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

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INTERACTIONS IN A FUSION REACTOR DESIGN

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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\(_2\)O 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\(_4\)SiO\(_4\), and LiTiO\(_3\)) showed that these oxides present minimal safety related problems when used with H\(_2\)O; 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\(_8\) (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

<table>
<thead>
<tr>
<th>Case</th>
<th>Composition</th>
<th>State&lt;sup&gt;a&lt;/sup&gt;</th>
<th>Temp/&lt;sup&gt;°&lt;/sup&gt;K</th>
<th>Temp/&lt;sup&gt;°&lt;/sup&gt;K</th>
<th>Reaction</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Li&lt;sub&gt;7&lt;/sub&gt;Pb&lt;sub&gt;2&lt;/sub&gt;</td>
<td>s</td>
<td>773</td>
<td>298</td>
<td>Modest</td>
</tr>
<tr>
<td>2</td>
<td>Li&lt;sub&gt;7&lt;/sub&gt;Pb&lt;sub&gt;2&lt;/sub&gt;</td>
<td>s</td>
<td>773</td>
<td>369</td>
<td>Vigorous</td>
</tr>
<tr>
<td>3</td>
<td>Li&lt;sub&gt;7&lt;/sub&gt;Pb&lt;sub&gt;2&lt;/sub&gt;</td>
<td>s</td>
<td>873</td>
<td>368</td>
<td>Vigorous</td>
</tr>
<tr>
<td>4</td>
<td>Li&lt;sub&gt;7&lt;/sub&gt;Pb&lt;sub&gt;2&lt;/sub&gt;</td>
<td>l</td>
<td>1103</td>
<td>368</td>
<td>Very Vigorous</td>
</tr>
<tr>
<td>5</td>
<td>Li&lt;sub&gt;0.62&lt;/sub&gt;Pb&lt;sub&gt;0.38&lt;/sub&gt;</td>
<td>l</td>
<td>773</td>
<td>368</td>
<td>Vigorous</td>
</tr>
<tr>
<td>6</td>
<td>Li&lt;sub&gt;0.17&lt;/sub&gt;Pb&lt;sub&gt;0.83&lt;/sub&gt;</td>
<td>l</td>
<td>773</td>
<td>368</td>
<td>Very Modest</td>
</tr>
<tr>
<td>7</td>
<td>Li</td>
<td>l</td>
<td>773</td>
<td>368</td>
<td>H&lt;sub&gt;2&lt;/sub&gt; Detonation</td>
</tr>
<tr>
<td>8</td>
<td>Li&lt;sup&gt;b&lt;/sup&gt;</td>
<td>l</td>
<td>773</td>
<td>368</td>
<td>Detonation</td>
</tr>
</tbody>
</table>

<sup>a</sup> s = solid, l = liquid

<sup>b</sup> injected under water
blanket designs and have provided specific design proposals to reduce the overall hazard potential of a \( \text{Li}_{17}\text{Pb}_{83} \) 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 \( \text{Li}_{17}\text{Pb}_{83} \) (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.
STEAM GENERATOR TUBE RUPTURE

- HIGH PRESSURE TWO-PHASE BLOWDOWN
- LIQUID METAL ENTRAINMENT 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
LIQUID METAL SPILL IN CONTAINMENT

LIQUID METAL COMPONENT

LIQUID METAL POUR

HYDROGEN GENERATION

WATER

LIQUID METAL MIXING IN WATER

STEAM GENERATION

CONCRETE BASEMAT

LIQUID-METAL/CONCRETE INTERACTIONS
- **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**
![Westinghouse Steam Generator Diagram](image)

<table>
<thead>
<tr>
<th></th>
<th>Plant Steam Generator</th>
<th>Model Steam Generator</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Rating MW</strong></td>
<td>293</td>
<td>70</td>
</tr>
<tr>
<td><strong>Unit Length ft (m)</strong></td>
<td>85.6 (26.1)</td>
<td>81.6 (24.9)</td>
</tr>
<tr>
<td><strong>Tube Length ft (m)</strong></td>
<td>77.1 (23.5)</td>
<td>77.1 (23.5)</td>
</tr>
<tr>
<td><strong>Active Tube ft (m)</strong></td>
<td>67.5 (20.6)</td>
<td>67.5 (20.6)</td>
</tr>
<tr>
<td><strong>Tube O.D. in (cm)</strong></td>
<td>.812 (2.1)</td>
<td>.812 (2.1)</td>
</tr>
<tr>
<td><strong>Tube I.D. in (cm)</strong></td>
<td>.436 (1.1)</td>
<td>.436 (1.1)</td>
</tr>
<tr>
<td><strong>No. of Tubes</strong></td>
<td>3366</td>
<td>804</td>
</tr>
<tr>
<td><strong>Shell O.D. in (cm)</strong></td>
<td>92 (234)</td>
<td>47 (119)</td>
</tr>
<tr>
<td><strong>Dry Weight Tons (Mg)</strong></td>
<td>382 (347)</td>
<td>118 (107)</td>
</tr>
</tbody>
</table>
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\textsuperscript{(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\textsuperscript{(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

\[
\text{Li} + \frac{1}{2} \text{H}_2 \text{O} + \text{LiOH} + \frac{1}{2} \text{H}_2 - 49 \text{ kcal/gmole of Li} \quad (\theta 25^\circ C) \tag{1}
\]

and for lithium-lead with water

\[
\text{Li}_{17}\text{Pb}_{83} + 0.17 \text{H}_2\text{O} + i_f + 0.17 \text{LiOH} + 0.085 \text{H}_2 + 0.83 \text{Pb} - 8.33 \text{ kcal/gmole of Li}_{17}\text{Pb}_{83} \quad (\theta 25^\circ C) \tag{2}
\]

where \(i_f\) is the heat of formation of \(\text{Li}_{17}\text{Pb}_{83}\) (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

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

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

$$C_L[T_{BO} - T_0] + x_i_{WO} = x[C_{LH} + C_H][T_f - T_0] + xQ + \left[1 - x\right]C_L[T_f - T_0] \quad \text{for } x < 1 \quad (3c)$$

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.
THERMODYNAMIC EQUILIBRIUM TEMPERATURE ($T_f$) VS. $X$ FOR Li BREEDER

$X = \frac{n_{H_2O}}{n_{Li}}$

- Partially vaporized LiOH
- Partially vaporized Li
- $P = 25$ psia
- $P = 1000$ psia
- $P = 2400$ psia

Temperature ($T_f$) in °C

- 1800
- 1600
- 1400
- 1200
- 1000
- 800
- 600
- 400
- 0.1

- 0.5
- 1.0
- 5.0
- 10.0
FIGURE 6

THERMODYNAMIC EQUILIBRIUM TEMPERATURE ($T_f$) vs. $X$ FOR $\text{Pb}_{83}\text{Li}_{17}$ BREEDER

$$Q_R = -8.33 \frac{\text{kcal}}{\text{g mole of } \text{Li}_{17}\text{Pb}_{83}}$$

$$Q_R = -6.36 \frac{\text{kcal}}{\text{g mole of } \text{Li}_{17}\text{Pb}_{83}}$$

$p = 25$ psia
$p = 1000$ psia
$p = 2400$ psia

$X = \frac{n_{\text{H}_2\text{O}}}{n_{\text{Li}}}$
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 Li₁₇Pb₈₃ 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 Li₁₇Pb₈₃)) is arrived at by assuming that the heat of formation of Li₁₇Pb₈₃ (iₚ) is negligible. The other value of Q (-6.36 kcal/(gmole of Li₁₇Pb₈₃)) is arrived at by including an estimate of the heat of formation, iₚ. This estimate of the heat of formation of Li₁₇Pb₈₃ is given by

\[ iₚ = ΔG + TΔS \]  (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 vaporization 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 initial shell side, liquid-metal breeder volume and temperature are taken to be $2.78 \times 10^7$ 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.

$$ S_{wo} = S_{wb} $$

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

$$ \dot{m}_w = A_b \rho_{wb} V_{wb} $$

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

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)

\[ \dot{m}_{bp} = \rho_b A_{prv} \left[ \frac{2}{K_{p_b}} (P - P_\infty) \right]^{1/2} \] (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 gener-
ators.

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 un-
reacted 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 mecha-
nisms 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 H₂ 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

\[ \frac{dm_R}{dt} = \dot{m}_{br} + \dot{m}_w. \] (9)

Reaction zone energy balance

\[ \frac{dE_R}{dt} = -Q_c - Q_r - p \frac{dV_r}{dt} + \dot{m}_{br} \dot{v}_b + \dot{m}_w \dot{v}_w \] (10)

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

\[ Q_r = h_t A_{tr}(t)(T_r - T_w). \] (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

\[ Q_c = 4\pi R^2 \frac{k_n}{\lambda_n} (T_r - T_n). \] (12)
The penetration depth, \( \lambda \), 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

\[
\frac{\mathrm{d}m_n}{\mathrm{d}t} = \dot{m}_{br} - \dot{m}_{bp},
\]  

(13)

and the nonreaction zone energy balance is

\[
\frac{\mathrm{d}E_n}{\mathrm{d}t} = Q_c - Q_n - P \frac{\mathrm{d}V_n}{\mathrm{d}t} - \dot{m}_{br} \cdot b - \dot{m}_{bp} \cdot b
\]

(14)

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

\[
Q_n = h_n A_{t_n} (T_n - T_w).
\]

(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, \( A_{\text{prv}} \). 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 \( A_{\text{prv}} \) 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 (\( A_{\text{prv}} = 0.005 \text{ m}^2 \)) with the other two curves (\( A_{\text{prv}} = 0.01 \text{ m}^2 \) and \( A_{\text{prv}} = 0.05 \text{ m}^2 \)). One notes that the system pressure quickly approaches the limiting pressure of the high pressure water (17 MPa), for smaller values of \( A_{\text{prv}} \). Another trend illustrated in this, and which is exhibited in the results of every calculation, is that the system pressure quickly (\(< 1 \times 10^{-4} \text{ s}\)) reaches a maximum pressure (\( P_{\text{max}} \)), and levels off near \( P_{\text{max}} \) for the early part of the calculation. In Fig. 8, we have plotted the maximum system pressure as a function of \( A_{\text{prv}} \) 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 (\( \dot{m}_{\text{bp}} \)) is proportional to \( A_{\text{prv}} \) and the square root of the liquid-metal breeder density (\( \rho_B \))

\[
\dot{m} \propto A_{\text{prv}} (\rho_B)^{1/2} .
\]

If the abscissa of Fig. 8 was \( \rho_B^{-1/2} A_{\text{prv}} \) instead of \( A_{\text{prv}} \), 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)

- Aprv = 0.05
- Aprv = 0.01
- Aprv = 0.005

Figure 7
MAXIMUM PRESSURE FOR Li-17 Pb-83 AND Li

Figure 8
MASS OF H₂ GENERATED AT 1s INTO ACCIDENT

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 temperature 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
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 $A_{p,r}$. 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 ($\sim 1800$ K). When the reaction zone temperature decreases to 1800 K (in roughly 10 ms), the reaction zone volume is approximately $0.01 \text{ m}^3$. 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
Figure 11

Reaction Zone Temperature for Li-17Pb-83 and Li

\[ x = 1.0 \]
\[ A_{prv} = 0.005 \text{ m}^2 \]

\[ T_r (K) \]

\[ \text{Time (s)} \]

- Li-17Pb-83
- Li
MAX. REACTION ZONE TEMPERATURE AS FUNCTION OF $x$

Li-17 Pb-83 BREEDER
$A_{prv} = 0.005 \text{ m}^2$

$x = \frac{\dot{n}_{H_2O}}{\dot{n}_{Li}}$

Figure 12
Fig. 6 \( Q_R = -6.36 \text{ kcal/gmole of Li}_{17}\text{Pb}_{83} \), 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\(_{17}\text{Pb}_{83}\)) 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

\[
\frac{dN_H}{dt} = A \frac{D_H}{R_0 T_y} \frac{dP_H}{dn} 
\]

\(15\)
where: \( \frac{dN_H}{dt} \) 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

\[
\frac{d}{dt} \left( \frac{W^2}{2} \right) = 3.8 \times 10^3 \exp \left( \frac{-84300}{R_0 T_V} \right)
\]  

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.

