Modeling of Lithium-Lead/Water Interactions in a Fusion Reactor Design: Part II. Modeling Improvements

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UWFDM-649

FUSION TECHNOLOGY INSTITUTE

UNIVERSITY OF WISCONSIN

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Prepared for EG&G Idaho Inc. and the Department of Energy Idaho Operations Office under DOE Contract DE-AC07-76ID01570.

Abstract

Two major improvements have been made to our dynamic parametric model for liquid metal/water reactions in a steam generator, which we introduced in a previous report (UWFDM-559). Because of the results of large scale lithium-lead experiments carried out at HEDL, we have altered the chemical reaction on which our model is based, from the LiOH redox reaction to the Li_2O reaction. The effect of this modification is to roughly double the amount of hydrogen produced during the accident. The hydrogen production rate seems to be a more serious problem than we had originally estimated. The second change made to our model was to allow the liquid metal to be a compressible fluid. As a result of this change, our model predicts that a pressure wave will be generated within a few milliseconds of accident initiation. This pressure wave effect should be considered for the structural integrity of the steam generator. Finally, the temperature response is quite similar to that in the original study indicating that the initial peak reaction zone temperature for a lithium-lead pool is lower than that for a lithium pool. In both cases the reaction zone temperature decreases to near the surrounding temperature quickly after the transient begins (~ 10 s).

Introduction

In this paper, we discuss improvements that were made to the computational model of lithium-lead/water interactions, MARSBURN. This paper is intended as a supplementary report to our original work.[1]

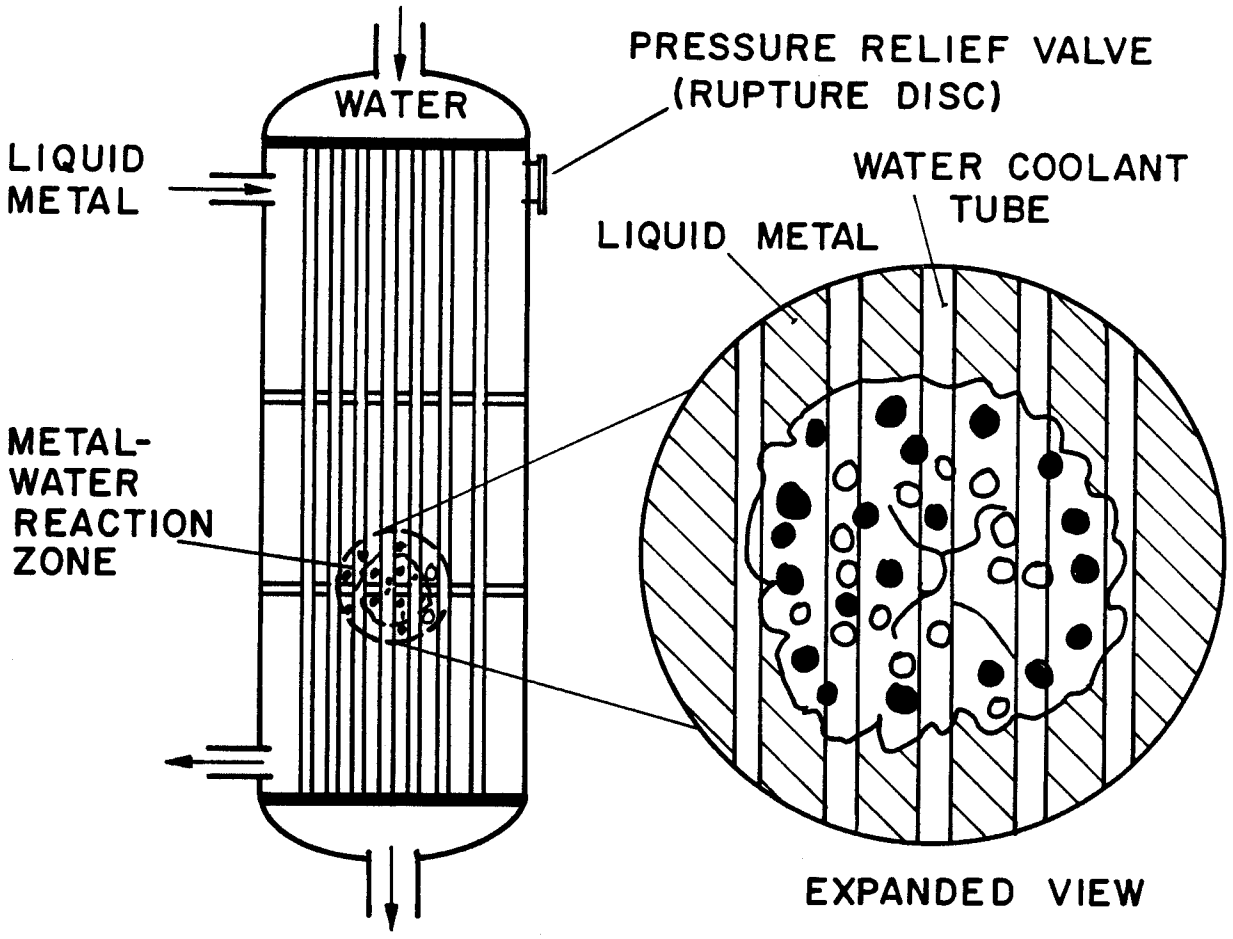
Our work in the modeling of lithium-lead/water interactions is based on a specific accident scenario in a conceptual fusion reactor design. We consider the effect of a steam tube rupture accident in a liquid-metal/water steam generator. The steam generator is nominally considered to be a Westinghouse design and acts as the main heat transfer unit in the primary loop of the reactor. The MARS[2] (Mirror Advanced Reactor Study) conceptual fusion reactor design utilized the lithium-lead alloy, $Li_{17}Pb_{83}$ (hereon designated as "lithium-lead") as the primary breeder and coolant. The model we have developed predicts the temperature and pressure history and the hydrogen generation rate due to an assumed guillotine break of a steam tube and the resulting liquid-metal/water chemical reaction (Fig. 1). The model is applied to both a lithium and lithium-lead coolant in order to obtain a general comparison between these two materials.

