL = 0
0132            END IF
0133      C
0134      C       That's all folks!
0135            IF  ( DEBUG(3) )  THEN
0136              WRITE ( IDBOUT,1001 )  MH2O, MSTM, MLMB, FRPRV
0137       1001     FORMAT ( ' MH2O MSTM MLMB FRPRV ' / 1P4G11.4 )
0138              WRITE ( IDBOUT,1002 )  MPBF, UMLIF, UMH2OF, MLIOHF, MH2F
0139       1002     FORMAT ( ' MPBF UMLIF UMH2OF MLIOHF MH2F ' / 1P5G11.4 )
0140             WRITE ( IDBOUT,1003 )  VNRF, VRF, VGASF, P
0141       1003     FORMAT ( ' VNRF VRF VGASF P ' / 1P4G11.4 )
0142              WRITE ( IDBOUT,1004 )
0143       1004     FORMAT ( ' EXITING MASS ' )
0144            END IF
0145      C
0146       200  CONTINUE
0147            RETURN
0148            END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	739	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	139	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	48	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	1106	

ENTRY POINTS

Address	Type	Name
0-00000000		MASS

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
5-00000038	R*8	APLI	4-00000008	R*8	APRV	4-00000020	R*8	DELTAI	AP-00000038@	R*8	DELTAT
5-00000010	R*8	DLI	5-00000008	R*8	DLIOH	5-00000000	R*8	DLMB	5-00000018	R*8	DPB
AP-00000004@	R*8	FRH2O	AP-0000005C@	R*8	FRPRV	AP-00000008@	R*8	FRSTM	AP-00000070@	I*4	ICONTL
3-0000001C	I*4	IDBOUT	AP-0000002C@	I*4	IPRV	2-00000010	R*8	MASLMB	2-00000018	R*8	MASPRV
AP-00000058@	R*8	MH2F	AP-00000020@	R*8	MH2I	AP-0000003C@	R*8	MH2O	2-00000000	R*8	MH2OL
AP-00000034@	R*8	MINERT	2-00000008	R*8	MLI	AP-00000054@	R*8	MLIOHF	AP-0000001C@	R*8	MLIOHI
AP-00000044@	R*8	MLMB	AP-00000048@	R*8	MPBF	AP-00000010@	R*8	MPBI	AP-00000040@	R*8	MSTM
4-00000030	I*4	NPIPES	AP-0000006C@	R*8	P	4-00000044	R*8	PEPS	AP-00000028@	R*8	PI
4-00000010	R*8	PPRV	5-00000028	R*8	TCLMB	5-00000030	R*8	TDLMB	AP-0000000C@	R*8	TEMPR
4-0000003C	R*8	TEPS	4-00000028	R*8	TIMEND	AP-00000050@	R*8	UMH2OF	AP-00000018@	R*8	UMH2OI
AP-0000004C@	R*8	UMLIF	AP-00000014@	R*8	UMLII	AP-00000068@	R*8	VGASF	AP-00000060@	R*8	VNRF
AP-00000024@	R*8	VNRI	4-0000004C	R*8	VRO	AP-00000064@	R*8	VRF	AP-00000030@	R*8	VRI
4-00000034	R*8	VTOT	4-00000000	R*8	X	4-00000018	R*8	XLCPRV	5-00000020	R*8	XLMBHF

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
0-00000105	100	0-000002E2	200	0-00000141	300	1-00000000	1000'	1-00000012	1001'	1-00000033	1002'
1-0000005D	1003'	1-0000007A	1004'								

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name
R*8	MTH$DSQRT		PCONTL

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE PCONTL (
0007         1  PI, PF,
0008         2  DELTAT
0009         3  )
0010    C
0011    C     This subroutine decreases the timestep in order to lower the
0012    C  pressure increase during the timestep.
0013            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0014            IMPLICIT INTEGER ( I-L,N )
0015            LOGICAL DEBUG(7)
0016            COMMON /DEB/ DEBUG, IDBOUT
0017    C
0018            IF  ( DEBUG(6) )  WRITE ( IDBOUT,1000 )  DELTAT
0019    C
0020            DELTAT = DELTAT * PI  / PF
0021    C
0022            IF  ( DEBUG(6) )  WRITE ( IDBOUT,1001 ) DELTAT
0023     1000     FORMAT ( '********** THE ORIGINAL DELTAT = ', 1P1G11.4 )
0024     1001     FORMAT ( '             IS NOW =              ', 1P1G11.4 )
0025    C
0026    C     That's all folks!
0027            RETURN
0028            END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	101	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	82	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	215	

ENTRY POINTS

Address	Type	Name
0-00000000		PCONTL

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
AP-0000000C@	R*8	DELTAT	3-0000001C	I*4	IDBOUT	AP-00000008@	R*8	PF	AP-00000004@	R*8	PI

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)

LABELS

Address	Label	Address	Label
1-00000000	1000'	1-00000029	1001'

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE ENERRZ (
0007          1 TEMPRI, TEMPNI, DELTAT, PI, P, VRF, MPBI, UMLII,
0008          1 UMH2OI, MLIOHI, MH2I, MH2O, MSTM, MLMB, MPBF, UMLIF, UMH2OF,
0009          1 MLIOHF, MH2F, VRI, URZI, SESTM, SEH2OL,
0010          2
0011          3 QCOND, PVDOT, URZF, ENGIN, QFCRZ, TEMPRF, DRDT )
0012    C
0013    C     This subroutine solves an energy balance on the reaction
0014    C  zone.  The reaction zone end of timestep energy is determined
0015    C  by the change in energy during the timestep.  The end of timestep
0016    C  average reaction zone temperature is then determined.
0017            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0018            IMPLICIT INTEGER ( I-L,N )
0019            DOUBLE PRECISION  P(10), VRF(10), PV(10)
0020            LOGICAL DEBUG(7)
0021            COMMON /DEB/ DEBUG, IDBOUT
0022            COMMON /INPUT/
0023          1 X, APRV,
0024          2 PPRV, XLCPRV,
0025          3 DELTAI, TIMEND, NPIPES, VTOT,
0026          4 TEPS, PEPS, VRO
0027            COMMON /PROP/
0028          1 DLMB, DLIOH, DLI, DPB,
0029          2 XLMBHF,
0030          3 TCLMB, TDLMB,
0031          4 APLI
0032            IF  ( DEBUG(4) )  THEN
0033              WRITE ( IDBOUT,1000 )
0034     1000       FORMAT ( ' ENTERING ENERRZ ' )
0035            END IF
0036    C
0037    C     The energy balance can be expressed as:
0038    C  URZF = URZI + DELTAT* ( -PVDOT - QCOND + ENGIN - QFCRZ )
0039    C
0040    C
0041    C  ***** QFCRZ *****
0042    C     This is the change in reaction zone energy due to forced
0043    C  convection to unbroken steam tubes.  This quantity is very
0044    C  approximate.  So we assume it is not a function of TEMPRF
0045    C  for simplicity.
0046            QFCRZ = 1.36D5 * ( VRF(10) + VRI ) * ( TEMPRI - 648. )
0047    C
0048    C  ***** PVDOT *****
0049    C     This is the energy change due to the work the fluid in the
0050    C  reaction zone does as it expands.  There are 10 parts to this
0051    C  quantity for each of the 10 subtimesteps.
0052            DELT = DELTAT * .1
0053            PV(1) = .5 * ( P(1) + PI ) * ( VRF(1) - VRI ) / DELT
0054            DO 100  I = 2,10
0055              PV(I) = .5 * ( P(I) + P(I-1) ) * ( VRF(I) - VRF(I-1) )
0056         1            / DELT
0057     100    CONTINUE
```