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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:

\[ \lambda_i = \lambda_{PWR} \quad (A.1) \]

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:

\[
\lambda_0 = C_1\lambda_1.
\]  

(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 \((\lambda_{SG})\) 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

\[
E_U = \frac{\lambda}{\mu + \lambda}
\]  

(A.3)

where \(\mu\) is the reciprocal of the time needed to repair the component after an accident, and \(\lambda\) 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 ($\lambda_{SG}$) 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:

$$\lambda_{SG} = 2.3 \times 10^{-5} \text{ hr}^{-1}$$
$E_{\text{tot}} = 4.2\%$.

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 ($\lambda = 2.75 \times 10^{-5} \text{ hr}^{-1}$), for the duplex tube design. The probability of a small leak, small reaction is $2.7 \times 10^{-7} \text{ hr}^{-1}$, and the probability of a large leak, large reaction is $1.6 \times 10^{-8} \text{ hr}^{-1}$. 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 $1 \times 10^{-12}$ 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 divided 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 H₂O 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 H₂O into the reaction zone. The amount of liquid-metal breeder flowing into the reaction zone and reacting is determined by the amount of H₂O 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:

\[
\frac{dE_R}{dt} = -Q_C - Q_r - p \frac{dV_r}{dt} + \dot{m}_{br} \dot{i}_b + \dot{m}_w \dot{i}_w. \tag{10}
\]

First, the energy flow terms on the right hand side of this equation over the timestep interval \(\Delta t\) 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:

\[
E_{Rf} = E_{Ri} + \Delta t(-Q_C - Q_r - p \frac{dV_r}{dt} + \dot{m}_{br} \dot{i}_b + \dot{m}_w \dot{i}_w). \tag{11}
\]

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 valve (m²).

PPRV - the set point pressure at which the pressure relief valve opens (N/m²).

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 (m³).

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 = 1.0E0
THE DEFAULT VALUE OF AFRV = 5.0000E-03 M2
THE DEFAULT VALUE OF PFRV = 1.7243E+05 PA
THE DEFAULT VALUE OF TIMEND = 10.00 SEC
THE DEFAULT VALUE OF NPIPES = 1
THE DEFAULT VALUE OF VRV = 1.0000E-05 M2
ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF Y

ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF AFRV

ENTER A 1 IF YOU WANT TO CHANGE THE DEFAULT VALUE OF TIMEND

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

ENTER THE NEW BREEDER DENSITY = K63

ENTER THE NEW BREEDER HEAT OF FORMATION = J/HOLE

ENTER THE NEW BREEDER THERMAL CONDUCTIVITY = W/M-K

ENTER THE NEW BREEDER THERMAL DIFFUSIVITY = MS/SEC

ENTER THE BREEDER ATOMIC FRACTION OF LI

ENTER A 1 IF YOU WANT GENERAL OUTPUT

ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE MOLAR COMPONENTS
OF THE REACTION ZONE AND THE FLOW RATES INTO AND OUT OF THE SYSTEM

ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE THE ENERGY STATICS OF THE TWO ZONES

ENTER A 1 IF YOU WANT VEDUS OUTPUT

PROGRAM EXECUTION NOW BEGINS

THERE ARE 22 LINES IN THESE OUTPUT FILES

TIME vs. TEMPERATURE IN LOGICAL UNIT NO. 11
TIME vs. PRESSURE IS IN LOGICAL UNIT NO. 12
TIME vs. MOSS AND BREEDER FLOW RATES IS IN LOGICAL UNIT NO. 13
THE GENERAL OUTPUT FILE IS IN LOGICAL UNIT NO. 20
THE VEDUS OUTPUT IS IN LOGICAL UNIT NO. 15

THE MAXIMUM PRESSURE = 1.4786E+07 PA
THE MAXIMUM REACTION ZONE TEMPERATURE = 2103. K
FOR X = 1.0E0 AND AFRV = 5.0000E-03 M2

END OF RUN
THE PROGRAM VARIABLES ARE:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>THE MIXING PARAMETER</td>
<td>1.299</td>
</tr>
<tr>
<td>PRESSURE RELIEF VALVE AREA</td>
<td>0.0000E+00 M2</td>
</tr>
<tr>
<td>PRV PRESSURE SET POINT</td>
<td>1.7243E+05 N/M2</td>
</tr>
<tr>
<td>CALCULATION END TIME</td>
<td>1.000E+00 SEC</td>
</tr>
<tr>
<td>NUMBER OF BROKEN STEAM TUBES</td>
<td>1</td>
</tr>
<tr>
<td>THE INITIAL REACTION ZONE VOLUME</td>
<td>1.0000E-05 M3</td>
</tr>
<tr>
<td>THE BREEDER IS COMPOSED OF 100.0% Li AND 0.0000E+00% Pd</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>REACTION ZONE TEMPERATURE</td>
<td>2163.4 K</td>
</tr>
<tr>
<td>NONREACTION ZONE TEMPERATURE</td>
<td>673.0 K</td>
</tr>
<tr>
<td>SYSTEM PRESSURE</td>
<td>1.8931E+04 PA</td>
</tr>
<tr>
<td>REACTION ZONE VOLUME</td>
<td>1.0000E-05 M3</td>
</tr>
<tr>
<td>GAS VOLUME</td>
<td>1.0000E-05 M3</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>MOLAR FLOWRATE - H2O</td>
<td>722.1 MOLES/SEC</td>
</tr>
<tr>
<td>MOLAR FLOWRATE TO R.Z. - LMA</td>
<td>722.1 MOLES/SEC</td>
</tr>
<tr>
<td>MOLAR FLOWRATE OUT OF PRV</td>
<td>1.2792E+05 MOLES/SEC</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>MASS OF Li IN R.Z.</td>
<td>6.7395E-04 MOLES</td>
</tr>
<tr>
<td>MASS OF Pd IN R.Z.</td>
<td>6.0000E+00 MOLES</td>
</tr>
<tr>
<td>MASS OF UNREACTION Li IN R.Z.</td>
<td>6.0000E+00 MOLES</td>
</tr>
<tr>
<td>MASS OF UNREACTION H2O IN R.Z.</td>
<td>9.8000E+00 MOLES</td>
</tr>
<tr>
<td>MASS OF LiHR IN R.Z.</td>
<td>3.4699E-04 MOLES</td>
</tr>
<tr>
<td>R.Z. EXPANSION VELOCITY</td>
<td>82.65 M/SEC</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>CONDUCTION ENERGY</td>
<td>1.4037E+07 J/SEC</td>
</tr>
<tr>
<td>FLUID EXPANSION WORK</td>
<td>2.4930E+05 J/SEC</td>
</tr>
<tr>
<td>ENERGY FLOW INTO R.Z.</td>
<td>1.4457E+05 J/SEC</td>
</tr>
<tr>
<td>ENERGY FLOW OUT OF R.Z.</td>
<td>1.2765E+07 J/SEC</td>
</tr>
<tr>
<td>CONVECTION ENERGY OUT OF R.Z.</td>
<td>66.32 J/SEC</td>
</tr>
<tr>
<td>CONVECTION ENERGY OUT OF R.Z.</td>
<td>5.9666E+00 J/SEC</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>FINAL ENERGY OF R.Z.</td>
<td>-76.42 J</td>
</tr>
<tr>
<td>FINAL ENERGY OF R.Z.</td>
<td>2.9293E+16 J</td>
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<table>
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</thead>
<tbody>
<tr>
<td>INITIAL ENERGY OF R.Z.</td>
<td>8.0303E+00 J</td>
</tr>
<tr>
<td>INITIAL ENERGY OF R.Z.</td>
<td>2.9269E+10 J</td>
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</tbody>
</table>

<table>
<thead>
<tr>
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<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>SUM OF ENERGY CHANGE TOTAL</td>
<td>-1.258 J</td>
</tr>
<tr>
<td>TOTAL INTERNAL ENERGY</td>
<td>-1.258 J</td>
</tr>
</tbody>
</table>
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 loca-
tion 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 com-
ment. 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/m²). Each line of output in logical unit number 13
consists of the time (s) and the mass of H₂ in the reaction zone (mole). Each
line of output in logical unit 14 consists of the time (s), the molar flow
rate of H₂O 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

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

and the nonreaction zone energy balance

\[ E_{Nf} = E_{Nf} + \Delta t(Q_c - Q_n - p \frac{dV_r}{dt} - \dot{m}_{br} i_b - \dot{m}_{bp} i_b) \]  \hspace{1cm} (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.
\( E_{N1} = \text{initial energy of N.Z.} \)

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

\[
E_{Rf} - E_{Ri} + E_{Nf} - E_{N1} = \Delta t (-Q_r - Q_n + \dot{m}_w i_w - \dot{m}_{bp} i_{bp}). \quad (B.3)
\]

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

\[
\sum_j (E_{Rfj} - E_{Rij} + E_{Nfj} - E_{N1j}) = \sum_i \Delta t_j (-Q_{rj} - Q_{nj} + \dot{m}_{wj} i_{wj} - \dot{m}_{bpj} i_{bpj}). \quad (B.4)
\]

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

\[
E_{Rij} = E_{Rf(j-1)} \quad (B.5)
\]

and

\[
E_{N1j} = E_{N1(j-1)}, \quad (B.6)
\]

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

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

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

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\[ E_{Rfj} - E_{Nfj} - E_{Nfo} = \sum_j \Delta t_j (-Q_{rj} - Q_{nj} + \dot{m}_{wj} w_j - \dot{m}_{bj} b_j). \] (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.
First we provide a list containing descriptions of the major program variables. The variables followed by an asterisk (*) appear written in various similar forms in various subroutines, as subroutine dummy variables (i.e., in the subroutine MDRIVE, the variable MH20 appears as MH20A).

- B. o. t. is defined as beginning of timestep.
- E. o. t. is defined as end of timestep.
- LMB is defined as liquid metal breeder.
- R. Z. is defined as reaction zone.
- N. Z. is defined as nonreaction zone.