Large-Scale Experiments at HEDL

Recently a couple of large-scale lithium-lead/water and lithium/water experiments have been carried out at the Hanford Engineering Development Laboratory.[3-5] Examining the results of these tests, it was found that the chemical reaction, on which our model was based, was not valid for a liquid metal rich environment. We had based our model on the equation

$$Li + H_2O \rightarrow LiOH + \frac{1}{2} H_2 - 49 \text{ kcal/mole } (@ 25^0C) . \qquad (1)$$

STEAM GENERATOR TUBE RUPTURE



- HIGH PRESSURE TWO-PHASE BLOWDOWN

- LIQUID METAL ENTRAINED IN EXPANDING MIXING ZONE

Fig. 1

But the HEDL tests indicated that in the presence of excess lithium, the water and lithium would react as

$$2\ Li + H_2O \rightarrow Li_2O + H_2 - 75\ kcal/mole\ (@\ 25^0C)\ . \qquad (2)$$

Only when the reaction occurs in an excess of water is Eq. (1) considered valid. Since the accident being modeled consists of the injection of high pressure steam from a broken steam tube into a large volume of lithium-lead (the shell side of the steam generator), the reaction will take place in the presence of excess lithium, as long as the mixing is adequate enough to disperse the steam into the lithium-lead. This is considered to be quite similar to the HEDL AWR-1 test.

The HEDL experiments were steady state experiments. The experiments consisted of a steady state injection of steam flow into a large (~ 20 ℓ) bath of lithium or lithium-lead. The insulated test chamber was exhausted into a gas sampling system to determine the amount of hydrogen produced. In both the lithium and lithium-lead tests, all of the steam injected into the system reacted to form hydrogen. Also in both tests, temperature readings from thermocouples placed at the point of steam injection up to 20 cm away showed temperatures within 20°C of each other except for the thermocouple placed at the point of steam injection. The temperature indicated by the thermocouples at the point of steam injection was higher than the other measured temperatures by as much as 100°C. As stated in the report from the lithium test: "These pool temperatures indicated a localized high temperature zone near the point of steam discharge, but otherwise good pool mixing occurred throughout the test."

This well mixed situation seems to result in the reaction zone being liquid metal rich. Because in a steam tube rupture in the steam generator the geometry is quite similar to the AWR-1 test, we consider the reaction zone to be metal rich. Thus, Eq. (2) seems valid for the early phase of this accident.

Dynamic Parametric Model

The steam generator accident modeled is one in which there is a sudden and complete rupture of a steam tube ("guillotine break"), essentially leaving a two water flow path into the liquid metal. For our current calculations, our model contains these major assumptions:

1. We base our nominal calculations on the MARS design parameters. The initial pressure of the reactants is 17.0 MPa for the water and 0.17 MPa for the liquid-metal. Also, the initial shell side, liquid-metal volume and temperature are taken to be 55.5 m^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 at thermal equilibrium.
3. The flow rate of water into the reaction zone is calculated by the one-dimensional homogeneous equilibrium model (HEM) for critical flow, i.e.

$$S_{wo} = S_{wb} \tag{3}$$

$$V_{wb} = [2(i_{wo} - i_{wb})]^{1/2} \tag{4}$$

$$\dot{m}_w = A_b \rho_{wo} V_{wb} \tag{5}$$

where the enthalpy at the break, i_{wb}, is found knowing the upstream entropy, s_{wo} and pressure, p_{wo}.

4. The flow of the liquid-metal into the reaction zone is determined by a mixing parameter x. Thus x is defined as the ratio of the molar flow rate of water to twice the molar flow rate of lithium into the reaction zone. Thus when x = 1, water and lithium enter the reaction zone in stoichiometrically equal amounts.
5. The reactants, including hydrogen, remain in the reaction zone.
6. The system pressure is maintained below 17 MPa (the water backpressure) by a pressure relief valve. This is accomplished by allowing a portion of the unreacted liquid-metal to leave the nonreaction zone each timestep. The flow rate out through the valve is modeled by a quasisteady mechanical energy balance (Bernoulli's equation)

$$\dot{m}_{\ell m} = \rho_{\ell m} A_{prv} \left[\frac{2}{k\rho_{\ell m}} (P_{prv} - P_{\infty})\right]^{1/2} \tag{6}$$

where P_{prv} is the pressure at the pressure relief valve. K is the loss coefficient of the valve, and is a function of the length of pipe (L_{prv}) connected to the valve

$$K = \frac{4fL_{prv}}{D_{prv}} \tag{7}$$

where D_{prv} is the diameter of the pipe and f is the pipe friction factor, which for simplicity is taken to be equal to 0.005 for a commercial steel tube. If L_{prv} is chosen to equal 0, then the loss coefficient for flow through an orifice is

$$K = 2.69 \ . \tag{8}$$

7. We assume that the increase in pressure in the shell side of the steam generator suspends the normal flow of the liquid metal through the steam generator.
8. The thermodynamic and transport properties of the reactants and products are assumed to be simple functions of temperature. The gases are assumed to be perfect. For $x > 1$, any unreacted water is assumed to be superheated steam. This possibility is allowed although the AWR-1 test suggests it is not physically reasonable.
9. The liquid metal in the nonreaction zone is considered compressible.

This last assumption is a major improvement from the previous model. One of the implications of this change on the model is that pressure changes are propagated as waves traveling through the system at the speed of sound of the liquid metal. The other implication of this change on the model is that, at the end of each timestep, the change in volume of the nonreaction zone due to pressure compression is calculated and becomes part of the volume occupied by the gas in the reaction zone.

Because pressure changes are propagated through the system at the speed of sound of the liquid-metal, the pressure, as calculated at the break, is delayed in time before its presence is felt at the pressure relief valve. The

time delay (t_{delay}) is determined by

$$t_{delay} = S_{b\text{-}prv}/C_{\ell m} \tag{9}$$

where $S_{b\text{-}prv}$ is the distance from the break to the pressure relief valve, and $C_{\ell m}$ is the speed of sound of the breeder. We assume that the break occurs in the center of the steam generator, therefore $S_{b\text{-}prv}$ is given in one-dimensional geometry by

$$S_{b\text{-}prv} = (r_{SG}^2 + (L_{sg}/2)^2)^{1/2} \ . \tag{10}$$

Since the pressure relief due to flow out of the pressure relief valve must travel back to the break before its presence is felt by the gas in the reaction zone, a sharp pressure increase at the break is felt for $2*t_{delay}$ seconds before pressure relief is sensed at the break.

