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MODELING OF LITHIUM AND LITHIUM-LEAD
REACTIONS IN AIR USING LITFIRE

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LITHIUM AND LITHIUM-LEAD MODELING IN
MULTI-COMPARTMENT SYSTEMS

by

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ABSTRACT

LITFIRE is a computer code that simulates the combustion of lithium in various containment schemes. The accuracy of LITFIRE in predicting thermal and pressure responses of containment atmosphere and structures has been tested against small scale (100 kg. Li) spills performed at the Hanford Engineering Development Laboratory. The agreement between experiment and LITFIRE prediction was within 10%

Modifications to the code have been made to increase its utility in modeling fires in fusion reactor containments. The ability to monitor lithium-lead alloy reactions in air has been incorporated into LITFIRE. Also, the geometry has been made more flexible and the available options made compatible with one another. Preliminary comparisons indicate that lithium-lead alloys are less reactive than pure lithium and generate maximum cell gas temperatures that are nearly a factor of two lower than those resulting from pure lithium fires, for the same volume of liquid metal spilled.

Application of LITFIRE to fires in a prototypical fusion reactor was made. The predictions of LITFIRE indicate that fires limited to the torus of a tokamak fusion reactor would be much less severe than fires resulting from spills directly onto the containment building floor. However, the primary wall and surrounding structures would become hotter in spills inside the torus because they are directly exposed to radiative heating by the fire.

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2. R. W. Sawdye, J. A. Sefcik, M. S. Kazimi, "Reliability Requirements for Admissible Radiological Hazards from Fusion Reactors," Trans. Am. Nucl. Soc. 27, 65-66, November 1977.
3. D. A. Dube, M. S. Kazimi and L. M. Lidsky, "Thermal Response of Fusion Reactor Containment to Lithium Fire," 3rd Top. Meeting in Fusion Reactor Technology, May 1978.
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TABLE OF CONTENTS

ABSTRACT	1
ACKNOWLEDGEMENTS	4
TABLE OF CONTENTS	5
LIST OF FIGURES	7
LIST OF TABLES	9
Chapter 1 Introduction	10
1.1 Background on Lithium Fire Modeling	10
1.2 LITFIRE History and Development	13
1.3 LITFIRE Model Description	14
1.4 Scope of Present Work	20
Chapter 2 Development and Application of Single-Cell LITFIRE	21
2.1 Recent Changes to LITFIRE Model	21
2.2 Application of LITFIRE to Experiment	24
2.2.1 Description of HEDL Experiment	24
2.2.2 LITFIRE Geometry Used to Model Experiment	27
2.2.3 Comparison of LITFIRE to Experiment	27
2.3 Sensitivity of LITFIRE to New Modeling	37
2.3.1 Sensitivity to Aerosol Removal from Cell Gas	37
2.3.2 Sensitivity to Combustion Zone Transmissivity	40
2.4 Analysis of a Lithium Spill in UWMAK-III	46
2.4.1 Description of UWMAK and LITFIRE Geometries	46
2.4.2 Prediction of Lithium Fire Consequences	46
2.4.3 Comparison of Present Calculation to Previous Predictions	52
Chapter 3 Development and Application of Two-Cell LITFIRE	55
3.1 Motivation for Two-Cell Version of LITFIRE	55
3.2 Model Description	57
3.2.1 Two-Cell Geometry	57
3.2.2 Explanation of Two-Cell Gas Exchange	58
3.2.3 Coding Changes Required for Two-Cell Calculation	61
3.3 Comparison of One and Two Cell Results for HEDL Experiment	62