- APLI - atom percent of Li in the LMB.
- APRV - area of the pressure relief valve. (M2)
- DELTAT (*) - the length of the timestep. (SEC)
- DLI - density of the liquid Li. (KG/M3)
- DLIOH - density of the liquid LiOH. (KG/M3)
- DLMB - density of the LMB. (KG/M3)
- DPB - density of the liquid Pb. (KG/M3)
- DROT - the time derivative of the radius; it is a measure of how fast the R. Z. is expanding. (M/SEC)
- DSEH2 - temperature derivative of the specific energy of the H2 gas. (J/MOLE-K)
- DSEH2O - temperature derivative of the specific energy of water vapor. (J/MOLE-K)
- DSELI - temperature derivative of the specific energy of the liquid Li. (J/MOLE-K)
- DSEPb - temperature derivative of the specific energy of the liquid Pb. (J/MOLE-K)
DSLIOH - temperature derivative of the specific energy of the LIOH. ( J/MOLE*K )
ENGIN - the internal energy of the H2O and LMB flowing into the reaction zone. ( J/SEC )
ENGOUT - the internal energy of the LMB flowing out of the nonreaction zone. ( J/SEC )
FRH2O (*) - the flow rate of the water from the broken steam tube(s). ( KG/SEC )
FRPRV (*) - the flow rate of unreacted LMB flowing through the pressure relief valve. ( KG/SEC )
FRSTM (*) - the flow rate of steam from the broken steam tube(s). ( KG/SEC )
HVAP - this is the saturated vapor enthalpy of H2O. ( J/MOLE )
IPRV - this is a flag that describes the condition of the pressure relief valve.
MASLMB - mass of the LMB flowing into the R. Z. ( KG )
MASPRV - mass of the LMB flowing through the pressure relief valve. ( KG )
MH2I (*), MH2F (*) - moles of H2 gas in the R. Z. at the b. o. t. and e. o. t. ( MOLE )
MH2D (*) - moles of H2O flowing into the R. Z. during the timestep. ( MOLE )
MH2DL - moles of liquid H2O flowing into the R.Z. during the timestep. ( MOLE )
MH2OFR - molar flowrate of H2O into the R. Z. during the timestep. ( MOLE/SEC )
MLI - moles of LI flowing into the R.Z. during the timestep ( MOLE )
MLIOHI (*), MLIOHF (*) - moles of LIOH in the R. Z. at the b. o. t. and e. o. t. ( MOLE )
MLMB (*) - moles of LMB flowing into the R.Z. during the timestep. ( MOLE )
MLMBFR - molar flowrate of LMB into the R. Z. during the timestep. ( MOLE/SEC )
MLMBNF - moles of LMB in the N. Z. at the e. o. t. ( MOLE )
MN2O - moles of LMB in the system at the beginning of the program ( MOLE )
MPBI (*), MPBF (*) - moles of PB in the R. Z. at the b. o. t.
and e. o. t. ( MOLE )

MPRVFR - molar flowrate of LMB out of the pressure relief
valve during the timestep. ( MOLE/SEC )

MSTM (*) - moles of steam flowing into the R. Z. during the
timestep ( MOLE )

NOUT - an internal count of the number of runs through the
driving DD loop.

NPipes - the number of broken steam tubes.

PBREAK - the pressure at the steam tube break. ( N/M2 )

PEND - penetration depth; a conduction length scale ( M )

PEPS - the pressure epsilon; a convergence measure. ( N/M2 )

PI (*), PF (*) - the b. o. t. and e. o. t. system pressure
(N/M2 )

PPRV - the set point pressure at which the pressure relief
valve ruptures. ( N/M2 )

PVDOT - the product of the pressure and the time derivative
of the R. Z. volume. ( J/SEC )

QCOND - the conductive heat transfer between the reaction
and nonreaction zones. ( J/SEC )

QFCNZ - the convective heat transfer from the N. Z. to
unbroken steam tubes. ( J/SEC )

QFCRZ - the convective heat transfer from the R. Z. to
unbroken steam tubes. ( J/SEC )

RADRZI, RADRZF, RADV - the b. o. t., e. o. t., and average
R. Z. radius ( M )

SEH20L - the specific energy of the liquid H2O. ( J/MOLE )

SEH2 - the specific energy of the H2 gas. ( J/MOLE )

SELI - the specific energy of the liquid LI. ( J/MOLE )

SELOH - the specific energy of the LIOH. ( J/MOLE )

SEPB - the specific energy of the liquid PB. ( J/MOLE )

SESTM - the specific energy of the steam ( J/MOLE )

SUMQ - the time integral of the time rate of change of
system energy. ( J )
SUMU - the total system energy. (J)
TCLMB - the thermal conductivity of the LMB (W/M-K)
TDLMB - the thermal diffusivity of the LMB (M2/SEC)
TEMPNI (*), TEMPNF (*) - the b. o. t. and e. o. t. temperature of the N. Z. (K)
TEMPRI (*), TEMPRF (*) - the b. o. t. and e. o. t. temperature of the R. Z. (K)
TEPS - the temperature epsilon; a convergence measure. (K)
TIMEND - the length of the accident scenario. (SEC)
TVAP - the vaporization temperature of the superheated steam. (K)
UMH2O1 (*), UMH2OF (*) - the unreacted amount of H2O in the R. Z. at the b. o. t. and e. o. t.
           (MOLE)
UMLII (*), UMLIF (*) - the unreacted amount of LI in the R. Z. at the b. o. t. and e. o. t. (MOLE)
UNZI, UNZF - the b. o. t. and e. o. t. internal energy of the N. Z. (J)
UNZQ - the internal energy of the system at the beginning of the program (J)
URZI, URZF - the b. o. t. and e. o. t. internal energy of the R. Z. (J)
VGASF - the volume of the gas in the R. Z. at the e. o. t. (M3)
VNRI (*), VNRF (*) - the b. o. t. and e. o. t. volume of the N. Z. (M3)
VRI (*), VRF (*) - the b. o. t. and e. o. t. volume of the R. Z. (M3)
VTOT - total volume of the system. (M3)
X - the mixing ratio; it is the ratio of the flow rate of H2O to flow rate of LI that enters the R. Z. during a timestep.
XH2OHF - the heat of formation of the H2O. (J/MOLE)
XLCPRV - the loss coefficient of the pressure relief valve.
XLMBHF - the heat of formation of the LMB. (J/MOLE)
C ****************************************************
C This is the main driving routine of the MARSBURN program.
C
C IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
C IMPLICIT INTEGER ( I-L,N )
C PARAMETER ( IWRITE = 6 )
C PARAMETER ( IOUT = 20, ITEMP = 11, IPRES = 12, IMH2 = 13,
C IFLOW = 14 )
C LOGICAL DEBUG(7)
C COMMON /DEB/, /DEBUG/, IDBOUT
C COMMON /INPUT/
C X, APRV,
C 2 PPRV, XLCPVR,
C 3 DELTAI, TIMEND, NPIPES, VTOT,
C 4 TEP5, PEPS, VR0
C COMMON /PROP/
C 1 DLMB, DLI0H, DLI, DPB,
C 2 XLMBH5,
C 3 TCLMB, TDLMB,
C 4 APLI
C
C First we set the default values for the common block
C variables.
C
C BEGINNING with INPUT.
C X = 1.
C APRV = .005
C PPRV = 1.72405
C XLCPVR = 2.69
C
C This is equivalent to the constant in the equation for the
C critical velocity for flow through an orifice.
C
C DELTAI = 1.0-4
C TIMEND = 10.
C NPIPES = 1.
C VTOT = 27.75
C TEP5 = 1.
C PEPS = 1.05
C VR0 = 1.0-5
C
C We must provide a volume at the beginning of the calculation for
C the first timestep water flow. This volume is equivalent to a
C spherical volume around the break with an effective radius of
C 1.34 cm. This radius is less than the tube pitch ( 1.84 cm ).
C Therefore the original break volume is confined to the region
C of one tube.
C
C Now we set the default values for the PROP common block.
C The default liquid metal breeder is LI-17 PB-83.
C
C DLMB = 8.97603
C DLI0H = 1.6303
C DLI = 510.
C DPB = 1.07104
C XLMBH5 = -1.42204
C TCLMB = 35.
C TDLMB = 2.270-5
C APLI = .17
The final default is the debug output logical unit number.

Now we call the INCHNG (input change) subroutine which prompts the user to set the rest of the common block variables and allows the user to change the default value of some of the common block variables.

CALL INCHNG

Now we set the initial values of program variables for the first timestep.

TEMPRI = 673.
TEMPNI = 673.
PI = 1.72405
VNRI = VTOT - VR0
VRI = VR0
MPBI = 0.
UMLII = 0.
UMH2O1 = 0.
MLIGHTI = 0.
MINERT = PI * VR0 / ( TEMPRI * 8.314 )

This is the initial gas in the reaction zone since the initial reaction zone volume must be nonzero. The gas is inert and is only present to keep the pressure calculations consistent.

Mh2i = 0.
DELTAT = DELTAI
NOUT = 0
NFLAG = 0

WRITE ( IWRITE,110 )
FORMAT ( ' PROGRAM EXECUTION NOW BEGINS ' )

CALL DRIVE ( TEMPRI, TEMPNI, PI, VNRI, VRI,
MPBI, UMLII, UMH2O1, MLIGHTI, Mh2i, MINERT,
DELTAT, NOUT, NFLAG,
PMAX, TMAX )

WRITE ( IWRITE,100 ) NOUT,ITEMP,IPRES,IMH2,IFLOW
FORMAT ( ' THERE ARE ','i5,' LINES IN THESE OUTPUT FILES' )
TIME vs. TEMP of R.Z. AND N.Z. IS IN LOGICAL UNIT NO. '
TIME vs. PRESSURE IS IN LOGICAL UNIT NO. 'i2'
TIME vs. MASS H2 IS IN LOGICAL UNIT NO. 'i2 /
TIME vs. H2O and BREEDER FLOW RATES IS IN LOGICAL ',
UNIT NO. ', 'i2 )

WRITE ( IWRITE,101 ) IOUT, IDBOUT
FORMAT ( ' THE GENERAL OUTPUT FILE IS IN LOGICAL UNIT',
1 ' NO. ', 'i2 / THE DEBUG OUTPUT IS IN LOGICAL UNIT',
2 ' NO. ', 'i2 )
WRITE ( IWRITE,102 ) PMAX, TMAX, X, APRV
FORMAT ( 5X,'i10X, THE MAXIMUM PRESSURE = ',1P1G11.4,
N/M2 '/ 10X, THE MAXIMUM REACTION ZONE',
TEMPERATURE = ',1P1G11.4,' k' / 10X, 'FOR X = ',
1P1G11.4, ' AND APRV = ',1P1G11.4, ' M2 ' )

C           That's all folks!
STOP
END

PROGRAM SECTIONS

<table>
<thead>
<tr>
<th>Name</th>
<th>Bytes</th>
<th>Attributes</th>
</tr>
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<tbody>
<tr>
<td>$CODE</td>
<td>557</td>
<td>PIC CON REL LCL SHR EXE RD NOWRT LONG</td>
</tr>
<tr>
<td>$DATA</td>
<td>577</td>
<td>PIC CON REL LCL SHR NOEXE RD NOWRT LONG</td>
</tr>
<tr>
<td>$LOCAL</td>
<td>188</td>
<td>PIC CON REL LCL NOSHR NOEXE RD WRT QUAD</td>
</tr>
<tr>
<td>DEB</td>
<td>32</td>
<td>PIC OVR REL GBL SHR NOEXE RD WRT LONG</td>
</tr>
<tr>
<td>INPUT</td>
<td>84</td>
<td>PIC OVR REL GBL SHR NOEXE RD WRT LONG</td>
</tr>
<tr>
<td>PROP</td>
<td>64</td>
<td>PIC OVR REL GBL SHR NOEXE RD WRT LONG</td>
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Total Space Allocated 1502

ENTRY POINTS

Address  Type  Name
0-00000000  MARSPRG$MAIN

VARIABLES

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<th>Address</th>
<th>Type</th>
<th>Name</th>
<th>Address</th>
<th>Type</th>
<th>Name</th>
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<tr>
<td>5-00000038</td>
<td>R*8</td>
<td>APLI</td>
<td>4-00000008</td>
<td>R*8</td>
<td>APRV</td>
<td>4-00000020</td>
<td>R*8</td>
<td>DELTAI</td>
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<td>R*8</td>
<td>DLI</td>
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<td>DLI</td>
<td>5-00000000</td>
<td>R*8</td>
<td>DLI</td>
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<td>2-00000000</td>
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<td>R*8</td>
<td>DLI</td>
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<td>MPBI</td>
<td>2-00000074</td>
<td>I*4</td>
<td>INFOR</td>
<td>2-00000070</td>
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<td>2-00000000</td>
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SUBROUTINE INCHNG

This subroutine sets the values of the logical vector DEBUG, the common block OUT, and allows the user to change the default values of X, APRV, PPRV, TIMEND, NPIPES, VRO, DLMB, XLMBHF, TCLMB, TOLMB, and APLI.