The change in volume due to the pressure compression (ΔV_{NR}) is determined by the definition of the bulk modulus (B)

$$B = \frac{dP}{dV} /V_{NR} = \Delta PV_{NR}/\Delta V_{NR} \tag{11}$$

where ΔP is the difference between the system pressure and the reference pressure (0.17 MPa). Because the bulk modulus is a function of the liquid-metal density and sound speed, the change in volume due to pressure compression is given by

$$\Delta V_{NR} = \Delta PV_{NR}/(\rho_{\ell m} C_{\ell m}^2) \ . \tag{12}$$

In our model, ΔV_{NR} is calculated utilizing the following assumptions. We assume that the reaction zone is small enough to neglect the effect of compression of the liquids in the reaction zone. We also assume that the temperature of the nonreaction zone varies so little that thermal expansion can be neglected. At each timestep, ΔV_{NR} is determined by a one-dimensional calculation. ΔV_{NR} is the sum of individual volume changes each of which is a function of the separate calculated pressure points as they propagate through the system.

We employ two control volumes and a specified mixing parameter in order to keep the modeling of the dynamic process relatively simple and unambiguous. Consistent with this approach is the use of a 1-D HEM critical flow model for water inflow and Bernoulli's equation for liquid-metal outflow. Because the pressure transient within the shell side of the steam generator is expected to be large, the assumption of the suspension of normal flow of liquid metal through the steam generator is reasonable. Because the transient caused by the tube rupture occurs over such short times ($\sim$ 1 s), the retention of H_2 in the reaction zone is reasonable. Also, because the experiments at HEDL were based on a volume of liquid-metal which equaled 0.02 m^3, and because the volume of liquid-metal in our model equals 55.5 m^3, it is safe to assume that there is sufficient lithium in the system for the system to be considered lithium rich throughout the calculation (i.e., $x < 1$).

One should notice that this last assumption may not be consistent with the two zone model of the shell side of the steam generator. According to the two zone model, later in the accident sequence, the reaction zone would be rich in reaction products, namely Li_2O. One may then expect the

$$Li_2O + H_2O \rightarrow 2\ LiOH \tag{12}$$

reaction to occur if $x > 1$. But one should realize that the two zone model is simply a calculational device to model the energy transfer from a region near the break to a region far from the break. The assumption that the mixing is sufficient to limit the chemical reaction to

$$2\ Li + H_2O \rightarrow Li_2O + H_2 \tag{13}$$

is based on experimental observations. The model can follow this empirical observation for a user input of $x \leq 1$.

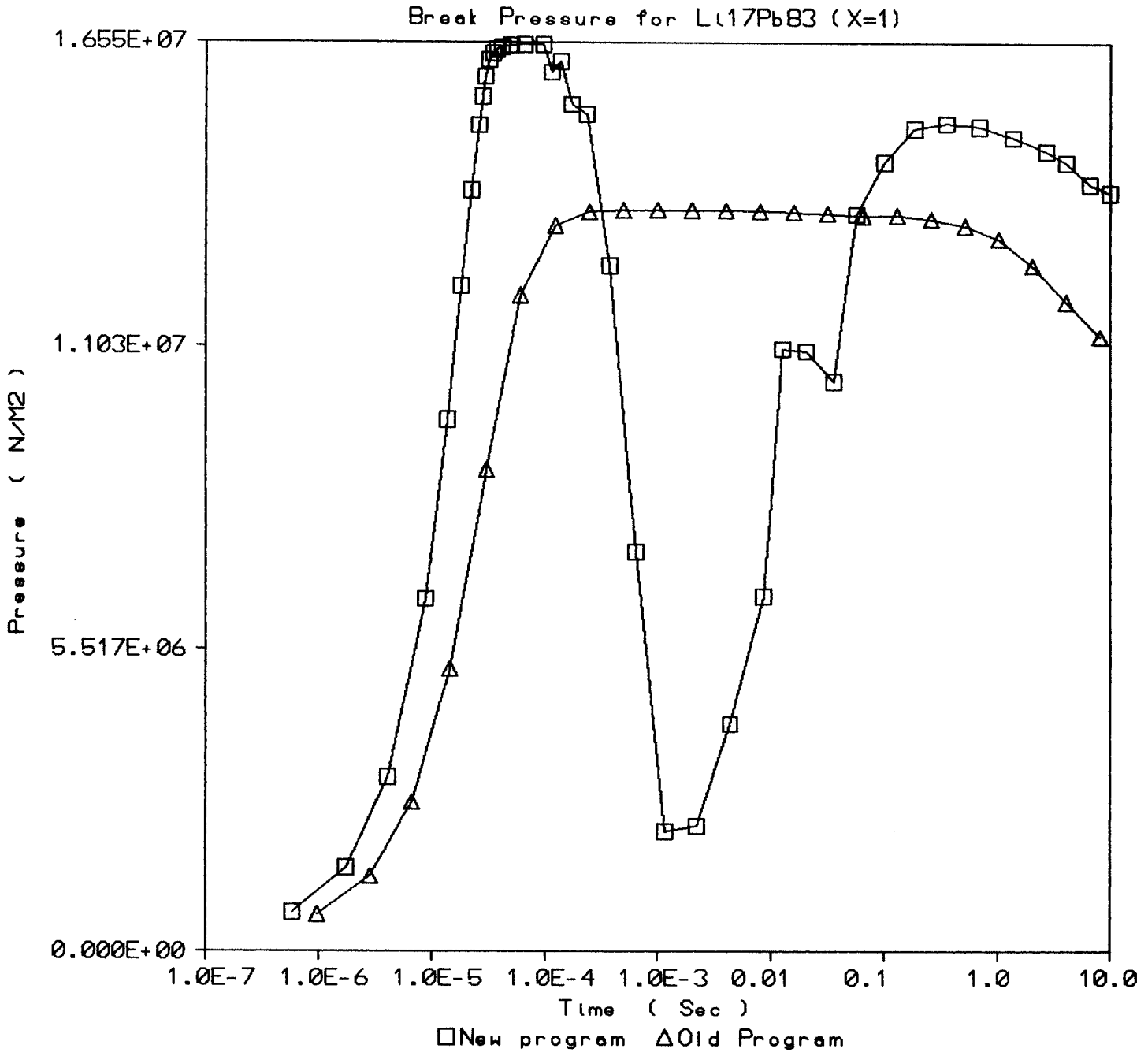
Based on the aforementioned assumptions, we solve mass and energy balances on the two zones to determine shell side pressure, reaction and nonreaction zone temperature, and the mass of hydrogen generated, all as functions of time from the initiation of the accident. The new program uses the mixing parameter, x, the relief valve area, A_{prv}, the relief valve pipe length, L_{prv}, and the distance from the break to the relief valve, S_{b-prv}, as the main variables. The new program varies from the old in two areas. The first difference is the result of basing the program on the Li_2O reaction instead of the LiOH reaction (Eq. (1) is used in place of Eq. (2)). The second difference is the result of allowing the liquid-metal in the nonreaction zone to be compressible.