```
0058    C
0059            PVDOT = 0.
0060            DO 200  J = 1,10
0061              PVDOT = PVDOT + PV(J)
0062     200    CONTINUE
0063            PVDOT = PVDOT * .1
0064    C
0065    C  ***** ENGIN *****
0066    C     This is the energy of the H2O and the breeder flowing into
0067    C  the reaction zone during the timestep.
0068            PAVE = ( PI + P(10) ) * .5
0069    C
0070            CALL SENER (
0071           1  TEMPNI, PAVE,
0072           2
0073           3  SEH2, SELIOH, SEH2O, SEPB, SELI,
0074           3  DSEH2, DSLIOH, DSEH2O, DSEPB, DSELI )
0075    C
0076    C     The temperature at which the liquid metal breeder internal
0077    C  energy is determined at is the temperature of the nonreaction
0078    C  zone, since this is the origin of the LMB.
0079            ENGIN = ( MSTM * SESTM + ( MH2O - MSTM ) * SEH2OL  +
0080           1          MLMB * ( ( 1 - APLI ) * SEPB  + APLI * SELI +
0081           2          XLMBHF ) ) / DELTAT
0082    C
0083    C  ***** URZI *****
0084    C     This is the internal energy of the reaction zone contents
0085    C  at the beginning of the timestep.  It is equal to the final
0086    C  internal energy of the reaction zone from the last timestep.
0087    C
0088    C     Now we are ready for the temperature iteration loop.
0089            TEMP = TEMPRI
0090     300    CONTINUE
0091    C
0092    C  ***** QCOND *****
0093    C     This is the heat transfered from the reaction zone to the
0094    C  nonreaction zone due to conduction.  It is a function of the
0095    C  reaction zone final temperature.
0096              RADRZF = .62 * ( VRF(10) ** ( 1. / 3. ) )
0097              RADRZI = .62 * ( VRI ** ( 1. / 3. ) )
0098              RADAVG = .75 * ( RADRZF ** 4. - RADRZI ** 4. ) /
0099           1              ( RADRZF ** 3. - RADRZI ** 3. )
0100    C
0101              DRDT = ( RADRZF - RADRZI ) / DELTAT
0102    C
0103              PEND = 1.77 * DSQRT ( DELTAT * TDLMB )
0104    C
0105    C
0106              QCOND = 6.23 * TCLMB * ( TEMP + TEMPRI - 2. * TEMPNI )
0107           1             * ( RADAVG ** 2. ) / PEND
0108    C
0109    C  ***** URZF *****
0110    C     We now sum up the energy flows to determine the end of
0111    C  timestep reaction zone internal energy.
0112              URZF = URZI + DELTAT * ( ENGIN - QFCRZ - PVDOT - QCOND )
0113    C
0114    C  ***** TEMPRF *****
```

```
0115     C     We now determine the end of timestep temperature of the
0116     C  reaction zone from the value of URZF.
0117               CALL ROOT (
0118           1  TEMPRI, URZF, PAVE,
0119           1  MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,
0120           2
0121           3  TEMPRF )
0122     C
0123               IF  ( ( DABS ( TEMPRF - TEMP ) ) .GT. TEPS )  THEN
0124     C      If this condition is true it means that the temperature used
0125     C  to calculate QCOND is not the end of timestep temperature.
0126     C  Thus we must iterate until this condition is false.
0127                 TEMP = TEMPRF
0128                 GO TO 300
0129               END IF
0130     C
0131     C     That's all folks!
0132               IF  ( DEBUG(4) )  THEN
0133                 WRITE ( IDBOUT,1001 ) URZI, QCOND, PVDOT
0134      1001         FORMAT ( ' URZI QCOND PVDOT ' / 1P3G11.4 )
0135                 WRITE ( IDBOUT,1002 ) QFCRZ, ENGIN, PEND
0136      1002         FORMAT ( ' QFCRZ ENGIN PEND ' / 1P3G11.4 )
0137                 WRITE ( IDBOUT,1003 ) URZF, TEMPRF
0138      1003         FORMAT ( ' URZF TEMPRF ' / 1P2G11.4 )
0139                 WRITE ( IDBOUT,1004 )
0140      1004         FORMAT ( ' EXITING ENERRZ ' )
0141               END IF
0142     C
0143               RETURN
0144               END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	872	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	121	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	372	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	1545	

ENTRY POINTS

Address	Type	Name
0-00000000		ENERRZ

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
5-00000038	R*8	APLI	4-00000008	R*8	APRV	2-00000050	R*8	DELT	4-00000020	R*8	DELTAI
AP-0000000C@	R*8	DELTAT	5-00000010	R*8	DLI	5-00000008	R*8	DLIOH	5-00000000	R*8	DLMB
5-00000018	R*8	DPB	AP-00000078@	R*8	DRDT	2-00000088	R*8	DSEH2	2-00000098	R*8	DSEH2O
2-000000A8	R*8	DSELI	2-000000A0	R*8	DSEPB	2-00000090	R*8	DSLIOH	AP-0000006C@	R*8	ENGIN
2-000000D8	I*4	I	3-0000001C	I*4	IDBOUT	2-000000DC	I*4	J	AP-0000004C@	R*8	MH2F
AP-0000002C@	R*8	MH2I	AP-00000030@	R*8	MH2O	AP-00000048@	R*8	MLIOHF	AP-00000028@	R*8	MLIOHI
AP-00000038@	R*8	MLMB	AP-0000003C@	R*8	MPBF	AP-0000001C@	R*8	MPBI	AP-00000034@	R*8	MSTM
4-00000030	I*4	NPIPES	2-00000058	R*8	PAVE	2-000000D0	R*8	PEND	4-00000044	R*8	PEPS
AP-00000010@	R*8	PI	4-00000010	R*8	PPRV	AP-00000064@	R*8	PVDOT	AP-00000060@	R*8	QCOND
AP-00000070@	R*8	QFCRZ	2-000000C8	R*8	RADAVG	2-000000B8	R*8	RADRZF	2-000000C0	R*8	RADRZI
2-00000060	R*8	SEH2	2-00000070	R*8	SEH2O	AP-0000005C@	R*8	SEH2OL	2-00000080	R*8	SELI
2-00000068	R*8	SELIOH	2-00000078	R*8	SEPB	AP-00000058@	R*8	SESTM	5-00000028	R*8	TCLMB
5-00000030	R*8	TDLMB	2-000000B0	R*8	TEMP	AP-00000008@	R*8	TEMPNI	AP-00000074@	R*8	TEMPRF
AP-00000004@	R*8	TEMPRI	4-0000003C	R*8	TEPS	4-00000028	R*8	TIMEND	AP-00000044@	R*8	UMH2OF
AP-00000024@	R*8	UMH2OI	AP-00000040@	R*8	UMLIF	AP-00000020@	R*8	UMLII	AP-00000068@	R*8	URZF
AP-00000054@	R*8	URZI	4-0000004C	R*8	VRO	AP-00000050@	R*8	VRI	4-00000034	R*8	VTOT
4-00000000	R*8	X	4-00000018	R*8	XLCPRV	5-00000020	R*8	XLMBHF			