3.4	Effect of Crack Size on Lithium Fires in Two-Cell Geometry	62
3.5	Application of LITFIRE to a Lithium Spill in a Vacuum Torus	71
Chapter 4	Lithium-Lead Combustion in Air	74
4.1	Lithium-Lead use in Fusion Related Systems	74
4.2	Properties of Lithium-Lead	74
4.2.1	Physical Properties	74
4.2.2	Thermodynamic and Chemical Properties	76
4.3	Models of Lithium-Lead Air Reactions	79
4.3.1	Turbulent Pool Model	79
4.3.2	Layered Pool Model	84
4.4	Major Changes to LITFIRE Encompassing LiPb Combustion in Air . . .	86
4.5	LITFIRE Results	87
4.5.1	Comparison of Turbulent Pool with Layered Pool Combustion . . .	88
4.5.2	Comparison of LiPb with Pure Lithium Combustion	88
Chapter 5	Summary and Conclusions	97
5.1	Code Development and Verification	97
5.2	LITFIRE Applications	97
5.3	Lithium-Lead Combustion	98
5.4	Recommendations for Further Development	98
References	101
Appendices	103
Appendix A	LITFIRE Data: HEDL Experiments	103
Appendix B	LITFIRE Data: Two-Cell Calculations	110
Appendix C	LITFIRE Data: LiPb Combustion	114
Appendix D	Listing of LITFIRE	118
Appendix E	Sample Input/Output for LITFIRE	154
Appendix F	Glossary for LITFIRE	160

LIST OF FIGURES

Figure 1.1	Energy Flow in One-Cell LITFIRE	16
Figure 1.2	Energy Flow in Two-Cell LITFIRE	17
Figure 1.3	Mass Flow in LITFIRE	19
Figure 2.1	Diagram of Changes to LITFIRE	22
Figure 2.2	HEDL Experimental Test Facility	25
Figure 2.3	LITFIRE Geometry for HEDL Comparison	28
Figure 2.4a	LITFIRE/HEDL Comparison: Wall Temperature	29
Figure 2.4b	LITFIRE/HEDL Comparison: Cell Gas Pressure	30
Figure 2.4c	LITFIRE/HEDL Comparison: Pool Temperature	31
Figure 2.4d	LITFIRE/HEDL Comparison: Cell Gas Temperature	32
Figure 2.5	Combustion Zone-Pool Coupling	39
Figure 2.6	Sensitivity of Gas Temperature to Aerosol Removal	41
Figure 2.7	Sensitivity of Gas Emissivity to Aerosol Removal	42
Figure 2.8	Pool Temperature Sensitivity to EMCZ	44
Figure 2.9	Cell Gas Sensitivity to EMCZ	45
Figure 2.10	Maximum Pool-Combustion Zone Temperature Differences	47
Figure 2.11	LA-2 Pool Temperature and LITFIRE Predictions	48
Figure 2.12	LA-2 Cell Gas Temperature and LITFIRE Predictions	49
Figure 2.13	UWMAK-III Containment	50
Figure 2.14	LITFIRE Prediction for Fire in UWMAK-III	51
Figure 2.15	Comparison of Old and New LITFIRE Predictions	53
Figure 2.16	UWMAK-III Cell Gas Pressurization History	54
Figure 3.1	LITFIRE Two-Cell Geometry	56
Figure 3.2	Cell Gas Energy Balance and Flow Rate Diagram	60
Figure 3.3	One and Two Cell Predictions for LA-4 Steel Wall Liner	63
Figure 3.4	Pressurization History in Uwmak-III Two Cell Geometry	65
Figure 3.5	Temperature History in Uwmak-III Two Cell Geometry	66
Figure 3.6	Component Temperatures in Uwmak-III Two Cell GEometry	67
Figure 3.7	Cell Pressurization vs. Crack Size	68
Figure 3.8	Cell Gas Temperature vs. Crack Size	69

Figure 3.9	Maximum Secondary Cell Temperatures vs. Crack Size	70
Figure 3.10	UWMAK-III Torus Pressurization History	72
Figure 3.11	UWMAK-III Component Temperatures	73
Figure 4.1	Density of LiPb	75
Figure 4.2	Phase Diagram of LiPb	75
Figure 4.3	Activity of LiPb	77
Figure 4.4	Heat of Dissociation of Li from LiPb	78
Figure 4.5	Turbulent Pool: Heat Flow	80
Figure 4.6	Turbulent Pool: Mass Flow	81
Figure 4.7	Layered Pool: Heat Flow	82
Figure 4.8	Layered Pool: Mass Flow	83
Figure 4.9	Layered and Turbulent Pool Comparison: Cell Temperatures	90
Figure 4.10	Layered and Turbulent Pool Comparison: Pool Temperatures	91
Figure 4.11	Effect of Lead on Combustion Rate	92
Figure 4.12	Small Scale LiPb Spill Using HEDL Geometry	93
Figure 4.13	Alternate Breeder Consequences: Turbulent Pool Results	94
Figure 4.14	Alternate Breeder Consequences: Layered Pool Results	95
Figure 4.15	Cell Gas Temperature Profiles for Various Alloys	96