Before we can compare the results of the new model to the old model, we must point out that the figures used in our previous paper[1] are in error. Our old program contained an error in the mass balance subroutine, which resulted in a calculated amount of hydrogen that was larger than it should have

been. For a given value of the pressure relief valve area, A_{prv}, and the mixing parameter, x, the error in this mass balance subroutine caused the system pressure to be overestimated and the reaction zone temperature to be underestimated, when compared to the corrected program. Although the calculations shown in the previous paper are in error, for a given value of x and A_{prv}, the system pressure and the reaction zone temperature are in error by less than 20%, when compared to the corrected program variables. Thus the conclusions drawn in the previous paper, that the maximum temperature for lithium-lead during the accident is not a safety concern for the steam generator, and that the pressure characteristics govern the integral response, are still valid for the corrected program.

We are now ready to discuss the results of the new model. In Fig. 2, we have graphed the pressure at the steam tube break as a function of time, for both the old and new models. Both plots are functions of the same input variables, the liquid-metal breeder is lithium-lead, the area of the pressure relief value equals 0.005 m^2, and the mixing parameter equals 1. The old model pressure trace is calculated with the corrected mass balance subroutine. The old model is based on the assumption that the liquid metal is incompressible. Therefore, the pressure at the break is also the pressure throughout the system. This means that pressure relief occurs immediately, and results in the system pressure quickly reaching a maximum and leveling off. Since the new model is based on liquid metal being compressible, the dynamics of pressure wave propagation through the system are important during the early portion of the accident sequence. The new model calculation represented in Fig. 2 is based on the distance between the break and the pressure relief valve being 10 m. Since the speed of sound of lithium-lead is 1850 m/s, the pres-

Fig. 2

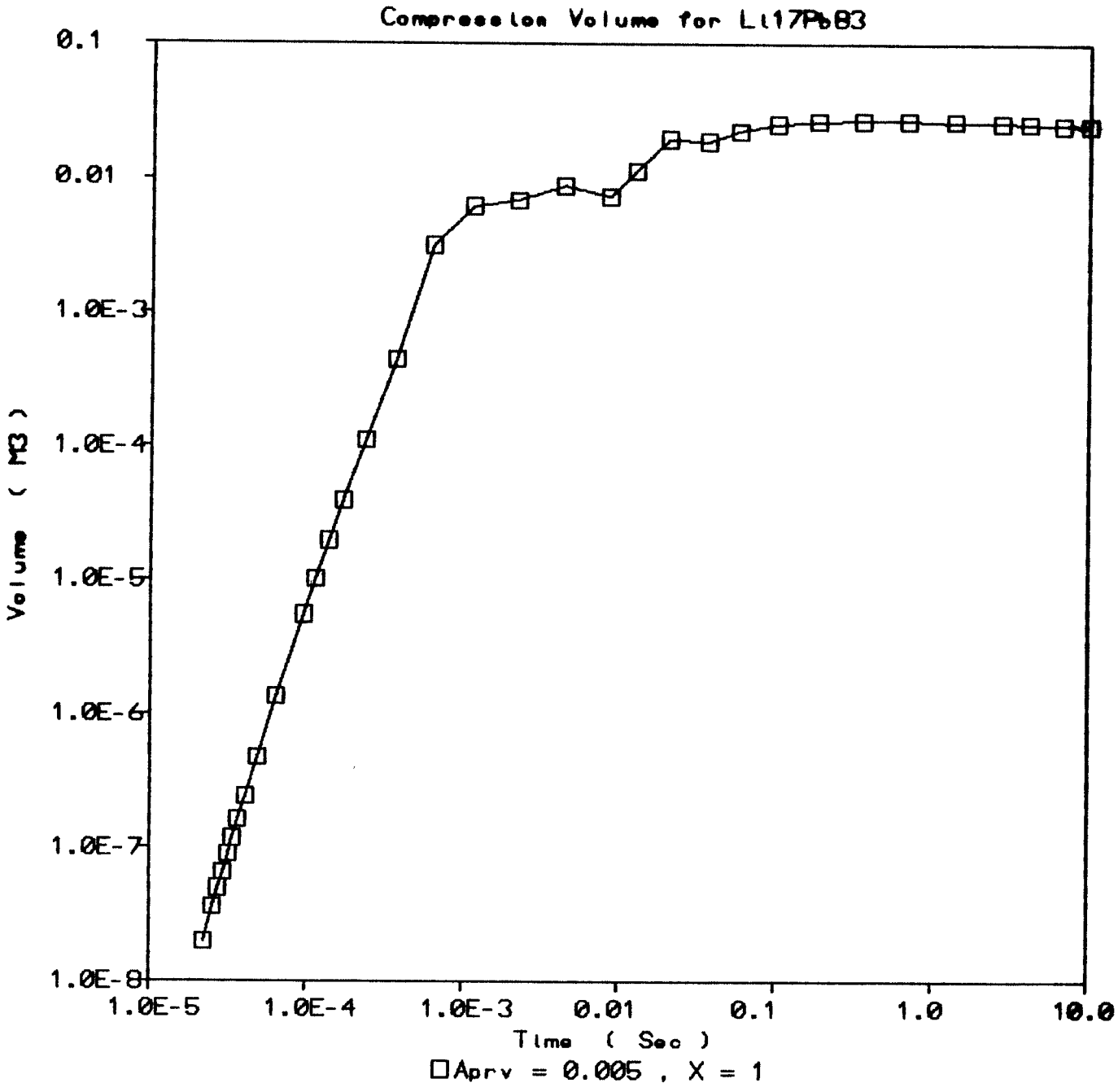

Break Pressure for Li17Pb83 (X=1)
1.655E+07
1.103E+07
5.517E+06
0.000E+00
Pressure (N/M2)
1.0E-7
1.0E-6
1.0E-5
1.0E-4
1.0E-3
0.01
0.1
1.0
10.0
Time (Sec)
□New program △Old Program