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)
AP-00000014@	R*8	P	80	(10)
2-00000000	R*8	PV	80	(10)
AP-00000018@	R*8	VRF	80	(10)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
**	100	**	200	0-0000013D	300	1-00000000	1000'	1-00000014	1001'	1-00000031	1002'
1-0000004E	1003'	1-00000066	1004'								

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name	Type	Name
R*8	MTH$DSQRT		ROOT		SENER

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE SENER (
0007           1  T, P,
0008           2
0009           3  SEH2,  SELIOH, SEH2O,  SEPB,  SELI,
0010           3  DSEH2, DSLIOH, DSEH2O, DSEPB, DSELI )
0011    C
0012    C     This subroutine calculates the specific energy and the
0013    C  temperature derivative of the specific energy for H2, LIOH,
0014    C  H2O, PB, and LI, as functions of the input temperature (T).
0015    C
0016    C     The constants used in the subroutine are taken from the
0017    C  JANAF tables.  The reference temperature is 273.15 K.
0018    C
0019            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0020            IMPLICIT INTEGER ( I-L,N )
0021    C  ***** H2 *****
0022    C     The specific heat at constant volume for an ideal diatomic
0023    C  gas is 5/2* ideal gas constant.
0024            SEH2 = 20.75 * ( T - 273.15 )
0025            DSEH2 = 20.75
0026    C
0027    C  ***** LIOH *****
0028    C     LIOH changes phase (melts) at 744.3 K.  For T .LE. 744.3
0029    C  the specific energy is curve fitted so that the specific energy
0030    C  and the temperature derivative of the specific energy are
0031    C  continuous at T=744.3 K.  The specific energy includes the
0032    C  heat of formation (4.7388D5 J/MOLE ).
0033            IF  ( T .GE. 744.3 )  THEN
0034              SELIOH = 86.78 * ( T - 744.3 ) - 4.243D5
0035              DSLIOH = 86.78
0036            ELSE
0037              SELIOH = -3.931D-2 * ( ( T - 273.15 ) ** 2. )  +
0038           1              123.8 * ( T - 273.15 )  - 4.739D5
0039              DSLIOH = -7.862D-2 * ( T - 273.15 ) + 123.8
0040            END IF
0041    C
0042    C  ***** H2O *****
0043    C     The water is assumed to be superheated steam.  The specific
0044    C  heat at constant volume is assumed to be 27. J/MOLE over the
0045    C  range of pressure and temperature.  The specific energy is
0046    C  equal to :
0047    C    27. * ( T - TVAP ) + HVAP + XH2OHF
0048    C  where: TVAP is the vaporation temperature, HVAP is the
0049    C  saturated steam enthalpy and XH2OHF is the water heat of formation.
0050    C  TVAP and HVAP are functions of pressure, the equations for which
0051    C  were determined by curve fitting data between pressures of
0052    C  1.724D5 and 1.6547D7 Pa.
0053            IF  ( P .EQ. 0. ) THEN
0054    C     P will equal 0 when the nonreaction zone  energy is being
0055    C  determined. Since the nonreaction zone does not contain any
0056    C  water the specific energy of the water in that case need not
0057    C  be determined.
```