IMPLICIT DOUBLE PRECISION ( A-H, I-O-Z )

IMPLICIT INTEGER ( I-L, N )

INTEGER DEBUG(7), INPUT(7)

CHARACTER*6 CINIT(6)

CHARACTER*6 NAME(7)

LOGICAL DEBUG(7)

COMMON /DEB/, DEBUG, IDBOUT

COMMON /OUT/, JOUT1, JOUT2, JOUT3

COMMON /INPUT/

X, APRV,

PPRV, XLCPRV,

DELTAL, TIMEND, NPIPES, VTOT,

TEPS, PEPS, VRO

COMMON /PROP/

DLMB, DLIH, DLI, DPB,

XLMBHF,

TCLMB, TOLMB,

APLI

PARAMETER ( IREAD = 5, IWRITE = 6 )

First we set the character arrays NAME and CINIT.

NAME(1) = 'DRIVE'

NAME(2) = 'DRIVE'

NAME(3) = 'MASS'

NAME(4) = 'ENERZ'

NAME(5) = 'ROOT'

NAME(6) = 'CONTL'

NAME(7) = 'ENERZ'

CINIT(1) = 'X'

CINIT(2) = 'APRX'

CINIT(3) = 'APRX'

CINIT(4) = 'TIMEND'

CINIT(5) = 'NPIPES'

CINIT(6) = 'VRO'

Now we see if the user wants to change any default values.

WRITE ( IWRITE, 100 ) X, APRV, PPRV, TIMEND, NPIPES, VRO

FORMAT ( 10X/

1 THE DEFAULT VALUE OF X = ', IPIG11.4/

2 THE DEFAULT VALUE OF APRV = ', IPIG11.4., M2 '/

3 THE DEFAULT VALUE OF PPRV = ', IPIG11.4., PA '/

4 THE DEFAULT VALUE OF TIMEND = ', IPIG11.4., SEC '/

5 THE DEFAULT VALUE OF NPIPES = ', I3 /

6 THE DEFAULT VALUE OF VRO = ', IPIG11.4., M3 '/

C
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 ' VALUE OF , 6A )
0062 READ ( IREAD,*) CINPUT(I)
0063 C
0064 10 CONTINUE
0065 C
0066 IF ( CINPUT(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 ( CINPUT(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 ( CINPUT(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 ( CINPUT(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 ( CINPUT(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 ( CINPUT(6) .EQ. 1 ) THEN
0097 WRITE ( IWRITE,107 )
0098 107 FORMAT ( ' ENTER THE NEW VALUE OF VRO' )
0099 READ ( IREAD,*) VRO
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 ' PB-83' / ' IF YOU WANT TO ENTER THE PROPERTIES OF',
0106 ' A DIFFERENT TYPE OF BREEDER ',/
0107 ' ENTER A 1 ' )
0108 READ ( IREAD,*) CINPUT(7)
0109 C
0110 IF ( CINPUT(7) .EQ. 1 ) THEN
0111 WRITE ( IWRITE,111 )
0112 111 FORMAT ( ' ENTER THE NEW BREEDER DENSITY - KG3 ' )
0113 READ ( IREAD,*) DLMB
0114 C
INCHNG

0115 WRITE ( IWRITE,112 )
0117 FORMAT ( ' ENTER THE NEW BREEDER HEAT OF FORMATION ',
0118 ' - J/MOLE ' )
0119 READ ( IREAD,* ) XLMBHF
0120 C
0121 WRITE ( IWRITE,113 )
0122 FORMAT ( ' ENTER THE NEW BREEDER THERMAL CONDUCTIVITY ',
0123 ' - W/M-K ' )
0124 READ ( IREAD,* ) TCLMB
0125 C
0126 WRITE ( IWRITE,114 )
0127 FORMAT ( ' ENTER THE NEW BREEDER THERMAL DIFFUSIVITY ',
0128 ' - M2/SEC ' )
0129 READ ( IREAD,* ) TDLMB
0130 C
0131 WRITE ( IWRITE,115 )
0132 FORMAT ( ' ENTER THE NEW BREEDER ATOMIC FRACTION OF LI',
0133 1 '/ 5X, 'I. E. ENTERING 1. IMPLIES A PURE LI',
0134 2 ' BREEDER.'/ 5X, 'ENTERING .5 IMPLIES LI-50',
0135 3 ' PB-50.' )
0136 READ ( IREAD,* ) APL1
0137 C
0138 END IF
0139 C
0140 C Now we set the type of output wanted for this run.
0141 WRITE ( IWRITE,200 )
0142 FORMAT ( ' ENTER A 1 IF YOU WANT GENERAL OUTPUT' )
0143 READ ( IREAD,* ) JOUT1
0144 C
0145 IF ( JOUT1 .NE. 1 ) GO TO 55
0146 WRITE ( IWRITE,201 )
0147 FORMAT( ' ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE ',
0148 ' MOLAR COMPONENTS / OFF OF THE REACTION ZONE AND THE',
0149 ' FLOWRATES INTO AND OUT OF THE SYSTEM' )
0150 READ ( IREAD,* ) JOUT2
0151 C
0152 WRITE ( IWRITE,202 )
0153 FORMAT( ' ENTER A 1 IF THE GENERAL OUTPUT IS TO INCLUDE',
0154 ' THE ENERGY STATIS OF THE TWO ZONES.' )
0155 READ ( IREAD,* ) JOUT3
0156 55 CONTINUE
0157 C
0158 C Finally we set the debug switches.
0159 WRITE ( IWRITE,300 )
0160 FORMAT ( ' ENTER A 1 IF YOU WANT DEBUG OUTPUT ' )
0161 READ ( IREAD,* ) JOUT4
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 ' FOR SUBROUTINE ', 6A )
0168 READ ( IREAD,* ) IDEBUG(I)
0169 C
0170 IF ( IDEBUG(I) .EQ. 1 ) THEN
0171 DEBUG(I) = .TRUE.
INCHNG

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

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<thead>
<tr>
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<th>Attributes</th>
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Total Space Allocated 3024

ENTRY POINTS

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SUBROUTINE DRIVE

1 TEMPR, TEMPNI, PI, VNRI, VRI,
1 MPBI, UMLII, UMH201, MLI0HI, MH2I, MINERT,
2 DELTAT, NOUT, NFLAG,
3 PMAX, Tmax

This subroutine contains the driving do loop. It also calls
the mass balance subroutine (MDRIVE),
the reaction zone energy balance (ENERRZ), and the nonreaction zone
energy balance (ENERNZ). It also contains statements that adjust
the length of the timestep (DELTAT) depending upon the size of the
pressure change over the timestep. Finally, it calls the sub-
routine OUTPUT.

IMPLICIT DOUBLE PRECISION (A-H,M,O-Z)
IMPLICIT INTEGER (I-L,N)
DOUBLE PRECISION P(10), VRP(10)
LOGICAL DEBUG(7)
PARAMETER (IWRITE = 6)
COMMON /DEB/ DEBUG, IDBOUT
COMMON /INPUT/

1 X, APRV,
2 PPRV, XLCPVR,
3 DELTAI, TIMEND, NPIPES, VTOT,
4 TEPS, PEPS, VRD
COMMON /PROP/

1 DLMB, DLIOH, DLL, DPB,
2 XLMBHF,
3 TCLMB, TDLMB,
4 APLI

To begin we set up the do loop.
IPRV = 0
TIME = 0.

SUMQ = 0.

MNZO = VNRI * DLMB / ( (1 - APLI) * .20721 +
APLI * 6.940-3 )
PDUM = 0.
The above PDUM is a dummy variable, used to tell SENER not
to carry out the equations to determine the specific energy of
the water, since that information will not be needed here.
CALL SENER

1 TEMPNI, PDUM,
2
3 SEH2, SELIOH, SEH2O, SEPB, SEFI,
3 DSEH2, DSLIOH, DSEH2O, DSEPB, DSEFI

UNZO = MNZO * ( (1 - APLI) * SEPB + APLI *

1 SELI + XLMBHF )

URZI = 0.
UNZI = UNZO
DO 100 WHILE ( TIME .LE. TIMEND )
TEMPAV = TEMPRI
CONTINUE

First a call to the mass balance subroutine.
CALL MDRI
1 TEMPAV, MPBI, UMLII, UMH2O1, MLIOHI, MH2I, VNRI, PI, IPRV,
2 VRI, MINERT, DELTAT,
3 MH20, MSTM, MLMB, MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,
3 FRPRV, VNRF, VRF, VGASF, P, ICONTL, SESTM, SEH2OL
IF ( ICONTL .EQ. 1 ) GO TO 200
This condition checks to see if DELTAT was adjusted during the
execution of MDRIVE. If it has, MDRIVE is reexecuted until
DELAT is not adjusted during execution of MDRIVE.

Now the call to the reaction zone energy balance.
CALL ENERZR ( TEMPRI, TEMPNII, DELTAT, PI, P, VRF, MPBI, UMLII,
1 UMH2O1, MLIOHI, MH2I, MH2O, MSTM, MLMB, MPBF, UMLIF, UMH2OF,
1 MLIOHF, MH2F, VRI, URZI, SESTM, SEH2OL,
2 QCOND, PVDOO, URZF, ENGIN, QFCRZ, TEMPRF, DRDT )

Now for the pressure control statements.

First we determine the end of timestep pressure.
PF = 8.314 * ( MH2F + MINERT + UMH2OF ) * TEMPRF / VGASF
PCHECK = ( PI + 1.6543D0 ) * .5
IF ( PF .GT. PCHECK ) THEN
If this condition is true, it means that the pressure has
increased more than half of the way to 1.6543D0 psia, which is the
water tube back pressure. This means that the system may
change too rapidly over the timestep. To be prudent then, the
timestep is decreased by a call to PCONT. And the balances are
recalculated.
CALL PCONT ( 1 PI, PF,
2 DELTAT
)
IF ( DEBUG(1) ) THEN
WRITE ( IDBOUT,1000 )
1000 FORMAT ( '***** PF is greater than PCHECK ' )
WRITE ( IDBOUT,1001 ) PF, PCHECK
1001 FORMAT ( ' PF PCHECK ' / 1P2G11.4 )
END IF
GO TO 200
END IF

The following code block checks if the condition is true, then calculating the mass balance
isothermally may not be a good assumption. To correct this, we
recalculate the mass balance with a different temperature, which
C is the final reaction zone temperature over this last iteration.

C

TEMPAV = TEMPRF

C

IF ( DEBUG(1) ) THEN

WRITE ( IDBOUT,1003 ) PF, P(10)

C

1003

FORMAT ( ' PF P(10) ' / 1P9.4 )

C

WRITE ( IDBOUT,1002 )

C

1002

FORMAT ( ' ***** nonisothermal pressure ' )

C

END IF

C

GO TO 200

C

END IF

C

The pressure control statements are now completed.

C

Now for the nonreaction zone energy balance.

C

IF ( NFLAG .EQ. 1 ) GO TO 300

C

If this condition is true, then the nonreaction zone temper-

C

ature has converged to the steam tube ambient temperature ( 648K ).

C

In this case, the nonreaction zone temperature will remain

C

at 648K, and it is not necessary to carry out the nonreaction

C

zone energy balance.

C

CALL ENERNZ ( VNRI, VNRNF, TEMPNI, DELTAT, PVDOT, QCOND, FRPRV, MLMB,

C

1 UNZI,

C

2

C

3 UNZF, TEMPNF, ENGOUT, QFCNZ )

C

Now for the temperature control statements.