sure wave takes roughly 5 ms to travel from the break to the outer region of the system. By keeping this fact in mind and by examining Fig. 3, it becomes possible to explain the oscillatory behavior of the break pressure during the first 10 ms of the accident sequence. In Fig. 3, we have plotted the volume change due to pressure compression for the same input variables. After initiation of the accident, the hydrogen generated by the chemical reaction causes a rapid increase in the system pressure at the break. This high pressure pulse propagates through the system at the speed of sound of the liquid metal, and compresses the liquid metal as the pressure wave travels through it. The change in volume due to the pressure compression is assumed to be occupied by the reaction zone hydrogen. From the ideal gas law,

$$P \propto V_{gas}^{-1} \; ; \tag{14}$$

therefore, as the compression volume increases, the break pressure decreases. Thus the behavior of the break pressure is explained by the following sequence of events. During the first 100 μs after the initiation of the accident, a high pressure wave is generated at the break due to hydrogen generation. From 100 μs to 5 ms after the initiation of the accident, the high pressure wave travels from near the break to the outer regions of the system. This causes the compression volume to increase by 4 orders of magnitude, during the same period. This, in turn, causes the break pressure to decrease, which causes a larger flow rate of water into the system and thus a more extensive reaction. Therefore the break pressure increases once again. By 10 ms into the accident, the effect of flow through the pressure relief valve is felt at the break. A balance between the flow of water into the system and the flow of

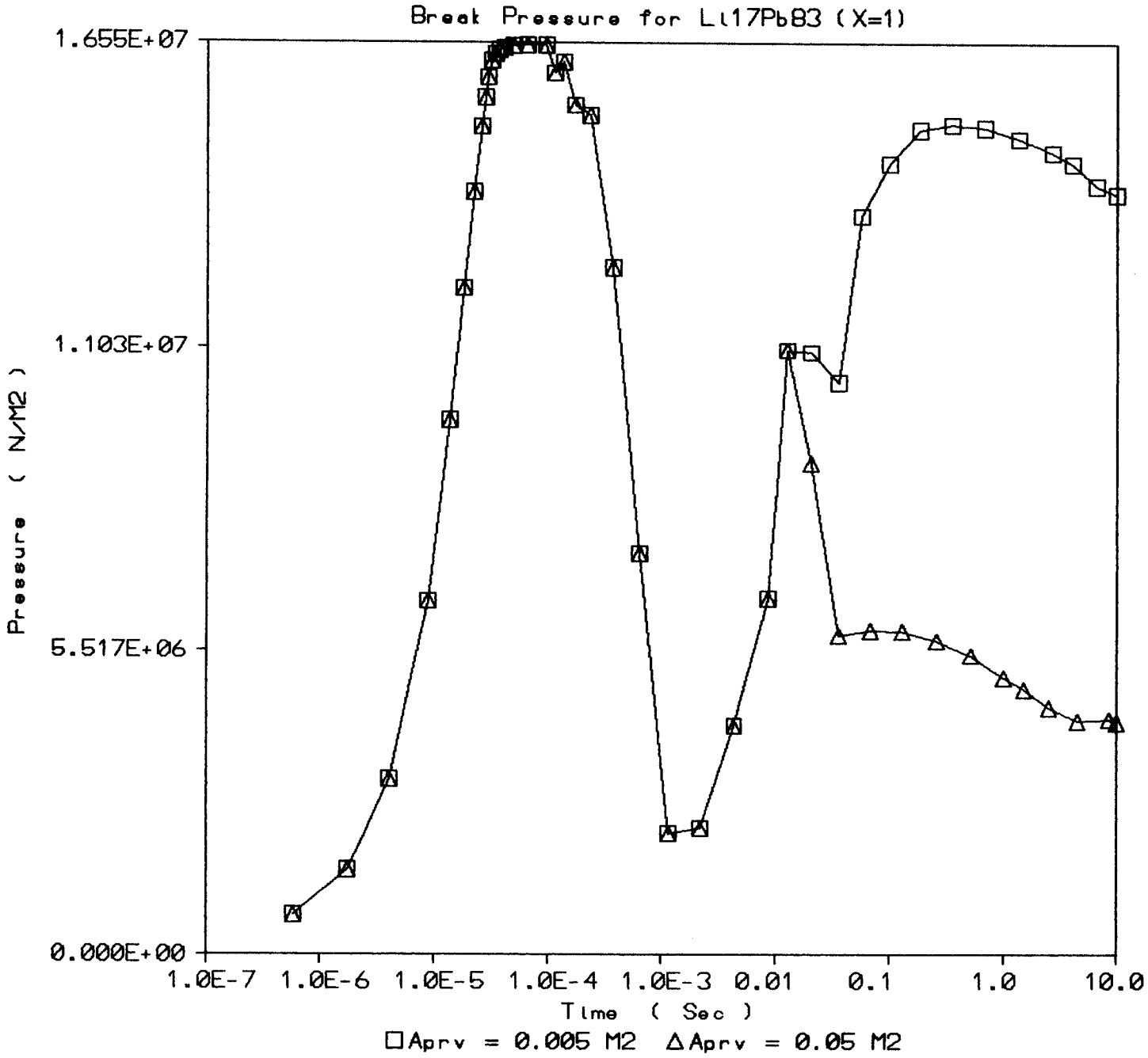
Fig. 3


Compression Volume for Li17Pb83
0.1
0.01
1.0E-3
1.0E-4
1.0E-5
1.0E-6
1.0E-7
1.0E-8
Volume (M3)
1.0E-5
1.0E-4
1.0E-3
0.01
0.1
1.0
10.0
Time (Sec)
□Aprv = 0.005 , X = 1

unreacted liquid metal out of the system through the pressure relief valve, is then quickly established. Once the balance is established, the compressible effects are suppressed and the break pressure for the new model mimics the break pressure for the old model.