```
0058     C
0059               SEH2O = 0.
0060               DSEH2O = 0.
0061             ELSE
0062               XH2OHF = -2.418D5
0063               TVAP = 308.84026 * DEXP ( ( DLOG( P ) - 5.9053292 )
0064          1         ** 2. / 163.65165 )
0065               HVAP = 5.0249453D4 * DEXP ( -1. * (( P - 4.5033433D6 )
0066          1         ** 2. / 1.6713273D15 ) )
0067               SEH2O = 27. * ( T - TVAP ) + HVAP + XH2OHF
0068               DSEH2O = 27.
0069             END IF
0070     C
0071     C  ***** PB *****
0072     C     We assume that T .GT. Tmelt = 600.6 K.
0073               SEPB = 30.3 * ( T - 600.6 )  +  1.394D4
0074               DSEPB = 30.3
0075     C
0076     C  ***** LI *****
0077     C     We assume that T .GT. Tmelt = 453.7 K.
0078               SELI = 29.7 * ( T - 453.7 )  +  7.85D3
0079               DSELI = 29.7
0080     C
0081               RETURN
0082               END
```

93

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	469	PIC CON REL LCL SHR EXE RD NOWRT LONG
2	$LOCAL	24	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
	Total Space Allocated	493	

ENTRY POINTS

Address	Type	Name
0-00000000		SENER

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
AP-00000020@	R*8	DSEH2	AP-00000028@	R*8	DSEH2O	AP-00000030@	R*8	DSELI	AP-0000002C@	R*8	DSEPB
AP-00000024@	R*8	DSLIOH	2-00000010	R*8	HVAP	AP-00000008@	R*8	P	AP-0000000C@	R*8	SEH2
AP-00000014@	R*8	SEH2O	AP-0000001C@	R*8	SELI	AP-00000010@	R*8	SELIOH	AP-00000018@	R*8	SEPB
AP-00000004@	R*8	T	2-00000008	R*8	TVAP	2-00000000	R*8	XH2OHF			

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name
R*8	MTH$DEXP	R*8	MTH$DLOG

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE ROOT (
0007         1  TI, UF, P,
0008         1  MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,
0009         2
0010         3  TF )
0011    C
0012    C     This subroutine determines the end of timestep temperture by
0013    C  Newton's method for finding the roots of an equation.
0014            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0015            IMPLICIT INTEGER ( I-L,N )
0016            LOGICAL DEBUG (7)
0017            COMMON /INPUT/
0018         1  X, APRV,
0019         2  PPRV, XLCPRV,
0020         3  DELTAI, TIMEND, NPIPES, VTOT,
0021         4  TEPS, PEPS, VRI
0022            COMMON /DEB/ DEBUG, IDBOUT
0023            IF  ( DEBUG(5) )  THEN
0024              WRITE ( IDBOUT,1000 )
0025     1000       FORMAT ( ' ENTERING ROOT ' )
0026              WRITE ( IDBOUT,1001 ) TI, UF, MPBF, UMLIF
0027     1001       FORMAT ( ' TI UF MPBF UMLIF ' / 1P4G11.4 )
0028              WRITE ( IDBOUT,1002 ) UMH2OF, MLIOHF, MH2F
0029     1002       FORMAT ( ' UMH2OF MLIOHF MH2F ' / 1P3G11.4 )
0030            END IF
0031    C
0032    C     Newton's method for finding roots gives:
0033    C
0034    C    TF = TI - F(TI) / ( dF(TI)/dT )
0035    C
0036    C  where,
0037    C  F(TI) = UF - ( MPBF*SEPB + UMLIF*SELIF + UMH2OF*SEH2O +
0038    C           MLIOHF*SELIOH + MH2F*SEH2F )
0039    C
0040    C
0041    C  and,
0042    C  dF(TI)/dT = MPBF*DSEPB + UMLIF*DSELI + UMH2OF*DSEH2O +
0043    C               MLIOHF*DSLIOH + MH2F*DSEH2
0044    C
0045            TDUM = TI
0046     100    CONTINUE
0047    C
0048            CALL SENER (
0049         1  TDUM, P,
0050         2
0051         3  SEH2, SELIOH, SEH2O, SEPB, SELI,
0052         3  DSEH2, DSLIOH, DSEH2O, DSEPB, DSELI )
0053    C
0054            TF = TDUM  +  ( UF - ( MH2F * SEH2  +  MLIOHF * SELIOH  +
0055         1       UMH2OF * SEH2O  +  MPBF * SEPB  +  UMLIF * SELI ) ) /
0056         2       ( MH2F * DSEH2  +  MLIOHF * DSLIOH  +  UMH2OF * DSEH2O
0057         3       +  MPBF * DSEPB  +  UMLIF * DSELI )
```

```
0058     C
0059              IF  ( DEBUG(5) )  THEN
0060                WRITE ( IDBOUT,1003 )  TF
0061       1003       FORMAT ( ' ITERATION TF ' / 1P1G11.4 )
0062              END IF
0063     C
0064     C
0065              IF  ( ( DABS ( TF - TDUM ) ) .GT. TEPS )  THEN
0066     C       If this condition is true, then we must reiterate until
0067     C    TF - TDUM converges to TEPS .
0068     C
0069                TDUM = TF
0070                GO TO 100
0071              END IF
0072     C
0073              IF  ( DEBUG(5) )  THEN
0074                WRITE ( IDBOUT,1004 )  TF
0075       1004       FORMAT ( ' TF ' / 1P1G11.4 )
0076                WRITE ( IDBOUT,1005 )
0077       1005       FORMAT ( ' EXITING ROOT ' )
0078              END IF
0079     C
0080     C       That's all folks!
0081              RETURN
0082              END
```


PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	412	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	131	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	140	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	799	

ENTRY POINTS

Address	Type	Name
0-00000000		ROOT

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
3-00000008	R*8	APRV	3-00000020	R*8	DELTAI	2-00000030	R*8	DSEH2	2-00000040	R*8	DSEH20
2-00000050	R*8	DSELI	2-00000048	R*8	DSEPB	2-00000038	R*8	DSLIOH	4-0000001C	I*4	IDBOUT
AP-00000020@	R*8	MH2F	AP-0000001C@	R*8	MLIOHF	AP-00000010@	R*8	MPBF	3-00000030	I*4	NPIPES
AP-0000000C@	R*8	P	3-00000044	R*8	PEPS	3-00000010	R*8	PPRV	2-00000008	R*8	SEH2

2-00000018	R*8	SEH2O	2-00000028	R*8	SELI	2-00000010	R*8	SELIOH	2-00000020	R*8	SEPB
2-00000000	R*8	TDUM	3-0000003C	R*8	TEPS	AP-00000024@	R*8	TF	AP-00000004@	R*8	TI
3-00000028	R*8	TIMEND	AP-00000008@	R*8	UF	AP-00000018@	R*8	UMH2OF	AP-00000014@	R*8	UMLIF
3-0000004C	R*8	VRI	3-00000034	R*8	VTOT	3-00000000	R*8	X	3-00000018	R*8	XLCPRV

ARRAYS

Address	Type	Name	Bytes	Dimensions
4-00000000	L*4	DEBUG	28	(7)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
0-000000AB	100	1-00000000	1000'	1-00000012	1001'	1-0000002F	1002'	1-0000004E	1003'	1-00000065	1004'
1-00000072	1005'										

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name
	SENER

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE ENERNZ (
0007         1  VNRI, VNRF, TEMPNI, DELTAT, PVDOT, QCOND, FRPRV, MLMB, UNZI,
0008         2
0009         3  UNZF, TEMPNF, ENGOUT, QFCNZ )
0010    C
0011    C     This subroutine solves an energy balance on the nonreaction
0012    C  zone.  The nonreation zone end of timestep energy is determined
0013    C  by the change in energy during the timestep.  The end of timestep
0014    C  average nonreaction zone temperature is then determined.
0015            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0016            IMPLICIT INTEGER ( I-L,N )
0017            LOGICAL DEBUG(7)
0018            COMMON /DEB/ DEBUG, IDBOUT
0019            COMMON /INPUT/
0020         1  X, APRV,
0021         2  PPRV, XLCPRV,
0022         3  DELTAI, TIMEND, NPIPES, VTOT,
0023         4  TEPS, PEPS, VRO
0024            COMMON /PROP/
0025         1  DLMB, DLIOH, DLI, DPB,
0026         2  XLMBHF,
0027         3  TCLMB, TDLMB,
0028         4  APLI
0029            IF  ( DEBUG(7) ) THEN
0030              WRITE ( IDBOUT,1000 )
0031     1000       FORMAT ( ' ENTERING ENERNZ ' )
0032            END IF
0033    C
0034    C     The energy balance can be expressed as :
0035    C  UNZF = UNZI + DELTAT * ( PVDOT + QCOND - ENGOUT - QFCNZ )
0036    C
0037    C
0038    C  ***** QFCNZ *****
0039    C     This is the change in the nonreaction zone energy due to
0040    C  forced convection to unbroken steam tubes.  This function is
0041    C  very approximate.
0042            QFCNZ = 4.3D5 * ( VNRF + VNRI ) * ( TEMPNI - 648. )
0043    C
0044    C  ***** PVDOT *****
0045    C     This is just the work due to expansion as calculated in
0046    C  ENERRZ, with an opposite sign.
0047    C
0048    C  ***** QCOND *****
0049    C     This is the heat flow due to conduction as calcculated in
0050    C  ENERRZ, again with an opposite sign.
0051    C
0052    C  ***** ENGOUT *****
0053    C     This is the energy of the breeder flowing out of the nonreaction
0054    C  zone through the pressure relief valve (FRPRV) and to the reaction
0055    C  zone (MLMB).
0056            P = 0.
0057            CALL SENER (
```