LIST OF TABLES

Table 1.1	Comparison of Alternate Coolants and Breeders	11
Table 1.2	Lithium Reactions of Interest	12
Table 1.3	LITFIRE Version and Available Options	15
Table 2.1	Summary of HEDL Test Conditions	26
Table 2.2	Experimental Gas Composition During LA-5	34
Table 2.3	Comparison with LITFIRE and Experimental Combustion Rates	35
Table 2.4	Estimation of LA-4 "Combustion Zone" Temperature	38
Table 3.1	Combustion Characteristics of Various Crack Sizes	64
Table 4.1	Summary of Lithium-Lead Calculations	89

1. INTRODUCTION

1.1. Background on Lithium Fire Modeling

The study of lithium fires is primarily due to lithium's presence in proposed fusion reactors as a tritium breeder and/or coolant. A major safety concern of using lithium is the potentially large amount of energy that could be released into the containment from lithium-air or lithium-water chemical reactions. This energy may be sufficient to cause melting and/or volatilization of structural materials as well as substantial pressurization of the containment building. Aside from the structural damage itself, another safety concern is volatilization of radioactive structural materials, such as the first wall of a tokamak torus. The high temperatures, coupled with possible pressurization of the containment, may lead to failure of the containment integrity. Therefore, lithium fires are a possible mechanism for release of radioactive particles outside the containment [1]. In addition, the reaction products of lithium air or water interactions (LiOH , Li_3N , Li_2O) are themselves corrosive and can also damage the reactor's structural materials.

As a result of these safety concerns with pure lithium, other lithium based alloys have been proposed as coolants and/or breeders. Among these are several lithium-lead alloys (Li_7Pb_2 , $\text{Li}_{17}\text{Pb}_{83}$, LiPb_4), as well as LiAl and Li_2O . Limited preliminary studies indicate that these alloys are less reactive and may be safer to use than pure lithium [2]. A comparison of alternate coolants and breeders appears in Table 1.1. For an extensive analysis of the relative hazards associated with many of the proposed breeder/coolant combinations see the discussion in chapter five of Piet, et al., [3]. Table 1.2 lists the important chemical reactions with lithium or LiPb compounds.

Several experiments of lithium combustion in various atmospheres have been performed to determine the consequences of such reactions as well as to formulate an engineering database for the combustion of lithium. These experiments are on a small scale (1 to 100 kg.-Li burned) when compared to a fusion reactor inventory of approximately 400,000 kg.-Li (for UWMAC-III) [4]. The results of these experiments were used to calibrate many of the empirical relations found in LITFIRE, the computer code that is the basis for the present work.

Since the lead component of LiPb is effectively inert, these compounds are expected to react with the same materials as pure lithium. Experiments using LiPb as reactant have been limited to small tests (0.05 kg.- LiPb) in water and one test in air using a blow torch as the heat source [5]. Other experiments involving LiPb combustion in an air atmosphere are in progress but data from these will not be available in time for use in the present work [6].