C

This first temperature control case is when TEMPRF and TEMPNF

C

converge to one temperature and remain at this temperature.

C

This is caused by either the value of X being too large or too

C

small. This causes the reaction rate to be too small, so that

C

the system reaches an equilibrium condition. This will cause

C

cannot work properly because the timestep decreases

C

significantly. If this happens, we halt the program.

C

IF ( DELTAT .LT. 1.0-12 ) THEN

C

WRITE ( IWRITE,1004 ) TIME, TEMPRF, TEMPNF, PF

C

1004

FORMAT ( ' PROGRAM EXECUTION HALTED ',1P9.4,

C

' SECONDS INTO THE ACCIDENT '/5X, ' BECAUSE EQUILITION',

C

2 ' BRIUM WAS REACHED BETWEEN THE TWO ZONES - WITH '/

C

5X, 'REACTION ZONE TEMPERATURE = ',1P9.4 /

C

5X, 'NONREACTION ZONE TEMPERATURE = ',1P9.4/

C

5X, 'SYSTEM PRESSURE = ',1P9.4 )

C

GO TO 101

C

END IF

C

IF ( ( TEMPNF - 648. ) .LE. .01 ) THEN

C

NFLAG = 1

C

TEMPNF = 648.

C

END IF

C

This alerts the program that the nonreaction zone temperature

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 C
0177 IF ( TEMPNF .GE. TEMPRF ) THEN
0178 DELTAT = DELTAT * .5
0179 GO TO 200
0180 END IF
0181 C To correct this, we must readjust the timestep size and
0182 C return to the beginning of the loop.
0183 C
0184 C SUMU = UNZF + URZF - UNZ0
0185 C SUMQ = DELTAT * ( ENGIN - ENGOUT - QFCRZ - QCFCN )
0186 C 1
0187 C SUMQ
0188 C These are the sum of the energy changes in the reaction
0189 C zone and nonreaction zone. If energy is conserved these will
0190 C be equal .
0191 C
0192 C MH2OFR = MH2O / DELTAT
0193 C MLMBFR = MLMB / DELTAT
0194 C 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 ( 1
0202 TIME, TEMPF, TEMPNF, PF, VRF(10), VGSF, MHH2OFR, MLMBFR,
0203 MPRVFR, MH2F, MBBF, UMLIF, UMH2OF, MLI0HF,
0204 QCOND, PVDOT, ENGOUT, ENGIN, URZF, UNZF, QFCRZ, QCFCNZ,
0205 DROTT, SUMQ, SUMU, URZI, UNZI,
0206 NOUT, NFLAG, PMAX, TMAX
0207 3 )
0208 C Finally, we reset the loop.
0209 C First we increase DELTAT. This is done so that the timestep
0210 C does not remain smaller than it needs to be.
0211 C DELTAT = 2. * DELTAT
0212 C PI = PF
0213 VRI = VRF(10)
0214 VNRI = VNRF
0215 TEMPI = TEMPRF
0216 TEMPNI = TEMPNF
0217 UMLII = UMLIF
0218 UMH2OI = UMH2OF
0219 MPBI = MPBF
0220 MLIOHI = MLI0HF
0221 MH2I = MH2F
0222 URZI = URZF
0223 UNZI = UNZF
0224 IF ( PI .GT. PPRV ) IPRV = 1
0225 C This condition checks to see if the rupture disk has opened
0226 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  execution. 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**

<table>
<thead>
<tr>
<th>Name</th>
<th>Bytes</th>
<th>Attributes</th>
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<td>PIC CON REL LCL SHR NOEXE RD NOWRT LONG</td>
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<td>$LOCAL</td>
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<td>PIC CON REL LCL NOSHR NOEXE RD WRT QUAD</td>
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<td>$INPUT</td>
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<td>PIC OVR REL GBL SHR NOEXE RD WRT LONG</td>
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**VX4-11 FORTRAN V3.5-62**

**Page 18**

18-Jul-1984 00:20:42 VAX-11 FORTRAN V3.5-62
18-Jul-1984 00:19:51 DUAI:[NUKE.JIM]MARS.PRG.26
### ARRAYS

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### FUNCTIONS AND SUBROUTINES REFERENCED

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SUBROUTINE MDRLVE ( 
  TEMP, MPB, UMLIB, UMH20, MLIOH, MH2I, VNRI, PI, IPRV, 
  VRI, MINERT, 
  DELT, 
  MH2O, MSTMA, MLMBA, MPBF, UMLIF, UMH2OF, MLIOHF, MH2F, 
  PRPRA, VNRF, VRF, VGASF, P, ICONTL, SESTMA, SEH20L 
)

This subroutine contains a do loop that drives the reaction
and nonreaction zones mass balance.

Since the reaction rate is determined by the interaction of the
pressure and the inlet and outlet flows, the mass balances, which
are dependent upon these flows, are the most important balances
in the overall process. To mirror this, the mass balances are
carried out 10 times for each time the energy balances are
calculated.

IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
IMPLICIT INTEGER ( I-L,N )
DOUBLE PRECISION P(10), VRF(10), MSTM(10), UMH2O(10),
MLMB(10), PRPRA(10), SESTM(10)

LOGICAL DEBUG(7)
COMMON /DEBF/ DEBUG, IDOUT
IF (. DEBUG(2) ) THEN
  WRITE ( IDOUT,1010 )
END IF

1010 FORMAT ( ' ENTERING MDRLVE ' )

PB = PB
UMLIB = UMLIB
UMH2 = UMH20 
MLIOH = MLIOH
MH2I = MH2I
VNRI = VNRI
PRPRA = PRPRA

DO 100 I = 1,10
  CALL FLOWRT ( 
    PB, 
    3 FRH2O, FRSTM, SESTM(I), SEH20L )

  CALL MASS ( 
    1 FRH2O, FRSTM, TEMP, MPB, UMLIB, UMH20, MLIOH, 
    1 MH2B, VNRI, PB, IPRV, VRF, MINERT, 
    2 DELT, 
    3 MH2O(I), MSTM(I), MLMBA, MPBF, UMLIF, UMH2OF, MLIOHF, 
    3 MH2F, PRPRA(I), VNRF, VRF(I), VGASF, P(I), ICONTL )

  IF ( ICONTL .EQ. 1 ) THEN
    DELT = DELT * 10.
  END IF
   GO TO 200
0059  END IF
0060  C  This condition checks to see if DELT was adjusted during the
0061  C  execution of MASS. If it has, control is returned to DRIVE.
0062  MPBB = MPBF
0063  UMLIB = UMLIF
0064  UMH2OB = UMH2OF
0065  MLIOH = MLIOHF
0066  MH2B = MH2F
0067  VRNF = VRVF
0068  PB = P(I)
0069  VRB = VRF(I)
0070  100 CONTINUE
0071  C  Now we must determine the average flowrates over the total
0072  C  timestep.
0073  C  timestep.
0074  FRPRVA = 0.
0075  MSTMA = 0.
0076  MH2OA = 0.
0077  MLMB = 0.
0078  SESTMA = 0.
0079  DO 300 I = 1,10
0080  MSTMA = MSTMA(I) + MSTMA
0081  MH2OA = MH2OA(I) + MH2OA
0082  MLMB = MLMB(I) + MLMB
0083  FRPRVA = FRPRV(I) + FRPRVA
0084  SESTMA = SESTM(I) + SESTMA
0085  300 CONTINUE
0086  SESTMA = SESTMA * 1.1
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  That's all folks!
0094  C
0095  IF ( DEBUG(2) ) THEN
0096  WRITE ( IDBOUT,1000 ) MH2OA, MSTMA, MLMB, FRPRVA
0097  1000  FORMAT ( ' MH2OA MSTMA MLMB 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, VRNF, VGASF, SEH20L
0101  1002  FORMAT ( ' MH2F VRNF VGASF SEH20L '/1P4G11.4 )
0102  WRITE ( IDBOUT,1003 ) ( P(I), I = 1,10 )
0103  1003  FORMAT ( ' P '/1P4G11.4 )
0104  WRITE ( IDBOUT,1004 ) ( VRF(I), I = 1,10 )
0105  1004  FORMAT ( ' VRF '/1P4G11.4 )
0106  WRITE ( IDBOUT,1005 ) ( SESTM(I), I=1,10 )
0107  1006  FORMAT ( ' SESTM '/1P4G11.4 )
0108  WRITE ( IDBOUT,1005 )
0109  1005  FORMAT ( ' EXATING MDRIVE ')
0110  END IF
0111  200 CONTINUE
0112  RETURN
0113  END
### PROGRAM SECTIONS

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**Total Space Allocated**: 1735

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SUBROUTINE FLOWRT ( 
 1 P, 
 2 3 FRH2O, FRSTM, SESTM, SEH2OL )

This subroutine calculates the flowrate of all the H2O and the 
steam from the broken tube(s) by the homogeneous equilibrium model. 
FRH2O and FRSTM are evaluated as functions of pressure. These 
flows are from two separate flow paths, one path connected 
to the upper plenum and one to the lower plenum. The H2O from 
the upper plenum is superheated over the whole range of pressures, 
with the critical pressure at 8.997606 Pa. The H2O from the lower 
plenum is subcooled. This subroutine also determines the specific 
internal energy of the steam and liquid (SESTM and SEH2OL).

IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
IMPLICIT INTEGER ( I-L,N )
COMMON /INPUT/ 
X, APRV,
PPRV, XLCPRV,
DELTAL, TIMEND, NPIPES, VTOT,
TEPS, PEPS, VRO

IF ( P .LE. 7.54533D6 ) THEN
FRSTM = 1.947
FRH2O = 11.064
ELSE IF (( P .LE. 8.27366D6 ) .AND. ( P .GT. 7.54533D6 ) ) THEN
FRSTM = 1.947
FRH2O = -5.91814D-7 * P + 15.5294
ELSE IF (( P .LE. 8.997606D6 ) .AND. ( P .GT. 8.27366D6 ) ) THEN
FRSTM = 1.947
FRH2O = -6.3260D-7 * P + 15.8669
ELSE IF (( P .LE. 9.65260D6 ) .AND. ( P .GT. 8.997606D6 ) ) THEN
FRSTM = -6.2305D-7 * P + 15.781
FRH2O = -6.56489D-9 * P + 2.00607
ELSE IF (( P .LE. 1.034207D ) .AND. ( P .GT. 9.65260D6 ) ) THEN
FRSTM = -3.04613D-8 * P + 2.23673
FRH2O = -7.67044D-7 * P + 17.1709
ELSE IF (( P .LE. 1.1032D7 ) .AND. ( P .GT. 1.034207D ) ) THEN
FRSTM = -5.82609D-8 * P + 2.52423
FRH2O = -6.85942D-7 * P + 16.3321
ELSE IF (( P .LE. 1.1721D7 ) .AND. ( P .GT. 1.1032D7 ) ) THEN
FRSTM = -7.73585D-8 * P + 2.73492
FRH2O = -9.00871D-7 * P + 18.7032
ELSE IF (( P .LE. 1.241D7 ) .AND. ( P .GT. 1.1721D7 ) ) THEN
FRSTM = -1.16619D-7 * P + 3.19593
FRH2O = -8.22642D-7 * P + 17.7663
ELSE IF (( P .LE. 1.31D7 ) .AND. ( P .GT. 1.241D7 ) ) THEN
FRSTM = -1.45073D-7 * P + 3.54815
FRH2O = -8.69565D-7 * P + 18.3686
ELSE IF (( P .LE. 1.3789D7 ) .AND. ( P .GT. 1.31D7 ) ) THEN
FRSTM = -1.89695D-7 * P + 4.13277
FRH2O = -1.02496D-6 * P + 20.4043
ELSE IF ( ( P .LE. 1.4479D7 ) .AND. ( P .GT. 1.3789D7 ) ) THEN
    FRSTM = -2.33623D-7 * P + 4.73843
    FRH2O = -1.14391D-6 * P + 22.0445
ELSE IF ( ( P .LE. 1.5168D7 ) .AND. ( P .GT. 1.4479D7 ) ) THEN
    FRSTM = -3.2656D-7 * P + 6.08407
    FRH2O = -1.4395D-6 * P + 26.2715
ELSE IF ( ( P .LE. 1.5858D7 ) .AND. ( P .GT. 1.5168D7 ) ) THEN
    FRSTM = -4.50783D-7 * P + 7.96827
    FRH2O = -1.81478D-6 * P + 32.0191
ELSE IF ( ( P .LE. 1.6547D7 ) .AND. ( P .GT. 1.5858D7 ) ) THEN
    FRSTM = -1.18978D-6 * P + 19.6873
    FRH2O = -4.7029D-6 * P + 77.8189
ELSE
    FRH2O = 0.
    FRSTM = 0.
END IF