```
0058          1  TEMPNI, P,
0059          2
0060          3  SEH2, SELIOH, SEH2O, SEPB, SELI,
0061          3  DSEH2, DSLIOH, DSEH2O, DSEPB, DSELI )
0062             SELMB = ( 1. - APLI ) * SEPB  +  APLI * SELI  +  XLMBHF
0063             ENGOUT = ( MLMB / DELTAT  +  FRPRV / ( ( 1. - APLI )
0064          1           * .20721 + APLI * 6.94D-3 ) ) * SELMB
0065     C
0066     C  ***** UNZI *****
0067     C     This is the internal energy of the liquid metal breeder
0068     C  in the nonreaction zone at the beginning of the timestep.
0069     C  It equals the final internal energy of the nonreaction zone
0070     C  from the last timestep.
0071     C
0072     C  ***** UNZF *****
0073     C     We can now sum up the energy changes to determine the end
0074     C  of timestep nonreaction zone internal energy.
0075             UNZF = UNZI  +  DELTAT * ( PVDOT + QCOND - ENGOUT - QFCNZ )
0076     C
0077     C  ***** TEMPNF *****
0078     C     We can now determine the nonreaction zone end of timestep
0079     C  temperature from the value of UNZF.
0080     C
0081     C  Before we call ROOT though, we must input the correct list of
0082     C  the dummy variables shared with ROOT, so that ROOT performs
0083     C  properly.
0084             MH2N = 0.
0085             MLIOHN = 0.
0086             UMH2ON = 0.
0087             MLMBNF = VNRF * DLMB / ( ( 1. - APLI ) * .20721  +
0088          1           APLI * 6.94D-3 )
0089             MPBN = ( 1. - APLI ) * MLMBNF
0090             MLIN = APLI * MLMBNF
0091     C     Also, ROOT does not allow for the heat of formation of the
0092     C  of the breeder directly, so it must be inputted indirectly.
0093             UNZ = UNZF - MLMBNF * XLMBHF
0094             CALL ROOT (
0095          1  TEMPNI, UNZ, P,
0096          1  MPBN, MLIN, UMH2ON, MLIOHN, MH2N,
0097          2
0098          3  TEMPNF )
0099     C
0100             IF  ( DEBUG(7) )  THEN
0101               WRITE ( IDBOUT,1001 ) UNZI, UNZF, TEMPNF
0102      1001       FORMAT ( ' UNZI UNZF TEMPNF ' / 1P3G11.4 )
0103               WRITE ( IDBOUT,1002 ) ENGOUT, QFCNZ
0104      1002       FORMAT ( ' ENGOUT QFCNZ ' / 1P2G11.4 )
0105               WRITE ( IDBOUT,1003 )
0106      1003       FORMAT ( ' EXITING ENERNZ ' )
0107             END IF
0108     C
0109     C     That's all folks!
0110             RETURN
0111             END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	423	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	93	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	244	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	DEB	32	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	940	

ENTRY POINTS

Address	Type	Name
0-00000000		ENERNZ

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
5-00000038	R*8	APLI	4-00000008	R*8	APRV	4-00000020	R*8	DELTAI	AP-00000010@	R*8	DELTAT
5-00000010	R*8	DLI	5-00000008	R*8	DLIOH	5-00000000	R*8	DLMB	5-00000018	R*8	DPB
2-00000030	R*8	DSEH2	2-00000040	R*8	DSEH2O	2-00000050	R*8	DSELI	2-00000048	R*8	DSEPB
2-00000038	R*8	DSLIOH	AP-00000030@	R*8	ENGOUT	AP-0000001C@	R*8	FRPRV	3-0000001C	I*4	IDBOUT
2-00000060	R*8	MH2N	2-00000088	R*8	MLIN	2-00000068	R*8	MLIOHN	AP-00000020@	R*8	MLMB
2-00000078	R*8	MLMBNF	2-00000080	R*8	MPBN	4-00000030	I*4	NPIPES	2-00000000	R*8	P
4-00000044	R*8	PEPS	4-00000010	R*8	PPRV	AP-00000014@	R*8	PVDOT	AP-00000018@	R*8	QCOND
AP-00000034@	R*8	QFCNZ	2-00000008	R*8	SEH2	2-00000018	R*8	SEH2O	2-00000028	R*8	SELI
2-00000010	R*8	SELIOH	2-00000058	R*8	SELMB	2-00000020	R*8	SEPB	5-00000028	R*8	TCLMB
5-00000030	R*8	TDLMB	AP-0000002C@	R*8	TEMPNF	AP-0000000C@	R*8	TEMPNI	4-0000003C	R*8	TEPS
4-00000028	R*8	TIMEND	2-00000070	R*8	UMH2ON	2-00000090	R*8	UNZ	AP-00000028@	R*8	UNZF
AP-00000024@	R*8	UNZI	AP-00000008@	R*8	VNRF	AP-00000004@	R*8	VNRI	4-0000004C	R*8	VRO
4-00000034	R*8	VTOT	4-00000000	R*8	X	4-00000018	R*8	XLCPRV	5-00000020	R*8	XLMBHF

ARRAYS

Address	Type	Name	Bytes	Dimensions
3-00000000	L*4	DEBUG	28	(7)

LABELS

Address	Label	Address	Label	Address	Label	Address	Label
1-00000000	1000'	1-00000014	1001'	1-00000031	1002'	1-0000004A	1003'