The properties of lithium and lithium-lead compounds are not completely known over the temperature range of interest. For LiPb the data is minimal and is summarized in section 4.2 of

TABLE 1.1

Comparison of Alternate Coolants and Breeders

Material	(B = Breeder) (C = Coolant)	Advantages	Disadvantages
Lithium	B & C	Excellent heat transfer High boiling point Low melting point High specific heat Low viscosity Good neutron moderator No long-term activation products No neutron damage High breeding ratio possible Low density	Highly reactive with: air water concrete High electrical conductivity
Li_aPb_b	B	Lower chemical reactivity than lithium High breeding ratio possible Lead is a good neutron shield for magnets Tritium recovery feasible	Poor technology base High density Activation product: Pb^{205} Reactive with water or lithium coolant
Flibe ($34 \text{ BeF}_2 : 66 \text{ LiF}$)	B + C	Good neutron moderator Low vapor pressure Low electrical conductivity Low tritium solubility Low chemical reactivity (expected)	Scarcity of beryllium
LiAlO_2	B	Chemical stability	Requires neutron multiplication
Water	C	Substantial engineering experience and database	Reacts with Li, and LiPb alloys High pumping power High operating pressure

TABLE 1.2

Lithium Reactions of Interest

	Heat of Reaction, ΔH_{298} kcal/mole of product
<u>In Air</u>	
$4\text{Li} + \text{O}_2 \longrightarrow 2\text{Li}_2\text{O}$	-43
$2\text{Li} + \text{O}_2 \longrightarrow \text{Li}_2\text{O}_2$	-152
$6\text{Li} + \text{N}_2 \longrightarrow 2\text{Li}_3\text{N}$	-48
$2\text{Li} + 2\text{H}_2\text{O} \longrightarrow 2\text{LiOH} + \text{H}_2$	-49
$2\text{Li} + \text{H}_2 \longrightarrow 2\text{LiH}$	
$2\text{Li} + \text{LiOH} \longrightarrow 2\text{LiO}_2 + \text{H}_2$	
Note: Li_2O_2 is unstable above 250 °C	-151.3 (magnetite)
<u>In Concrete</u>	
$8\text{Li} + \text{Fe}_3\text{O}_4 \longrightarrow 3\text{Fe} + 4\text{Li}_2\text{O}$	-151.3 (magnetite)
$4\text{Li} + \text{SiO}_2 \longrightarrow \text{Si} + 2\text{Li}_2\text{O}$	(basalt)
$2\text{Li} + \text{H}_2 \longrightarrow 2\text{LiH}$	
<u>Others</u>	
$4\text{Li} + 3\text{CO}_2 \longrightarrow 2\text{Li}_2\text{CO}_3 + \text{C}$	-45
$n\text{Li} + m\text{Pb} \longrightarrow \text{Li}_n \text{Pb}_m$	-13n for $\frac{n}{m} < 1$

this report. However, work is continuously being done to expand the database, and two reports have been published that review the state of knowledge of these materials [7,8]. Property data in the present calculations have been taken from these two reports unless otherwise specified.

1.2. LITFIRE History and Development

The computer code LITFIRE, developed at MIT, is an analytic tool for calculating the consequences of lithium fires in various containment schemes. In its original form, LITFIRE was a modified version of SPOOL-FIRE [9] which modeled liquid-metal sodium fires in containment. The adaptation of SPOOL-FIRE to LITFIRE incorporated several major changes. These include allowance for nitrogen and water vapor reactions as well as changing sodium properties implicit in the code to lithium properties. In addition, the effect of aerosols in the containment on radiative heat transfer was included. By far the most important change to the modeling was the incorporation of a "combustion zone" above the lithium pool. It is in this zone that lithium combustion takes place, according to mass and heat transfer mechanisms described by Dube [1].

With these changes in tact LITFIRE was used to predict the consequences of a postulated lithium fire in a prototypical fusion reactor geometry. A sensitivity analysis was performed on many of the important parameters in LITFIRE and best estimates for these parameters were adopted. An analysis of strategies for mitigating the consequences of lithium fires was performed and found to have significant effects [1].

After the original study was completed, lithium combustion experiments were conducted at the Hanford Engineering Development Laboratory (HEDL). The geometry of these experiments differed significantly from the capabilities of LITFIRE and useful comparisons were not readily attainable. Several changes were made to LITFIRE to model the experimental setup and the predictions of LITFIRE were then compared to the experimental data. The new modifications brought the temperature field predictions to within 30% of the HEDL experimental results for a variety of lithium reactions. Details of the experiments and LITFIRE changes were documented by Tillack [10]. Other unverified extensions of the code were also developed at that time. They include the capacity for lithium-concrete reactions and a two compartment containment scheme with combustion in one cell and mass and heat transfer between the two cells.