C Now the total flowrates are determined by multiplying FRH2O
C and FRSTM by the number of broken pipes.
FRH2O = FRH2O * NPIPES
FRSTM = FRSTM * NPIPES

C Now to determine the specific energy of the H2O as it leaves
C the break and enters the reaction zone. The energy for the steam
C has been curve fitted to a parabolic form, with the independent
C variable being the pressure at the break. If the system pressure
C is less than the critical pressure (8.9976D6 Pa ), then the
C energy of the steam is determined at the critical pressure.
C The specific energy is determined from the 1st law as:
C
C U = Ib - P * V = 1 / 2 * ( VEL ) **2 + XH2OHF
C
C where, U is the specific energy, Ib is the back enthalpy,
C P * V is the pressure at the break times the specific volume
C at the break, 1/2 * ( VEL ) **2 is the kinetic energy of
C the water with VEL as the water velocity at the break, and
C XH2OHF is the heat of formation of the water. For the subcooled
C water from the lower plenum, the second and third terms of the
C above equation are negligible. Therefore SEH2OL is not a function
C of the break pressure.

XH2OHF = -2.418505
IF ( ( P .LE. 8.9976D6 ) THEN
    PBREAK = 8.9976D6
ELSE
    PBREAK = P
END IF

SESTM = 4.6404165D4 + 5.8535350D-4 * PBREAK + 1.0704336D-11
* ( PBREAK ** 2. ) + XH2OHF

SEH2OL = 2.31504 + XH2OHF
That's all folks!
RETURN
END
### PROGRAM SECTIONS

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Total Space Allocated: 1337

### ENTRY POINTS

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SUBROUTINE MASS (  
1 FRH2O, FRSTM, TEMPR, MPBI, UMLII, UMH2O1, MLIOHI, MH2I,  
1 VNRI, PI, IPRV, VRI, MINERT,  
2 DELTAT,  
3 MH2O, MSTM, MLMB, MPBF, UMLIF, UMH2OF, MLIOHF, MH2F,  
1 FRPRV, VNRV, VRV, VGASF, P, ICONTL )  
C  
C This subroutine evaluates the end of timestep masses of the  
C reaction products in the two zones, given the initial masses of  
C the constituents of the zones and the inlet flowrate of water.  
C On the basis of the end of timestep reaction zone composition  
C and the beginning of timestep pressure, the volumes of the  
C reaction and nonreaction zones and the flowrate out of the  
C pressure relief valve are determined.  
C  
C IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )  
C IMPLICIT INTEGER ( I-L,N )  
C LOGICAL DEBUG(7)  
C COMMON /DEB/ DEBUG, IDBOUT  
C COMMON /INPUT/  
C COMMON /APRV/  
C COMMON /XLPRV/  
C COMMON /DELTAT, TIMEND, NPIPES, VTOT/  
C COMMON /TEPS, PEPS, VRO/  
C COMMON /PROP/  
C COMMON /DLMB, DLIOH, DLI, DPB,  
C XLMBF,  
C TCLMB, TDLMB,  
C APLI  
C  
C IF ( DEBUG(3) ) THEN  
C WRITE ( IDBOUT,1000 )  
C FORMAT ( ' ENTERING MASS ' )  
C END IF  
C  
C REACTION ZONE MASS BALANCE ;  
C  
C First, from a mass balance on the reaction zone we can  
C determine the molar composition of the reaction zone at the  
C end of the timestep.  
C  
C MH2OL = 55.5 * FRH2O * DELTAT  
C MSTM = 55.5 * FRSTM * DELTAT  
C MH2O = MH2OL + MSTM  
C MLI = MH2O / X  
C MLMB = MLI / APLI  
C MPBF = ( 1. - APLI ) * MLMB + MPBI  
C IF ( X .LE. 1. ) THEN  
C UMLIF = MLI - MH2O + UMLII  
C UMH2OF = 0.  
C MLIOHF = MH2O + MLIOHI  
C MH2F = 2. * MH2O + MH2I  
C ELSE  
C UMLIF = 0.  
C UMH2OF = MH2O - MLI + UMH2O1
0058  MLI = MLI + MLI + MLI
0059  MH2F = 2 * MLI + MH2I
0060  END IF
0061  C  NONREACTION ZONE MASS BALANCE :
0062  C
0063  C  From a mass balance on the nonreaction zone, the time rate
0064  C  of change of the nonreaction zone mass is found to be due to
0065  C  the flow of breeder into the reaction zone and the flow of
0066  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  C  MASLMB = ( ( 1 - APLI ) * .20721 + APLI * 6.94D-3 ) * MLMB
0072  C
0073  C  The flow of breeder out of the pressure relief valve is
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 execution of this
0078  C  subroutine, since
0079  C  MASS maybe iterated upon many times during the execution of
0080  C  DRIVE and MDRIVE.
0081  C  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 /
0088  2  CONTINUE
0089  END IF
0090  C
0091  C  MASP = 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  C  VNRF = VNRI - ( MASP + MASLMB ) / DLMB
0099  C
0100  C  The volume of the reaction zone is the total breeder volume
0101  C  - the nonreaction zone volume.
0102  C  VRF = VRI + ( MASP + MASLMB ) / DLMB
0103  C
0104  C  We can now determine the volume of the gas ( H2 and H2Og )
0105  C  in the reaction zone.
0106  C  VGASF = VRF - 6.94D-3 * UMLIF / DLI - 2.31D-2 * MLIH
0107  C  1 /
0108  C
0109  C  ISOThERMAL PRESSURE :
0109  C
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.
P = 8.314 * ( MH2F + MINERT + UMH2OF ) * TEMPR / VGASF
IF ( P.GT. 1.654707 ) THEN

C If this condition is true, it means that the shell side
C pressure has exceeded the water back pressure. This condition
C is corrected by a call to PCONTL, which decreases the timestep.
C
CALL PCONTL ( 1 PI, P, 2 DELTAT, 3 )
ICONTL = 1
GO TO 200

C This variable alerts the calling routines MDRIVE and DRIVE
C that DELTAT has been adjusted.
ELSE
ICONTL = 0
END IF

C That's all folks!
IF ( DEBUG(3) ) THEN
WRITE ( IOUT,1001 ) MH2O, MSTM, MLMB, FRPRV
1001 FORMAT ( ' MH2O MSTM MLMB FRPRV ' / 1PG11.4 )
WRITE ( IOUT,1002 ) MPBF, UMLIF, UMH2OF, MLIOHF, MH2F
1002 FORMAT ( ' MPBF UMLIF UMH2OF MLIOHF MH2F ' / 1PG11.4 )
WRITE ( IOUT,1003 ) VNRF, VRF, VGASF, P
1003 FORMAT ( ' VNRF VRF VGASF P ' / 1PG11.4 )
WRITE ( IOUT,1004 ) END IF
1004 FORMAT ( ' EXITING MASS ' )
END IF

C
200 CONTINUE
RETURN
END
### PROGRAM SECTIONS

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**Total Space Allocated**: 1106

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## FUNCTIONS AND SUBROUTINES REFERENCED

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SUBROUTINE PCONTL ( 
  1 PI, PF, 
  2 DELTAT 
  3 )
C This subroutine decreases the timestep in order to lower the 
C pressure increase during the timestep.
C
IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )
IMPLICIT INTEGER ( I-L,N )
LOGICAL DEBUG(7)
COMMON /DEB/ DEBUG, IDBOUT
C IF ( DEBUG(6) ) WRITE ( IDBOUT,1000 ) DELTAT
C DELTAT = DELTAT * PI / PF
C IF ( DEBUG(6) ) WRITE ( IDBOUT,1001 ) DELTAT
1000 FORMAT ( '********** THE ORIGINAL DELTAT = ', 1P1G11.4 )
1001 FORMAT ( ' IS NOW = ', 1P1G11.4 )
C That's all folks!
RETURN
END
### PROGRAM SECTIONS

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**Total Space Allocated**: 215

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**SUBROUTINE ENERRZ**

1 TEMPR1, TEMPN1, DELTAT, PI, P, VRF, MPB1, UMLII,
2 UMH20I, MLIOHI, MHZ1, MH20, MSTR, MLMB, MPBF, UMLIF, UMH2OF,
3 MLIOHF, MH2F, VRI, URZI, SESTM, SEH20L,
4 QCOND, PVDOT, URZF, ENGIN, QFCRZ, TEMPRF, DRDT

This subroutine solves an energy balance on the reaction zone. The reaction zone end of timestep energy is determined by the change in energy during the timestep. The end of timestep average reaction zone temperature is then determined.

**IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )**

**DOUBLE PRECISION PI(10), VRF(10), PV(10)**

**LOGICAL DEBUG(7)**

**COMMON /DEB/ DEBUG, IDBOUT**

**COMMON /INPUT/**

1 X, APRV,
2 PPRV, XLCPRV,
3 DELTAT, TIMEND, NPIPS, VTOT,
4 TEP, PEPS, VR0

**COMMON /PROP/**

1 DLMB, DLIOH, DL1, DPB,
2 XLMBHF,
3 TCLMB, TDLMB,
4 API

**IF ( DEBUG(4) ) THEN**

**WRITE ( IDBOUT,1000 )**

**FORMAT (' ENTERING ENERRZ ' )**

**END IF**

The energy balance can be expressed as:

**URZF = URZI + DELTAT* ( -PVDOT - QCOND - ENGIN - QFCRZ )**

****** QFCRZ *******

This is the change in reaction zone energy due to forced convection to unbroken steam tubes. This quantity is very approximate. So we assume it is not a function of TEMPRF for simplicity.

**QFCRZ = 1.36D5 * ( VRF(10) + VRI ) * ( TEMPRI - 648. )**

****** PVDOT *******

This is the energy change due to the work the fluid in the reaction zone does as it expands. There are 10 parts to this quantity for each of the 10 subtimesteps.