FUNCTIONS AND SUBROUTINES REFERENCED

Type	Name	Type	Name
	ROOT		SENER

```
0001    C
0002    C
0003    C*****************************************************
0004    C
0005    C
0006            SUBROUTINE OUTPUT (
0007         1  TIME, TEMPRF, TEMPNF, PF, VRF, VGASF, MH2OFR, MLMBFR,
0008         1  MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, MLIOHF,
0009         1  QCOND, PVDOT, ENGOUT, ENGIN, URZF, UNZF, QFCRZ, QFCNZ,
0010         1  DRDT, SUMQ, SUMU, URZI, UNZI,
0011         2  NOUT, NFLAG, PMAX, TMAX
0012         3  )
0013    C
0014    C     This subroutine directs the output to different files.
0015    C  There are 5 different output files with these logical numbers
0016    C  set as parameters.
0017    C
0018    C     IOUT - is the general output file.
0019    C
0020    C     ITEMP - gives a list of TIME, TEMPRF, and TEMPNF.
0021    C
0022    C     IPRES - """""""""""""""" TIME and PF.
0023    C
0024    C     IMH2  - """""""""""""""" TIME and MH2F.
0025    C
0026    C     IFLOW - """""""""""""""" TIME, MH2O, and FRPRV.
0027    C
0028    C    These last 4 files will simply contain a list of numbers
0029    C  without comment.  This allows these lists to be easily con-
0030    C  nected to graphics programs.
0031            IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
0032            IMPLICIT INTEGER ( I-L,N )
0033            COMMON /OUT/ JOUT1, JOUT2, JOUT3
0034            COMMON /INPUT/
0035         1  X, APRV,
0036         2  PPRV, XLCPRV,
0037         3  DELTAI, TIMEND, NPIPES, VTOT,
0038         4  TEPS, PEPS, VRO
0039            COMMON  /PROP/
0040         1  DLMB, DLIOH, DLI, DPB,
0041         2  XLMBHF,
0042         3  TCLMB, TDLMB,
0043         4  APLI
0044            PARAMETER  ( IOUT = 20, ITEMP = 11, IPRES = 12, IMH2 = 13,
0045         1                 IFLOW = 14 )
0046            NOUT = NOUT + 1
0047    C
0048    C
0049    C
0050    C
0051    C
0052    C     First we determine if the current value of PF or TEMPRF
0053    C  is a maximum.
0054            IF  ( NOUT .EQ. 1 )  THEN
0055              PMAX = PF
0056              TMAX = TEMPRF
0057            END IF
```

```
0058            IF  ( PF .GE. PMAX )  PMAX = PF
0059            IF  ( TEMPRF .GE. TMAX )  TMAX = TEMPRF
0060    C
0061    C       Now we update the list output files.
0062            WRITE ( ITEMP,100 )  TIME, TEMPRF, TEMPNF
0063     100      FORMAT ( 10X, 1P1G11.4, 10X, 1P1G11.4, 10X, 1P1G11.4 )
0064            WRITE ( IPRES,101 ) TIME, PF
0065     101      FORMAT ( 10X, 1P1G11.4, 10X, 1P1G11.4 )
0066            WRITE ( IMH2,102 ) TIME, MH2F
0067     102      FORMAT ( 10X, 1P1G11.4, 10X, 1P1G11.4 )
0068            WRITE ( IFLOW,103 ) TIME, MH2O, FRPRV
0069     103      FORMAT ( 10X, 1P1G11.4, 10X, 1P1G11.4, 10X, 1P1G11.4 )
0070    C
0071    C     Now for the general output file.
0072    C  The composition of the general output file is determined by
0073    C  the value of the 3 control common variables JOUT1, JOUT2, and
0074    C  JOUT3.  These variables are set during the execution of INCHNG.
0075            IF  ( JOUT1 .NE. 1 )  GO TO 10
0076    C
0077    C     First we relate the program variables at the top of the out-
0078    C  put file.
0079            IF  ( NOUT .EQ. 1 )  THEN
0080              XAPLI =  100. * APLI
0081              APPB =  100. * ( 1. - APLI )
0082              WRITE ( IOUT,220 )  X, APRV, PPRV, TIMEND, NPIPES, VRO,
0083         1                        XAPLI, APPB
0084     220        FORMAT ( 5X, 'THE PROGRAM VARIABLES ARE :'/
0085         1               15X,' THE MIXING PARAMETER ------ ',1P1G11.4/
0086         2               15X,' PRESSURE RELIEF VALVE AREA - ',1P1G11.4,
0087         3               ' M2 ' /
0088         4               15X,' PRV PRESSURE SET POINT ----- ',1P1G11.4,
0089         5               ' N/M2 ' /
0090         6               15X,' CALCULATION END TIME ------- ',1P1G11.4,
0091         7               ' SEC '/
0092         8               15X,' NUMBER OF BROKEN STEAM TUBES ',I3 /
0093         9               15X,' THE INITIAL REACTION ZONE VOL',1P1G11.4,
0094         1              ' M3 ' / 15X, ' THE BREEDER IS COMPOSED OF ',
0095         2             1P1G11.4,' % LI  AND ',1P1G11.4, ' % PB '/
0096         3             5X / 5X / 5X )
0097            END IF
0098    C
0099    C
0100            IF  ( NFLAG .EQ. 0 )  THEN
0101              WRITE ( IOUT,200 ) TIME
0102              WRITE ( IOUT,201 )  TEMPRF, TEMPNF, PF, VRF, VGASF
0103              IF  ( JOUT2 .EQ. 1 )  WRITE ( IOUT,202 ) MH2OFR, MLMBFR,
0104         1        MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, MLIOHF, DRDT
0105              IF  ( JOUT3 .EQ. 1 )  WRITE ( IOUT,203 ) QCOND, PVDOT,
0106         1        ENGIN, ENGOUT, QFCRZ, QFCNZ, URZF, UNZF, URZI,
0107         2        UNZI, SUMQ, SUMU
0108    C
0109            ELSE
0110    C
0111              WRITE ( IOUT,200 ) TIME
0112              WRITE ( IOUT,201 ) TEMPRF, TEMPNF, PF, VRF, VGASF
0113              IF ( JOUT2 .EQ. 1 )  WRITE ( IOUT,202 ) MH2OFR, MLMBFR,
0114         1        MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, MLIOHF
```

```
0115            END IF
0116      C
0117       200  FORMAT ( 10X / 10X / '**********************************',
0118           1  '****************' / 5X, ' END OF TIMESTEP TIME ------- ',
0119           2  1P1G11.4, ' SEC ' / )
0120      C
0121       201  FORMAT ( 10X / 5X, ' REACTION ZONE TEMPERATURE -- ' ,
0122           1  1P1G11.4, ' K ' /
0123           2  5X, ' NONREACTION ZONE TEMPERATURE  ' , 1P1G11.4, ' K ' /
0124           3  5X/5X, ' SYSTEM PRESSURE ------------ ',1P1G11.4, ' PA '/
0125           4  5X/5X, ' REACTION ZONE VOLUME ------- ',1P1G11.4,' M3 '/
0126           5  5X,    ' GAS VOLUME ----------------- ',1P1G11.4,' M3 '/)
0127      C
0128      C
0129       202  FORMAT ( 5X/5X, ' MOLAR FLOWRATE - H2O ------- ',1P1G11.4,
0130           1  ' MOLES/SEC ' /
0131           2  5X, ' MOLAR FLOWRATE TO R.Z. - LMB ',1P1G11.4,' MOLES/SEC '/
0132           3  5X, ' MOLAR FLOWRATE OUT OF PRV -- ',1P1G11.4,' MOLES/SEC '/
0133           4  5X/5X,' MASS OF H2 IN R.Z. --------- ',1P1G11.4,' MOLES '/
0134           5  5X,    ' MASS OF PB IN R.Z. --------- ',1P1G11.4,' MOLES '/
0135           6  5X,    ' MASS OF UNREACTED LI IN R.Z. ',1P1G11.4,' MOLES '/
0136           7  5X,    ' MASS OF UNREACTED H2O IN R.Z.',1P1G11.4,' MOLES '/
0137           8  5X,    ' MASS OF LIOH IN R.Z. ------- ',1P1G11.4,' MOLES'/
0138           9  5X/5X,' R.Z. EXPANSION VELOCITY ---- ',1P1G11.4,' M/SEC'/)
0139      C
0140      C
0141       203  FORMAT ( 5X/5X, ' CONDUCTION ENERGY ---------- ', 1P1G11.4,
0142           1       ' J/SEC ' /
0143           2  5X,    ' FLUID EXPANSION WORK ------- ',1P1G11.4, ' J/SEC '/
0144           3  5X,    ' ENERGY FLOW INTO R.Z. ------ ',1P1G11.4, ' J/SEC '/
0145           4  5X,    ' ENERGY FLOW OUT OF N.Z. ---- ',1P1G11.4, ' J/SEC '/
0146           5  5X,    ' CONVECTION ENERGY OUT OF R.Z.',1P1G11.4, ' J/SEC '/
0147           6  5X,    ' CONVECTION ENERGY OUT OF N.Z.',1P1G11.4, ' J/SEC '/
0148           7  5X/5X,' FINAL ENERGY OF R.Z. ------- ',1P1G11.4, ' J '/
0149           8  5X,    ' FINAL ENERGY OF N.Z. ------- ',1P1G11.4, ' J '/
0150           9  5X/5X,' INITIAL ENERGY OF R.Z. ----- ',1P1G11.4, ' J '/
0151           1  5X,    ' INITIAL ENERGY OF N.Z. ----- ',1P1G11.4, ' J '/
0152           2  5X/5X,' SUM OF ENERGY CHANGE TOTAL - ',1P1G11.4, ' J '/
0153           3  5X,    ' TOTAL INTERNAL ENERGY ------ ',1P1G11.4, ' J ')
0154      C
0155      C
0156       10   CONTINUE
0157      C
0158      C     That's all folks!
0159            RETURN
0160            END
```