The inclusion of LiPb-water reactions in a prototypical breeder element was next incorporated into LITFIRE [2]. This modeling is substantially different from the combustion zone model for pool fires and has therefore been separated from the rest of the lithium fire modeling. As a result there are now two versions of LITFIRE, (LITFIRE-A) treating lithium-air and lithium-concrete reactions; and (LITFIRE-B) treating LiPb-water reactions. The addition of LiPb-air reactions is

part of the present work and will be incorporated into LITFIRE-A since much of the combustion zone modeling is identical to that of lithium-air reactions. Table 1.3 lists the versions and options of LITFIRE that are presently available and their state of verification with respect to experiment.

1.3. LITFIRE Model Description

LITFIRE generates the temperature and pressure profiles in an idealized geometry with a single heat source and various heat sinks. The heat source term represents the combustion of lithium. When combustion has ceased, or the reaction does not ignite, the hottest structural component (or the lithium pool itself) will act as a decaying heat source until all the temperatures reach equilibrium with ambient. The heat flow between nodes is one-dimensional and consists of conductive, convective, and radiative components when appropriate.

$$\text{convection} \quad \frac{dq}{dt} = h A (T_1 - T_2) \quad \text{Newton's Law of Cooling} \quad (1.1)$$

$h = h(\text{Gr,Pr}) = \text{heat transfer coefficient}$

$$\text{conduction} \quad \frac{dq}{dt} = k A \frac{dT}{dx} \quad \text{Fourier's Conduction Equation} \quad (1.2)$$

$k = k(T) = \text{thermal conductivity}$

$$\text{radiation} \quad \frac{dq}{dt} = \sigma A (T_1^4 - T_2^4) \quad \text{Stephan- Boltzman Law} \quad (1.3)$$

$\sigma = \text{Stephan-Boltzman Constant}$

In some cases one of the channels may be ignored if it is not of significant magnitude with respect to the other components.

Correlations for the heat transfer mechanisms are fairly simple and the combustion source term is highly idealized in order to: 1) permit greater flexibility for users; 2) base the calculations on available data, and; 3) to reduce computation time and costs. For a given geometry, there are enough user defined coefficients to accurately model the principal heat transfer mechanisms. However, the combustion zone model is fairly inflexible and is also the most simplified part of the LITFIRE model. The effect of surface layer formation, wicking, product buildup in the pool, and multiple species reactant competition are ignored or very crudely modeled. Significant improvements to multiple species combustion were added by Tillack [10] and are further discussed in chapter 2 of this report.