The effect of liquid metal compressibility is further illustrated by Fig. 4. In this figure, we have plotted the new model break pressure for two values of the pressure relief valve area. Up to 10 ms after the initiation of the accident, the break pressure response is identical for both values of A_{prv}. This should be expected since it takes roughly 10 ms for the effect of flow through the pressure relief valve to be felt at the break. After about 10 ms, a balance between water inflow and liquid metal outflow is quickly established, and the liquid metal compressibility becomes of negligible importance. Therefore, before the effect of pressure relief is felt at the break, the break pressure is only a function of the mixing parameter, which determines the extent of the reaction; and of the break to pressure relief valve distance, which determines the length of time that compressible effects are significant. The initial pressure wave at the relief valve is actually quite small due to pressure decay as $1/r^2$ from the break location. These facts are demonstrated in Fig. 5. In this figure, we have graphed the new model break pressure for $A_{prv} = 0.005$ m^2, and two differing values of the break to pressure relief valve distance. Here we assume that the shape of the steam generator does not change as S_{b-prv} changes, i.e. the ratio of the steam generator height to radius remains constant. For $S_{b-prv} = 5$ m, the compressible effects are minimal, and break pressure response approaches the incompressible liquid metal limit. For $S_{b-prb} = 25$ m, the compressible effects have a greater impact. In this case, it takes 27 ms for a pressure pulse to travel from the

Fig. 4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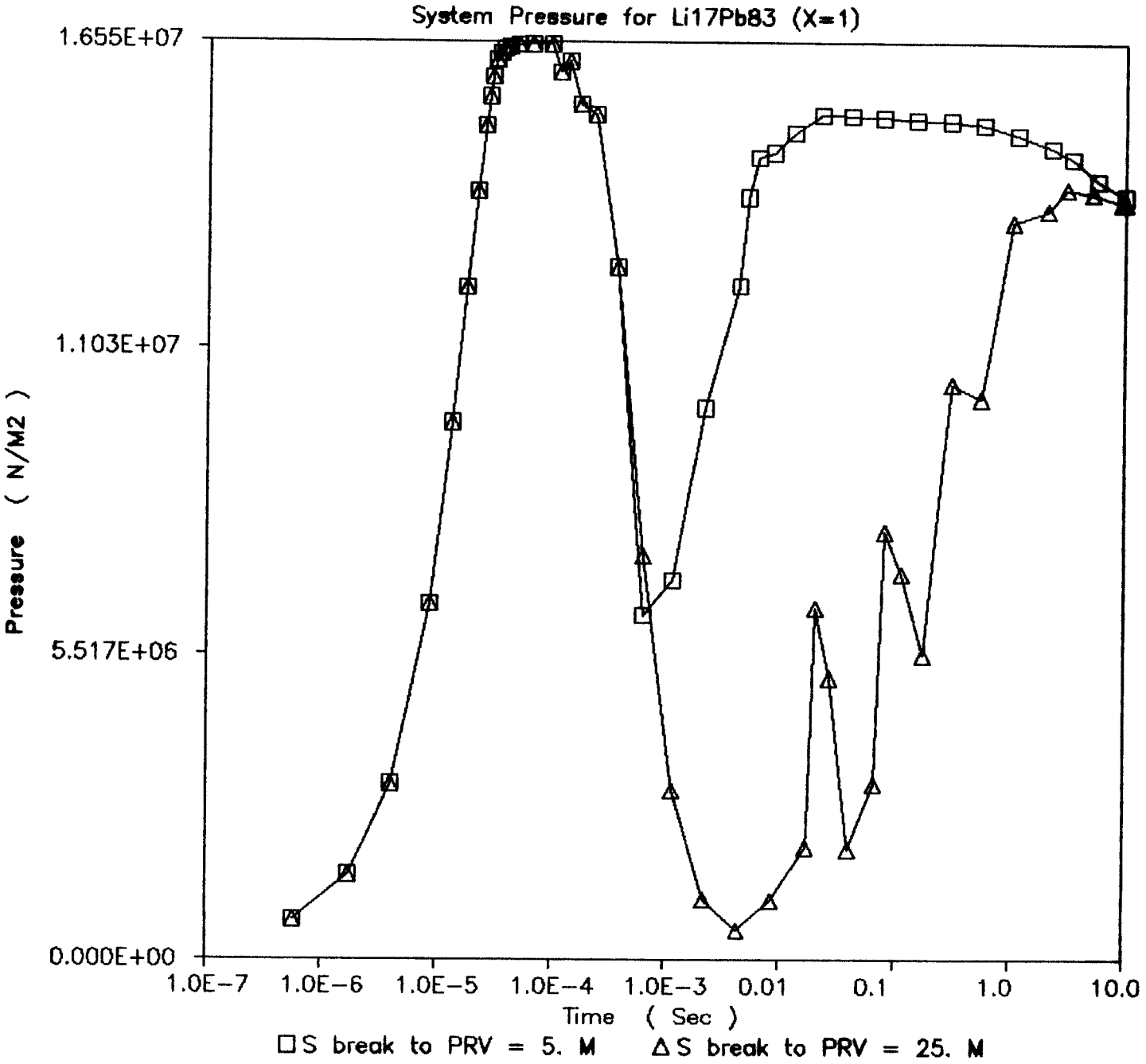
Pressure (N/M2)
1.0E-7
1.0E-6
1.0E-5
1.0E-4
1.0E-3
0.01
0.1
1.0
10.0
Time (Sec)
□Aprv = 0.005 M2 △Aprv = 0.05 M2

Fig. 5


System Pressure for Li17Pb83 (X=1)
1.655E+07
1.103E+07
5.517E+06
0.000E+00
Pressure (N/M2)
1.0E-7
1.0E-6
1.0E-5
1.0E-4
1.0E-3
0.01
0.1
1.0
10.0
Time (Sec)
□S break to PRV = 5. M
ΔS break to PRV = 25. M

break to the pressure relief valve and for the subsequent pressure relief to be felt back at the break. Therefore the balance between water inflow and liquid metal outflow will take place on a timescale greater than 27 ms. This is the the reason for the oscillating behavior displayed by the pressure trace from 20 ms to 1 s.