PROGRAM SECTIONS

	Name	Bytes	Attributes
0	$CODE	1012	PIC CON REL LCL SHR EXE RD NOWRT LONG
1	$PDATA	1827	PIC CON REL LCL SHR NOEXE RD NOWRT LONG
2	$LOCAL	32	PIC CON REL LCL NOSHR NOEXE RD WRT QUAD
3	OUT	12	PIC OVR REL GBL SHR NOEXE RD WRT LONG
4	INPUT	84	PIC OVR REL GBL SHR NOEXE RD WRT LONG
5	PROP	64	PIC OVR REL GBL SHR NOEXE RD WRT LONG
	Total Space Allocated	3031	

ENTRY POINTS

Address	Type	Name
0-00000000		OUTPUT

VARIABLES

Address	Type	Name	Address	Type	Name	Address	Type	Name	Address	Type	Name
5-00000038	R*8	APLI	2-00000018	R*8	APPB	4-00000008	R*8	APRV	4-00000020	R*8	DELTAI
5-00000010	R*8	DLI	5-00000008	R*8	DLIOH	5-00000000	R*8	DLMB	5-00000018	R*8	DPB
AP-0000005C@	R*8	DRDT	AP-00000048@	R*8	ENGIN	AP-00000044@	R*8	ENGOUT	2-00000008	R*8	FRPRV
3-00000000	I*4	JOUT1	3-00000004	I*4	JOUT2	3-00000008	I*4	JOUT3	AP-00000028@	R*8	MH2F
2-00000000	R*8	MH20	AP-0000001C@	R*8	MH2OFR	AP-00000038@	R*8	MLIOHF	AP-00000020@	R*8	MLMBFR
AP-0000002C@	R*8	MPBF	AP-00000024@	R*8	MPRVFR	AP-00000074@	I*4	NFLAG	AP-00000070@	I*4	NOUT
4-00000030	I*4	NPIPES	4-00000044	R*8	PEPS	AP-00000010@	R*8	PF	AP-00000078@	R*8	PMAX
4-00000010	R*8	PPRV	AP-00000040@	R*8	PVDOT	AP-0000003C@	R*8	QCOND	AP-00000058@	R*8	QFCNZ
AP-00000054@	R*8	QFCRZ	AP-00000060@	R*8	SUMQ	AP-00000064@	R*8	SUMU	5-00000028	R*8	TCLMB
5-00000030	R*8	TDLMB	AP-0000000C@	R*8	TEMPNF	AP-00000008@	R*8	TEMPRF	4-0000003C	R*8	TEPS
AP-00000004@	R*8	TIME	4-00000028	R*8	TIMEND	AP-0000007C@	R*8	TMAX	AP-00000034@	R*8	UMH2OF
AP-00000030@	R*8	UMLIF	AP-00000050@	R*8	UNZF	AP-0000006C@	R*8	UNZI	AP-0000004C@	R*8	URZF
AP-00000068@	R*8	URZI	AP-00000018@	R*8	VGASF	4-0000004C	R*8	VR0	AP-00000014@	R*8	VRF
4-00000034	R*8	VTOT	4-00000000	R*8	X	2-00000010	R*8	XAPLI	4-00000018	R*8	XLCPRV
5-00000020	R*8	XLMBHF									

LABELS

Address	Label	Address	Label	Address	Label	Address	Label	Address	Label	Address	Label
0-000003F3	10	1-00000000	100'	1-00000016	101'	1-00000025	102'	1-00000034	103'	1-000001BA	200'
1-00000227	201'	1-00000316	202'	1-000004E3	203'	1-0000004A	220'				

COMMAND QUALIFIERS

```
  FORTRAN /LIST MARSPRG.;26

  /CHECK=(NOBOUNDS,OVERFLOW,NOUNDERFLOW)
  /DEBUG=(NOSYMBOLS,TRACEBACK)
  /STANDARD=(NOSYNTAX,NOSOURCE_FORM)
  /SHOW=(NOPREPROCESSOR,NOINCLUDE,MAP)
  /F77  /NOG_FLOATING  /I4  /OPTIMIZE  /WARNINGS  /NOD_LINES  /NOCROSS_REFERENCE  /NOMACHINE_CODE  /CONTINUATIONS=19
```

COMPILATION STATISTICS

```
  Run Time:           20.81 seconds
  Elapsed Time:       87.85 seconds
  Page Faults:        1039
  Dynamic Memory:     143 pages
```