**DELT = DELTAT * .1**

**DO 100 I = 2,10**

**PV(I) = .5 * ( P(I) + PI ) * ( VRF(I) - VRI ) / DELT**

**100 CONTINUE**
C PVDOT = 0.
0060  DO 200 J = 1,10
0061        PVDOT = PVDOT + PV(J)
0062 200 CONTINUE
0063        PVDOT = PVDOT * .1
0064 C ***** ENGIN *****
0065 C This is the energy of the H2O and the breeder flowing into
0066 C the reaction zone during the timestep.
0067        PAVE = ( PI + P(10) ) * .5
0068 C CALL SENER (
0069 C        1 TEMPNI, PAVE,
0070 C        2
0071 C        3 SEH2, SELIOM, SEH2O, SEPB, SELI,
0072 C        3 DSEH2, DSLIOM, DSEH2O, DSEPB, DSELI )
0073 C The temperature at which the liquid metal breeder internal
0074 C energy is determined at is the temperature of the nonreaction
0075 C zone, since this is the origin of the LMB.
0076 C ENGIN = ( MSTM * SESTM + ( MH2O - MSTM ) * SEH2OL +
0077 C        1 MLMB * ( ( 1 - APLI ) * SEPB + APLI * SELI +
0078 C        2 XLMHBF ) ) / DELTAT
0079 C ***** URZI *****
0080 C This is the internal energy of the reaction zone contents
0081 C at the beginning of the timestep. It is equal to the final
0082 C internal energy of the reaction zone from the last timestep.
0083 C Now we are ready for the temperature iteration loop.
0084 C TEMP = TEMPRI
0085 300 CONTINUE
0086 C ***** QCND *****
0087 C This is the heat transferred from the reaction zone to the
0088 C nonreaction zone due to conduction. It is a function of the
0089 C reaction zone final temperature.
0090 C RADRZF = .62 * ( VRF(10) ** ( 1. / 3. ) )
0091 C RADRZI = .62 * ( VR1 ** ( 1. / 3. ) )
0092 C RADAVG = .75 * ( RADRZF ** 4. - RADRZI ** 4. ) /
0093 C        1 ( RADRZF ** 3. - RADRZI ** 3. )
0094 C DROT = ( RADRZF - RADRZI ) / DELTAT
0095 C PEND = 1.77 + DSQRT ( DELTAT * TDLMB )
0096 C QCND = 6.23 * TCLMB * ( TEMP + TEMPRI - 2. * TEMPNI )
0097 C        1 * ( RADAVG ** 2. ) / PEND
0098 C ***** URZF *****
0099 C We now sum up the energy flows to determine the end of
0100 C timestep reaction zone internal energy.
0101 C URZF = URZI + DELTAT * ( ENGIN - QFCRZ - PVDOT - QCND )
0102 C ***** TEMPRF *****
We now determine the end of timestep temperature of the reaction zone from the value of URZF.

CALL ROOT ( 1 TEMPRI, URZF, PAVE, 1 MPBF, UMLIF, UMHZOF, MLIOHF, MHZF, 3 TEMPRF )

IF ( ( DABS ( TEMPRF - TEMP ) ) .GT. TEPS ) THEN
  IF this condition is true it means that the temperature used to calculate QCOND is not the end of timestep temperature.
  Thus we must iterate until this condition is false.
  TEMP = TEMPRF
  GO TO 300
END IF

That's all folks!

IF ( DEBUG(4) ) THEN
  WRITE ( IDBOUT,1001 ) URZI, QCOND, PVDOT
  FORMAT ( ' URZI QCOND PVDOT '/ 1P3G11.4 )
  WRITE ( IDBOUT,1002 ) QFCRZ, ENGIN, PEND
  FORMAT ( ' QFCRZ ENGIN PEND '/ 1P3G11.4 )
  WRITE ( IDBOUT,1003 ) URZF, TEMPRF
  FORMAT ( ' URZF TEMPRF '/ 1P2G11.4 )
  WRITE ( IDBOUT,1004 )
  FORMAT ( ' EXITING ENERRZ ' )
END IF

RETURN

END
PROGRAM SECTIONS

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FUNCTIONS AND SUBROUTINES REFERENCED

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</table>
SUBROUTINE SENER ( 
  1 T, P, 
  2 3 SEH2, SELIOH, SEH20, SEPB, SELI, 
  3 DSEH2, DSL1OH, DSEH20, DSEPB, DSELI )

This subroutine calculates the specific energy and the 
temperature derivative of the specific energy for H2, LIOH, 
H20, PB, and LI, as functions of the input temperature (T).
The constants used in the subroutine are taken from the 
JANAF tables. The reference temperature is 273.15 K.

IMPLICIT DOUBLE PRECISION ( A-H,M-O-Z )
IMPLICIT INTEGER ( I-L,N )

***** H2 *****
The specific heat at constant volume for an ideal diatomic 
gas is 5/2* ideal gas constant.
SEH2 = 20.75 * ( T - 273.15 )
DSEH2 = 20.75

***** LIOH *****
LIOH changes phase (melts) at 744.3 K. For T .LE. 744.3
the specific energy is curve fitted so that the specific energy 
and the temperature derivative of the specific energy are 
continuous at T=744.3 K. The specific energy includes the 
heat of formation (4.738805 J/MOLE ).

IF ( T .GE. 744.3 ) THEN
  SELIOH = 86.78 * ( T - 744.3 ) - 4.24305
  DSLIOH = 86.78
ELSE
  SELIOH = -3.9310-2 * ( ( T - 273.15 ) ** 2. ) +
  123.8 * ( T - 273.15 ) - 4.73905
  DSLIOH = -7.8820-2 * ( T - 273.15 ) + 123.8
END IF

***** H2O *****
The water is assumed to be superheated steam. The specific 
heat at constant volume is assumed to be 27. J/MOLE over the 
range of pressure and temperature. The specific energy is 
equal to:
27. * ( T - TVAP ) + HVAP + XH20HF
where: TVAP is the vaporation temperature, HVAP is the 
saturated steam enthalpy and XH20HF is the water heat of formation.
TVAP and HVAP are functions of pressure, the equations for which 
could be determined by curve fitting data between pressures of 
1.72405 and 1.654707 Pa.
IF ( P .EQ. 0. ) THEN
  P will equal 0 when the nonreaction zone energy is being 
determined. Since the nonreaction zone does not contain any 
water the specific energy of the water in that case need not 
be determined.
C SEH20 = 0.
DSEH20 = 0.
ELSE
XH2OHF = -2.418D5
TVAP = 308.84026 * DEXP ( ( DLOG( P ) - 5.9053292 )
1
HVAP = 5.024945304 * DEXP ( -1. * (( P - 4.5033433D6 )
1
SEH20 = 27. * ( T - TVAP ) + HVAP + XH2OHF
DSEH20 = 27.
END IF
C ****** PB ******
C We assume that T .GT. Tmelt = 600.6 K.
SEPB = 30.3 * ( T - 600.6 ) + 1.394D4
DSEPB = 30.3
C ****** LI ******
C We assume that T .GT. Tmelt = 453.7 K.
SELI = 29.7 * ( T - 453.7 ) + 7.85D3
DSELI = 29.7
C RETURN
C END

PROGRAM SECTIONS

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Total Space Allocated 493

ENTRY POINTS

Address Type Name
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VARIABLES

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AP-00000004@ R8 T 2-00000008 R8 TVAP 2-000000000 R8 XH2OHF
SUBROUTINE ROOT

This subroutine determines the end of timestep temperature by Newton's method for finding the roots of an equation.

IMPLICIT DOUBLE PRECISION (A-H, O-Z)
IMPLICIT INTEGER (I-L, N)
LOGICAL DEBUG (7)
COMMON /INPUT/
X, APRV,
PPRV, XLCPVR,
DELTAI, TIMENO, NPIPES, VTOT,
TEPS, PEPS, VRI
COMMON /DEB/ DEBUG, IDBOUT
IF (DEBUG(5)) THEN
   WRITE (IDBOUT, 1000)
   FORMAT (' ENTERING ROOT ')
   WRITE (IDBOUT, 1001) TI, UF, MPBF, UMLIF
   FORMAT (' TI UF MPBF UMLIF / 1P4G11.4 ')
   WRITE (IDBOUT, 1002) UMH2OF, MLI0HF, MH2F
   END IF

Newton's method for finding roots gives:

TF = TI - F(TI) / (dF(TI)/dT)

where,
F(TI) = UF - (MPBF*SEPB + UMLIF*SELIF + UMH2OF*SEH2O + MLI0HF*SELIOH + MH2F*SEH2F)

and,
dF(TI)/dT = MPBF*DSEPB + UMLIF*DSELI + UMH2OF*DSEH2O + MLI0HF*DSELIOH + MH2F*DSEH2

TDUM = TI
CONTINUE

CALL SENER (TDUM, P,
SEH2, SELIOH, SEH2O, SEPB, SELI,
DSEH2, DSLIOH, DSEH2O, DSEPB, DSELI)

TF = TDUM + (UF - (MH2F * SEH2 + MLI0HF * SELIOH + UMH2OF * SEH2O + MPBF * SEPB + UMLIF * SELI)) / (MH2F * DSEH2 + MLI0HF * DSLIOH + UMH2OF * DSEH2O + MPBF * DSEPB + UMLIF * DSELI)
0058   C      IF ( DEBUG(5) ) THEN
0059     WRITE ( IDBOUT,1003 ) TF
0060  1003      FORMAT ( ' ITERATION TF ' / 1P1G11.4 )
0061     END IF
0062     C
0063     C      IF ( ( DABS ( TF - TDUM ) ) .GT. TEPS ) THEN
0064     C      If this condition is true, then we must reiterate until
0065     C      TF - TDUM converges to TEPS .
0066     C
0067     C      TDUM = TF
0068     C      GO TO 100
0069     C      END IF
0070     C
0071     C      IF ( DEBUG(5) ) THEN
0072     C      WRITE ( IDBOUT,1004 ) TF
0073     1004      FORMAT ( ' TF ' / 1P1G11.4 )
0074     C      WRITE ( IDBOUT,1005 )
0075     C      END IF
0076     C
0077     C      THAT'S ALL FOLKS!
0078     C     RETURN
0079     C     END

PROGRAM SECTIONS

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FUNCTIONS AND SUBROUTINES REFERENCED

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SENER
SUBROUTINE ENERNZ (
1 VNRI, VNRF, TEMPNI, DELTAT, PVDOT, QCOND, FRPRV, MLMB, UNZI,
2 3 UNZF, TEMPNF, ENGOUT, QFCNZ)

This subroutine solves an energy balance on the nonreaction zone. The nonreaction zone end of timestep energy is determined by the change in energy during the timestep. The end of timestep average nonreaction zone temperature is then determined.

IMPLICIT DOUBLE PRECISION (A-H,M,O-Z)
IMPLICIT INTEGER (I-L,N)
LOGICAL DEBUG(7)
COMMON /DEBDEBUG, IDBOUT
COMMON /INPUT/
X, APRV,
PRPRV, XLCPRV,
DELTAT, TIMEND, NPipes, VTOT,
TEPS, PEPS, VRO
COMMON /PROP/
DLMB, DLCH, DLI, DPB,
XLMBHF,
TCLMB, TDLMB,
APLi
IF (DEBUG(7)) THEN
WRITE (IDBOUT,1000)
1000 FORMAT ('ENTERING ENERNZ')
END IF

The energy balance can be expressed as:
UNZF = UNZI + DELTAT * (PVDOT + QCOND - ENGOUT - QFCNZ)

***** QFCNZ *****
This is the change in the nonreaction zone energy due to forced convection to unbroken steam tubes. This function is very approximate.
QFCNZ = 4.305 * (VNRF + VNRI) * (TEMPNI - 648.)