Despite the fact that the changes made to the model have a considerable effect on the early pressure response of the system, the effect on the temperature response of the system is minimal. This is exhibited in Fig. 6, where we have plotted the temperature of the reaction zone for the two models, under the same initial conditions as used in the first two figures. This figure shows that, after the compressible effects diminish, the new model reaction zone temperature converges to the incompressible flow model reaction zone temperature.

The only quantity that is significantly changed by the new model is the mass of hydrogen generated, which is presented in Fig. 7. As shown in this figure, the mass of hydrogen generated is elevated by roughly a factor of two over the old model. This increase in hydrogen generation is the reason why the two pressure traces shown in Fig. 2 do not converge to the same value. The reason that hydrogen generation is increased by a factor of two is due to the different chemical reaction. Comparing Eq. (1) to Eq. (2), one will notice that twice the amount of hydrogen is generated by the new model reaction (Eq. 2) as is generated by the old model reaction (Eq. 1), for equal amounts of water injected. Since the flow rate of water into the system is determined by the break pressure, the differing break pressure response for the two models (Fig. 1) is the reason why the mass of hydrogen generated by the new model is not exactly twice the mass of hydrogen generated by the old model.

Fig. 6

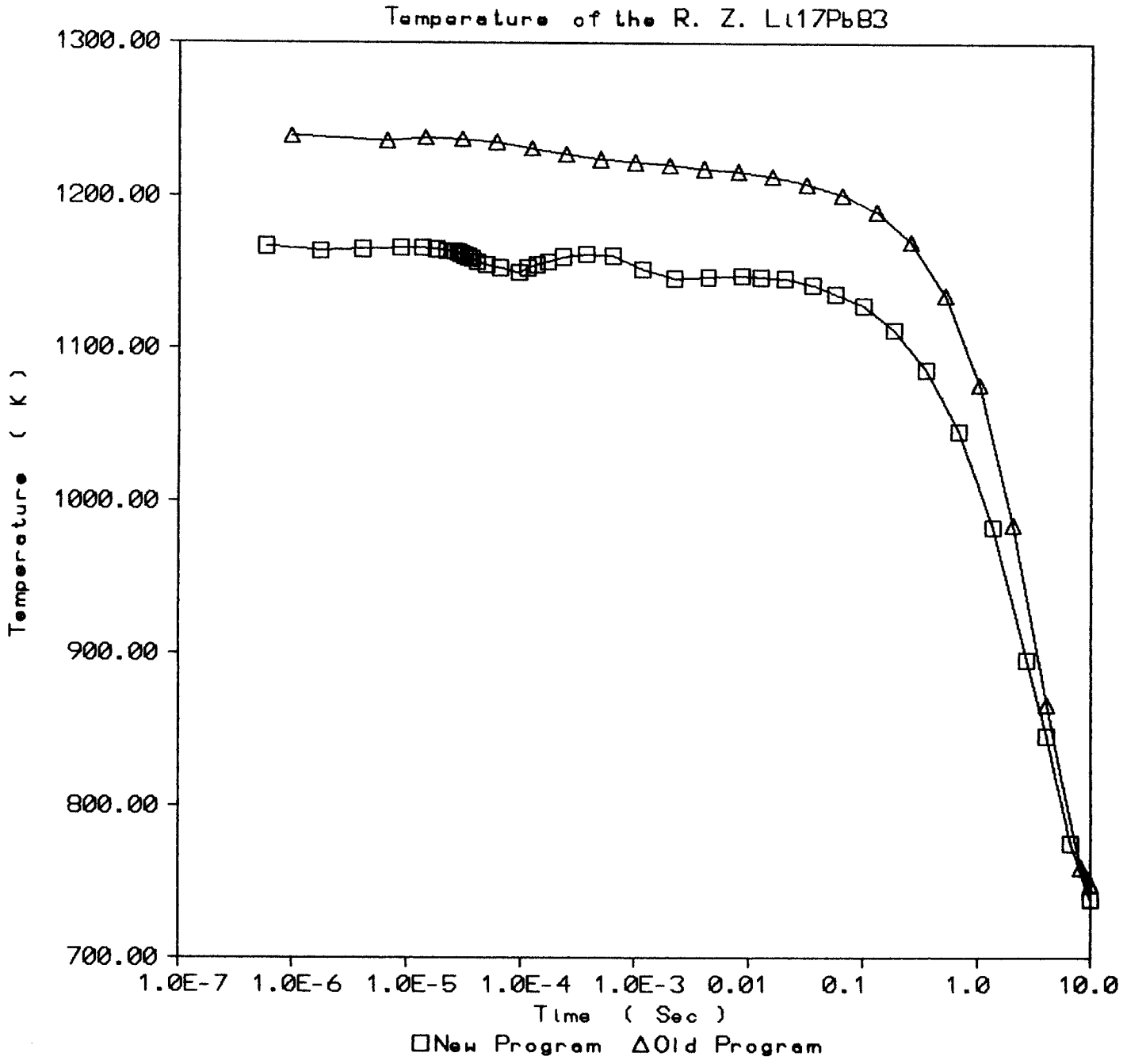
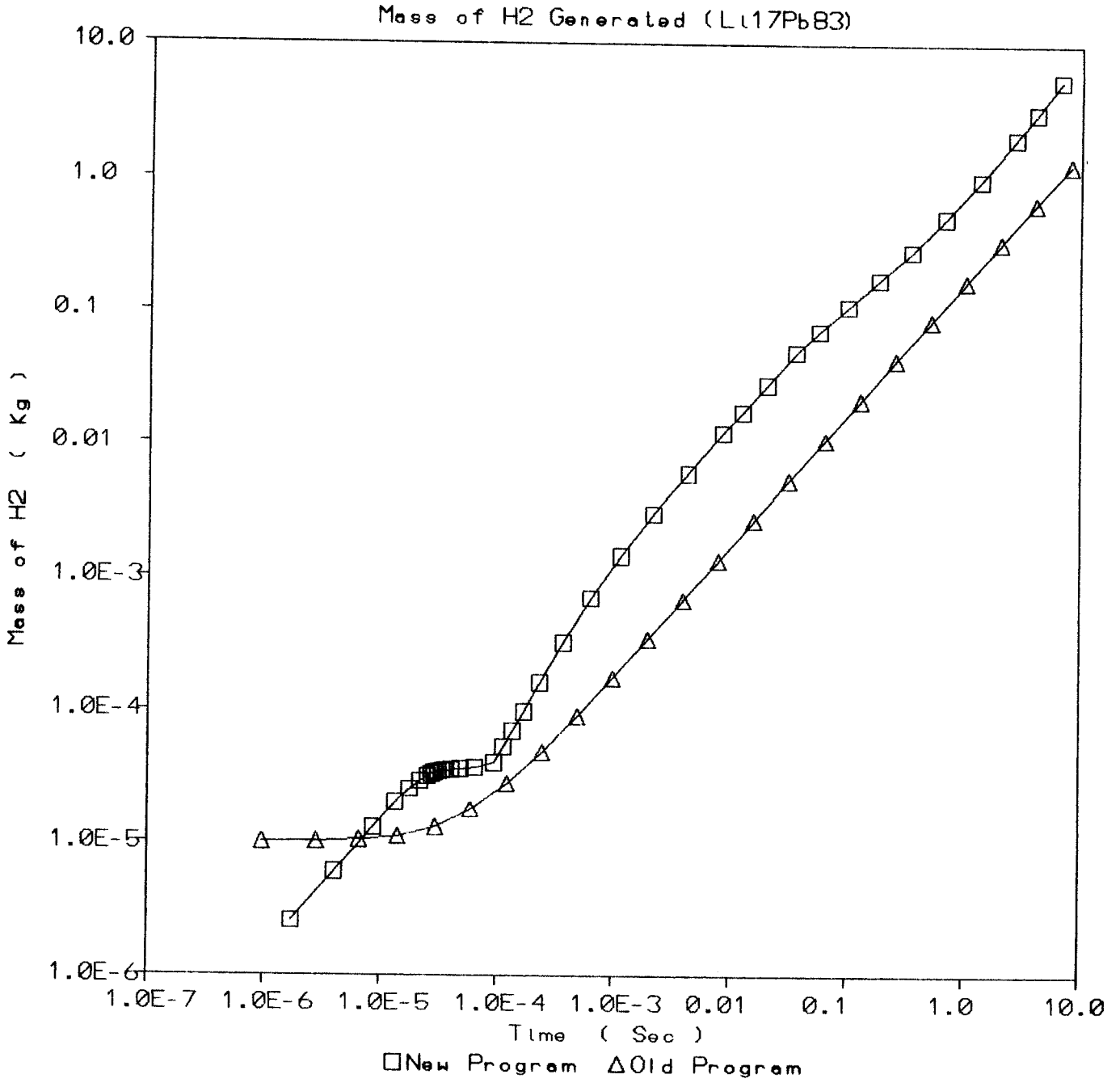