NOMENCLATURE

A an area

A_b the area of the steam tube break

A_{prv} the area of the pressure relief valve and a variable in dynamic model equations

A_t the surface area of a steam tube

C_1 the factor that determines the probability that the outer tube, of the duplex tube, will fail

C_2 the factor that determines the probability that the inner tube will fail due to the failure of the outer tube

C_3 the factor that determines the probability that the outer tube will fail, due to the failure of the inner tube

C_4 the factor that determines the probability that a small break will deteriorate into a large break

C_H the molar specific heat of hydrogen

C_L the molar specific heat of lithium

C_{LH} the molar specific heat of lithium hydroxide

E_R the total internal energy of the reaction zone

E_{tot} the overall unavailability of a steam generator design

h the overall heat transfer coefficient of the steam tube

i_b enthalpy of the liquid metal breeder entering the reaction zone

i_f the heat of formation of the liquid metal breeder, $Li_{17}Pb_{83}$

i_{wb} the enthalpy of the water/steam flowing through the steam tube break

i_{wf} the final enthalpy of the water in the Thermodynamic Equilibrium Model

i_{wo} the initial enthalpy of the water in the Thermodynamic Equilibrium Model

k_n the thermal conductivity of the nonreaction zone, liquid metal breeder

$\dot{m}_{bp}$ the molar flow rate of unreacted liquid metal breeder through the pressure relief valve

$\dot{m}_{br}$ the molar flow rate of liquid metal breeder into the reaction zone

$\dot{m}_w$ the molar flow rate of water into the reaction zone

m_n the total mass of the nonreaction zone

m_R the total mass of the reaction zone

N_H the number of moles of hydrogen

P the variable system pressure

P_ℓ the final quasi-steady pressure

P_{max} the maximum system pressure

P_∞ the pressure relief valve back pressure, assumed to be 1 atm

Q the heat of reaction

Q_c The conduction heat flow between the reaction zone and nonreaction zone

Q_n the convective heat flow from the nonreaction zone to unbroken steam tubes

Q_r the convective heat flow from the reaction zone to unbroken steam tubes

R the radius of the reaction zone

S_{wb} the entropy of the water at the tube break

S_{NO} the initial entropy of the water

T_f the final thermodynamic equilibrium temperature

T_n the average temperature of the nonreaction zone

T_{ni} the initial temperature of the nonreaction zone

T_0 the reference temperature in the Thermodynamic Equilibrium Model, chosen to be 0°C

T_r the average temperature of the reaction zone

T_w the average temperature of the water/steam in the steam tubes, assumed to be 648°K

V_r the volume of the reaction zone

v_{wb} the velocity of the water flowing through the steam tube break

x the mixing parameter. In the Thermodynamic Equilibrium Model it is defined as the molar ratio of water to Li in the initial mixture. In the Dynamic Model, it is defined as the ratio of the molar flow rate of H_2O to the molar flow rate of Li into the reaction zone per timestep.

α_n the thermal diffusivity of the liquid metal breeder

ΔG the Gibb's free energy of the $Li_{17}Pb_{83}$

ΔS the entropy of the $Li_{17}Pb_{83}$

Δt the length of the timestep is seconds

λ the probability of a specific accident scenario

λ_i the probability that the inner tube, of the duplex tube, will fail

λ_o the probability that the outer tube will fail

λ_{PWR} the probability that a PWR steam tube will fail

λ_{SG} the overall probability that a forced shutdown of the steam generator will occur

μ the reciprocal of the time needed to repair the steam generator, which has been shut down due to a specific accident scenario

λ the conduction length scale derived from boundary layer theory

ρ_b the density of the liquid metal breeder

ρ_{wb} the density of the water/steam flowing through the steam tube break

References

1. P.J. Krane, M.S. Kazimi, "An Evaluation of Accidental Water Reactions with Lithium Compounds in Fusion Reactor Blankets," Plasma Fusion Center and Department of Nuc. Engr., MIT (July 1981).

2. S.J. Piet et al., "Potential Consequences of Tokamak Fusion Reactor Accidents: The Materials Impact," Plasma Fusion Center, MIT (June 1982).

3. R.G. Clemmer, D.R. Armstrong, et al., "An Experimental Study of the Reaction of Li_7Pb_2 with Water," Trans. Am. Nucl. Soc. 32, 71 (1979).

4. R.G. Clemmer, D.R. Armstrong, et al., "The Reactions of Li-Pb Alloys with Water," Trans. Am. Nucl. Soc. 34, 55 (1980).

5. A.G. Rogers, B.L. Benedict, et al., "Liquid Li-Pb-Bi, A New Tritium Breeder," Eng. Fusion Research Proc., Chicago, October 1981.

6. L. Muhlestein, Private Communication (October 1982).

7. D.W. Jepson et al., "Fusion Reactor Blanket Material Safety Compatability Studies," Nuclear Tech. 20, 450 (August 1983).

8. J.L. Rouyer, "Safety Analysis," Commissariat a l'Energie Atomique, ARD 1-044-E1 (April 1983).

9. H. Klippel, "Safety Analysis of a $Li_{17}Pb_{83}$ Liquid Breeder Blanket," Ener. Centrum Nederland, FYS-FUS-82-6 (June 1982).

10. B.G. Logan et al., "Mirror Advanced Reactor Study Interim Design Report," UCRL-53333 (April 1983).

11. M. Corradini, G. Moses, "A Dynamic Model for Fuel-Coolant Mixing," ANS Int'l. Mtg., on LWR Severe Accident Evaluation, Boston (August 1983).

12. M. Berman, LWR Safety Semi-Annual Report, Sandia National Laboratories, SAND-82-15721, Chapter 2 (June 1983).

13. M. Corradini, "A Proposed Model for Fuel-Coolant Mixing," ANS Int'l. Thermal Reactor Safety Mtg., Chicago (August 1982).

14. L. Efferding, Private Communication, Westinghouse Corp. (Nov. 1982).

15. E.M. Larsen, Private Communication (December 1982).

16. M.L. Corradini, "Phenomenological Modeling of the Triggering Phase of Small-Scale Steam Explosion Experiments," Nucl. Sci. and Eng. 78, 1540170 (1981).

17. R. Bird et al., Transport Phenomena, Wiley & Sons, NY (1960).

18. L. Baker et al., "Studies of Metal-Water Reactions at High Temperatures," ANL-6548, Argonne National Lab (May 1982).

19. M. Corradini et al., "Modeling Lithium-Lead/Water Interactions," 5th Int'l. Topical Mtg. on Fusion Energy, Knoxville, TN (April 1983).

20. D.M. France et al., "Blowdown Tests in a Sodium Heated Steam Generator," ANS Transaction V45, Detroit (June 1983).

21. "IEEE Guide for General Principles of Reliability Analysis of Nuclear Power Generating Station Protection System," IEEE Std 352-1975.