***** PVDOT *****
This is just the work due to expansion as calculated in ENERRZ, with an opposite sign.

***** QCOND *****
This is the heat flow due to conduction as calculated in ENERRZ, again with an opposite sign.

***** ENGOUT *****
This is the energy of the breeder flowing out of the nonreaction zone through the pressure relief valve (FRPRV) and to the reaction zone (MLMB).
P = 0.
CALL SENER (
ENERNZ

18-Jul-1984 00:20:42  VAX-11 FORTRAN V3.5-62
18-Jul-1984 00:19:51  DUA1:[NUKE.JIM]MARSPEQ..26

0058 1 TEMPNI, P,
0059 2
0060 3 SEH2, SELI0H, SEH20, SEPB, SELI,
0061 3 DSEH2, DSLI0H, DSEH20, DSEP, DSELI )
0062 SELMB = ( 1. - APLI ) * SEP + APLI * SELI + XLMBHF
0063 ENGOUT = ( MLMB / DELTAT + FRPRV / ( ( 1. - APLI )
0064 1
0065 * .20721 + APLI * 6.94D-3 ) ) * SELMB
0066 C
0067 C ***** UNZI *****
0068 C This is the internal energy of the liquid metal breeder
0069 C In the nonreaction zone at the beginning of the timestep.
0070 C It equals the final internal energy of the nonreaction zone
0071 C from the last timestep.
0072 C
0073 C ***** UNZF *****
0074 C We can now sum up the energy changes to determine the end
0075 C of timestep nonreaction zone internal energy.
0076 C
0077 C UNZF = UNZI + DELTAT * ( PVDOT + QCOND - ENGOUT - QFCNZ )
0078 C
0079 C ***** TEMPNF *****
0080 C We can now determine the nonreaction zone end of timestep
0081 C temperature from the value of UNZF.
0082 C
0083 C Before we call ROOT though, we must input the correct list of
0084 C the dummy variables shared with ROOT, so that ROOT performs
0085 C properly.
0086 C
0087 C
0088
0089 C
0090 C
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 C
0094 C
0095 C
0096 C
0097 C
0098 C
0099 C
0100 C
0101 C
0102 C
0103 C
0104 C
0105 C
0106 C
0107 C
0108 C
0109 C
0110 C
0111 C

69
PROGRAM SECTIONS

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SUBROUTINE OUTPUT (  
  TIME, TEMPRF, TEMPNF, PF, VRF, VGASF, MH20FR, MLMBFR,  
  MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, MLI0HF,  
  QCND, PVDOT, ENGOUT, ENGIN, URFZ, UNZF, QFCRZ, QFCNZ,  
  DRDT, SUQM, SUMU, URZI, UNZI,  
  NOUT, NFLAG, PMAX, TMAX  
)  
This subroutine directs the output to different files. 
There are 5 different output files with these logical numbers set as parameters.  
IOUT is the general output file.  
ITEMP gives a list of TIME, TEMPRF, and TEMPNF.  
IPRES gives the TIME and PF.  
IMH2 gives the TIME and MH2F.  
IFLOW gives the TIME, MH2O, and FRPRV.  
These last 4 files will simply contain a list of numbers without comment.  
This allows these lists to be easily connected to graphics programs.  
IMPLICIT DOUBLE PRECISION ( A-H,M,O-Z )  
IMPLICIT INTEGER ( I-L,N )  
COMMON /OUT/ JOUT, JOUT2, JOUT3  
COMMON /INPUT/ X, APRV, PPRV, XLCPRV,  
3 DELTAI, TIMEND, NPIPEC, VTOT,  
4 TEPS, PEPS, VRO  
COMMON /PROP/ DLMB, DLI0H, DL1, DPB,  
2 XLMHBF,  
3 TCLMB, TDLMB,  
4 APLI  
PARAMETER ( IOUT = 20, ITEMP = 11, IPRES = 12, IMH2 = 13,  
  IFLOW = 14 )  
NOUT = NOUT + 1  
First we determine if the current value of PF or TEMPRF is a maximum.  
IF ( NOUT .EQ. 1 ) THEN  
  PMAX = PF  
  TMAX = TEMPRF  
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 ( ITEMPL,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 ( IMH,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 XAPL = 100. * APLI
0081 APPB = 100. * ( 1. - APLI )
0082 WRITE ( IOUT,220 ) X, APRV, PPRV, TIMEND, NPIPES, VRO.
0083 XAPL, 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 ------ ',13 /
0093 9 15X,' THE INITIAL REACTION ZONE VOL ------ ',1P1G11.4,/
0094 1 ' M3' /
0095 2 1P1G11.4,' % LI AND ',1P1G11.4, ' % PB' /
0096 3 5X / 5X / 5X )
0097 END IF
0098 C
0099 C IF ( NFLAG .EQ. 0 ) THEN
0100 WRITE ( IOUT,200 ) TIME
0101 WRITE ( IOUT,201 ) TEMPRF, TEMPNF, PF, VRF, VGASF
0102 IF ( JOUT2 .EQ. 1 ) WRITE ( IOUT,202 ) MH2OF, MLMBFR,
0103 MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, ML1OHF, DRDT
0104 1
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 2
0109 C
0110 ELSE
0111 C WRITE ( IOUT,200 ) TIME
0112 WRITE ( IOUT,201 ) TEMPRF, TEMPNF, PF, VRF, VGASF
0113 IF ( JOUT2 .EQ. 1 ) WRITE ( IOUT,202 ) MH2OF, MLMBFR,
0114 1 MPRVFR, MH2F, MPBF, UMLIF, UMH2OF, ML1OHF
END IF

200 FORMAT ( 10X / 10X / '******************************',
1        1 '**************' / 5X, ' END OF Timestep TIME ------ ',
1        2 1PI1G11.4, ' SEC ' / )

201 FORMAT ( 10X / 5X, ' REACTION ZONE TEMPERATURE -- ',
1        1 1PI1G11.4, ' K ' /
1        2 5X, ' NONREACTION ZONE TEMPERATURE ', 1PI1G11.4, ' K ' /
1        3 5X/5X, ' SYSTEM PRESSURE ---------------- ', 1PI1G11.4, ' PA ' /
1        4 5X/5X, ' REACTION ZONE VOLUME --------- ', 1PI1G11.4, ' M3 ' /
1        5 5X, ' GAS VOLUME ------------------- ', 1PI1G11.4, ' M3 ' / )

202 FORMAT ( 5X/5X, ' MOLAR FLOWRATE - H2O -------- ', 1PI1G11.4, ' MOLES/SEC ' /
1        1 5X, ' MOLAR FLOWRATE TO R.Z. - LMB ', 1PI1G11.4, ' MOLES/SEC ' /
1        2 5X/5X, ' MOLAR FLOWRATE OUT OF PRV -- ', 1PI1G11.4, ' MOLES/SEC ' /
1        3 5X, ' MASS OF H2 IN R.Z. -------- ', 1PI1G11.4, ' MOLES ' /
1        4 5X/5X, ' MASS OF PB IN R.Z. -------- ', 1PI1G11.4, ' MOLES ' /
1        5 5X, ' MASS OF UNREACTION LI IN R.Z. ', 1PI1G11.4, ' MOLES ' /
1        6 5X, ' MASS OF UNREACTION H2O IN R.Z. ', 1PI1G11.4, ' MOLES ' /
1        7 5X, ' MASS OF LIOH IN R.Z. -------- ', 1PI1G11.4, ' MOLES ' /
1        8 5X/5X, ' R.Z. EXPANSION VELOCITY ---- ', 1PI1G11.4, ' M/SEC ' /)

203 FORMAT ( 5X/5X, ' CONDUCTION ENERGY ----------------- ', 1PI1G11.4, ' J/SEC ' /
1        1 5X, ' FLUID EXPANSION WORK -------- ', 1PI1G11.4, ' J/SEC ' /
1        2 5X, ' ENERGY FLOW INTO R.Z. ------- ', 1PI1G11.4, ' J/SEC ' /
1        3 5X, ' ENERGY FLOW OUT OF N.Z. ----- ', 1PI1G11.4, ' J/SEC ' /
1        4 5X, ' CONVECTION ENERGY OUT OF R.Z. ', 1PI1G11.4, ' J/SEC ' /
1        5 5X, ' CONVECTION ENERGY OUT OF N.Z. ', 1PI1G11.4, ' J/SEC ' /
1        6 5X/5X, ' FINAL ENERGY OF N.Z. ------ ', 1PI1G11.4, ' J ' /
1        7 5X/5X, ' INITIAL ENERGY OF R.Z. ----- ', 1PI1G11.4, ' J ' /
1        8 5X/5X, ' INITIAL ENERGY OF N.Z. ----- ', 1PI1G11.4, ' J ' /
1        9 5X/5X, ' SUM OF ENERGY CHANGE TOTAL ---- ', 1PI1G11.4, ' J ' /
1        10 5X/5X, ' TOTAL INTERNAL ENERGY ------ ', 1PI1G11.4, ' J ' /)

That's all folks!

RETURN

END
**PROGRAM SECTIONS**

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**LABELS**

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OUTPUT

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18-Jul-1984 00:19:51 DUA1:[NUKE.JIM]MARSFRG.;26

COMMAND QUALIFIERS

FORTRAN /LIST MARSFRG.;26
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COMPILATION STATISTICS

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

***EOF***  54 PAGES COST $5.40 PROJ BALANCE $996.10 USER BALANCE $905.77
NOMENCLATURE

A an area
A\textsubscript{D} the area of the steam tube break
A\textsubscript{prv} the area of the pressure relief valve and a variable in dynamic model equations
A\textsubscript{t} the surface area of a steam tube
C\textsubscript{1} the factor that determines the probability that the outer tube, of the duplex tube, will fail
C\textsubscript{2} the factor that determines the probability that the inner tube will fail due to the failure of the outer tube
C\textsubscript{3} the factor that determines the probability that the outer tube will fail, due to the failure of the inner tube
C\textsubscript{4} the factor that determines the probability that a small break will deteriorate into a large break
C\textsubscript{H} the molar specific heat of hydrogen
C\textsubscript{L} the molar specific heat of lithium
C\textsubscript{LH} the molar specific heat of lithium hydroxide
E\textsubscript{R} the total internal energy of the reaction zone
E\textsubscript{tot} the overall unavailability of a steam generator design
h the overall heat transfer coefficient of the steam tube
i\textsubscript{b} enthalpy of the liquid metal breeder entering the reaction zone
i\textsubscript{f} the heat of formation of the liquid metal breeder, Li\textsubscript{17}Pb\textsubscript{83}
i\textsubscript{wb} the enthalpy of the water/steam flowing through the steam tube break
i\textsubscript{wf} the final enthalpy of the water in the Thermodynamic Equilibrium Model
i\textsubscript{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

\( P_{\text{max}} \) the maximum system pressure

\( P_\infty \) 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

\( S_{\text{WB}} \) the entropy of the water at the tube break

\( S_{\text{NO}} \) the initial entropy of the water

\( T_f \) the final thermodynamic equilibrium temperature

\( T_n \) the average temperature of the nonreaction zone

\( T_{\text{ni}} \) 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°C
\( V_r \) 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\(_2\)O to the molar flow rate of Li into the reaction zone per timestep.
\( \alpha_n \) the thermal diffusivity of the liquid metal breeder
\( \Delta G \) the Gibb's free energy of the Li\(_{17}\)Pb\(_{83}\)
\( \Delta S \) the entropy of the Li\(_{17}\)Pb\(_{83}\)
\( \Delta t \) the length of the timestep is seconds
\( \lambda \) the probability of a specific accident scenario
\( \lambda_i \) the probability that the inner tube, of the duplex tube, will fail
\( \lambda_o \) the probability that the outer tube will fail
\( \lambda_{PWR} \) the probability that a PWR steam tube will fail
\( \lambda_{SG} \) the overall probability that a forced shutdown of the steam generator will occur
\( \mu \) the reciprocal of the time needed to repair the steam generator, which has been shut down due to a specific accident scenario
\( \lambda \) the conduction length scale derived from boundary layer theory
\( \rho_B \) the density of the liquid metal breeder
\( \rho_{WB} \) the density of the water/steam flowing through the steam tube break
References


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


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