Temperature of the R. Z. Li17Pb83
1300.00
1200.00
1100.00
1000.00
900.00
800.00
700.00
Temperature (K)
1.0E-7
1.0E-6
1.0E-5
1.0E-4
1.0E-3
0.01
0.1
1.0
10.0
Time (Sec)
□New Program △Old Program

Fig. 7


Mass of H2 Generated (Li17Pb83)
10.0
1.0
0.1
0.01
1.0E-3
1.0E-4
1.0E-5
1.0E-6
Mass of H2 (Kg)
1.0E-7 1.0E-6 1.0E-5 1.0E-4 1.0E-3 0.01 0.1 1.0 10.0
Time (Sec)
□New Program △Old Program

Conclusions

Two major changes were made to our dynamic parametric model for liquid-metal/water reactions in a steam generator. The effect of allowing the liquid-metal to be a compressible fluid causes the system pressure to oscillate during the first few milliseconds after the initiation of the accident. The large pressure wave generated should be considered in the integrity of the steam generator tubes. After a balance has been established between the flow of water into the system through the broken steam tube and the flow of unreacted liquid-metal from the system through the pressure relief valve, the effect of liquid metal compressibility on the system becomes negligible.

The effect of altering the base chemical reaction to the Li_2O reaction instead of the LiOH reaction, is to roughly double the amount of hydrogen produced by the new model as opposed to the old model. Therefore the production of hydrogen by a ruptured steam tube accident in a lithium based liquid-metal steam generator is greater than originally estimated. For this contact mode of coolant injection into a large pool of liquid-metal this chemical reaction is considered reasonable based on the observation of the HEDL experiments. The parametric model should be used in this case with the mixing parameter, $x \leq 1$.

Finally, the conclusions from the original study concerning the temperature response using the parametric model are relatively unchanged. At early times the peak reaction zone temperature of the lithium-lead is significantly lower than that of a lithium pool. As time progresses ($t > 10$ s) the reaction zone temperature decreases during the mixing with the surrounding liquid-metal pool.

Nomenclature

A_b	the area of the steam tube break
A_{prv}	the area of the pressure relief valve and a variable in the model
B	the bulk modulus of the liquid-metal
$C_{\ell m}$	the speed of sound of the liquid-metal
D_{prv}	the diameter of the pressure relief valve pipe
f	a friction factor for the pressure relief valve pipe
i_{wb}	the enthalpy of the water/steam flowing through the steam tube break
i_{wo}	the initial enthalpy of the water/steam flowing through the steam tube break
k	the loss coefficient of the pressure relief valve
L_{prv}	the pressure relief valve pipe length
L_{sg}	the length of the steam generator
$\dot{m}_{\ell m}$	the molar flow rate of the liquid metal through the pressure relief valve
$\dot{m}_w$	the molar flow rate of water into the reaction zone
P_{prv}	the system pressure at the pressure relief valve
P_∞	the pressure relief valve backpressure
r_{sg}	the radius of the steam generator
S_{b-prv}	the distance from the break to the pressure relief valve
S_{wb}	the entropy of the water at the tube break
S_{wo}	the initial entropy of the water
t_{delay}	the length of time it takes a pressure wave to travel from the break to the pressure relief valve
V_{NR}	the volume of the nonreaction zone
V_{wb}	the velocity of the water flowing through the tube break
x	the mixing parameter; it equals the ratio of the molar flow rate of H_2O to twice the molar flow rate of Li into the reaction zone

ΔP the difference between the system pressure and the initial pressure

ΔV_{NR} the change in the nonreaction zone volume due to the pressure compression

$\rho_{\ell m}$ the density of the liquid metal

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

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5. Ibid., (Nov.-Dec. 1984).