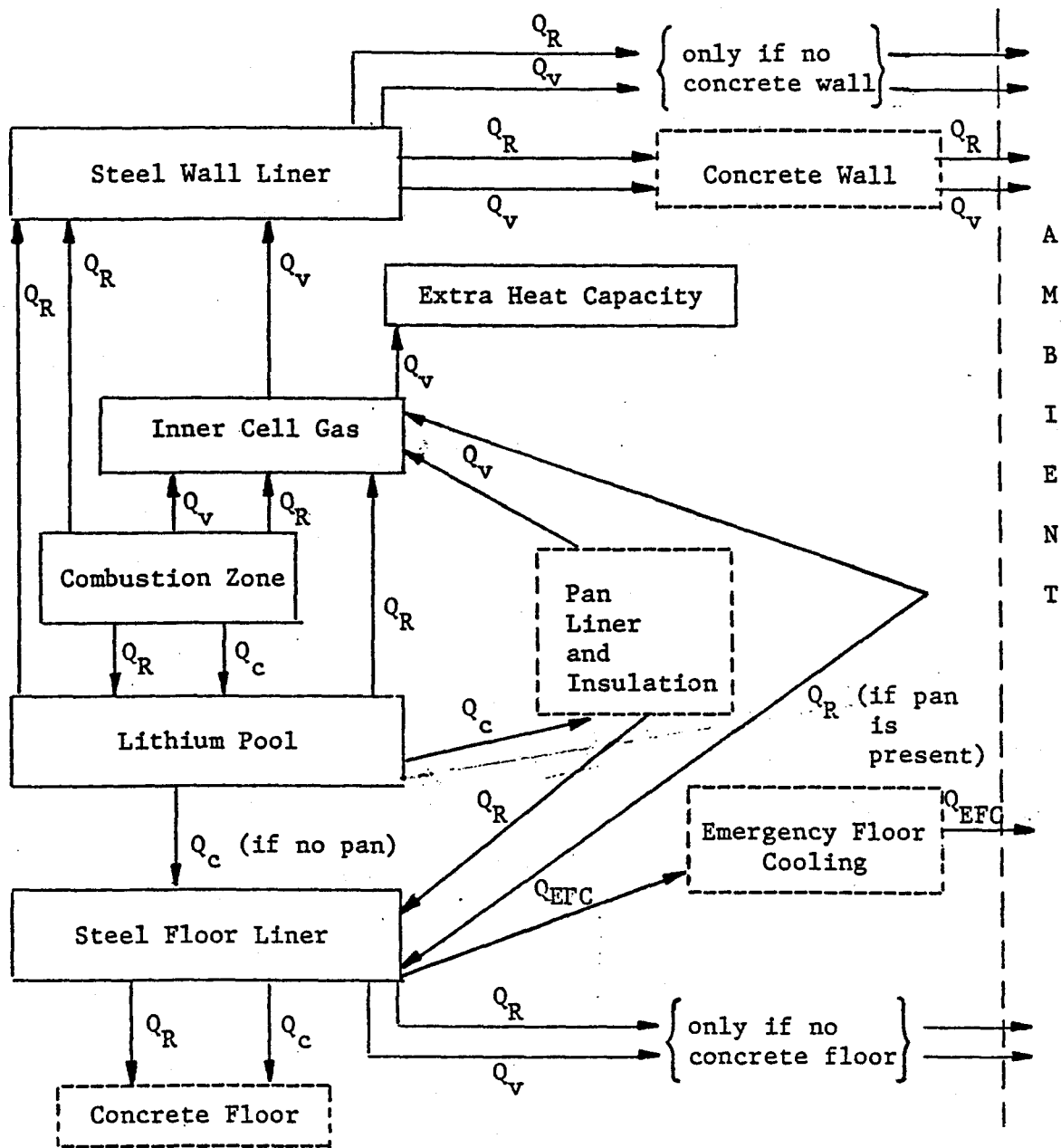
The idealized energy flows in LITFIRE (one and two cell versions) are shown in Figures 1.1 and 1.2. Each node has a heat capacity approximating that of its physical counterpart (average specific heat of the material times the total mass of the node) and a single, bulk averaged temperature. Heat transfer between two nodes is a function of temperature difference and the equivalent thermal resistance (for each heat transfer mechanism) of that specific pair of nodes.

Mass flows in LITFIRE are also lumped and are principally between the two cell gas nodes, the combustion zone and lithium pool, and the combustion zone and primary cell gas. These are

TABLE 1.3

LITFIRE Versions and Available Options

<u>Version</u>	<u>Reaction Modeled</u>	<u>Available Options</u>	<u>State of Verification</u>
LITFIRE-A	Li-Air	One or two cells Pan geometry Gas injections Emergency cooling of floor or cell gas SI or English units	Compared to small scale HEDL tests. (less than 100kg. Li)
LITFIRE-A	Li-Concrete	All of above except pan geometry	Unverified
LITFIRE-A	LiPb-Air	Same as Li-Air reactions	Unverified
LITFIRE-B	LiPb-Water	One cell SI or English units	Unverified



dashed lines indicate optional node

Q_R = radiative heat transfer

Q_V = convective heat transfer

Q_C = conductive heat transfer

Figure 1.1: Energy flow in single cell LITFIRE

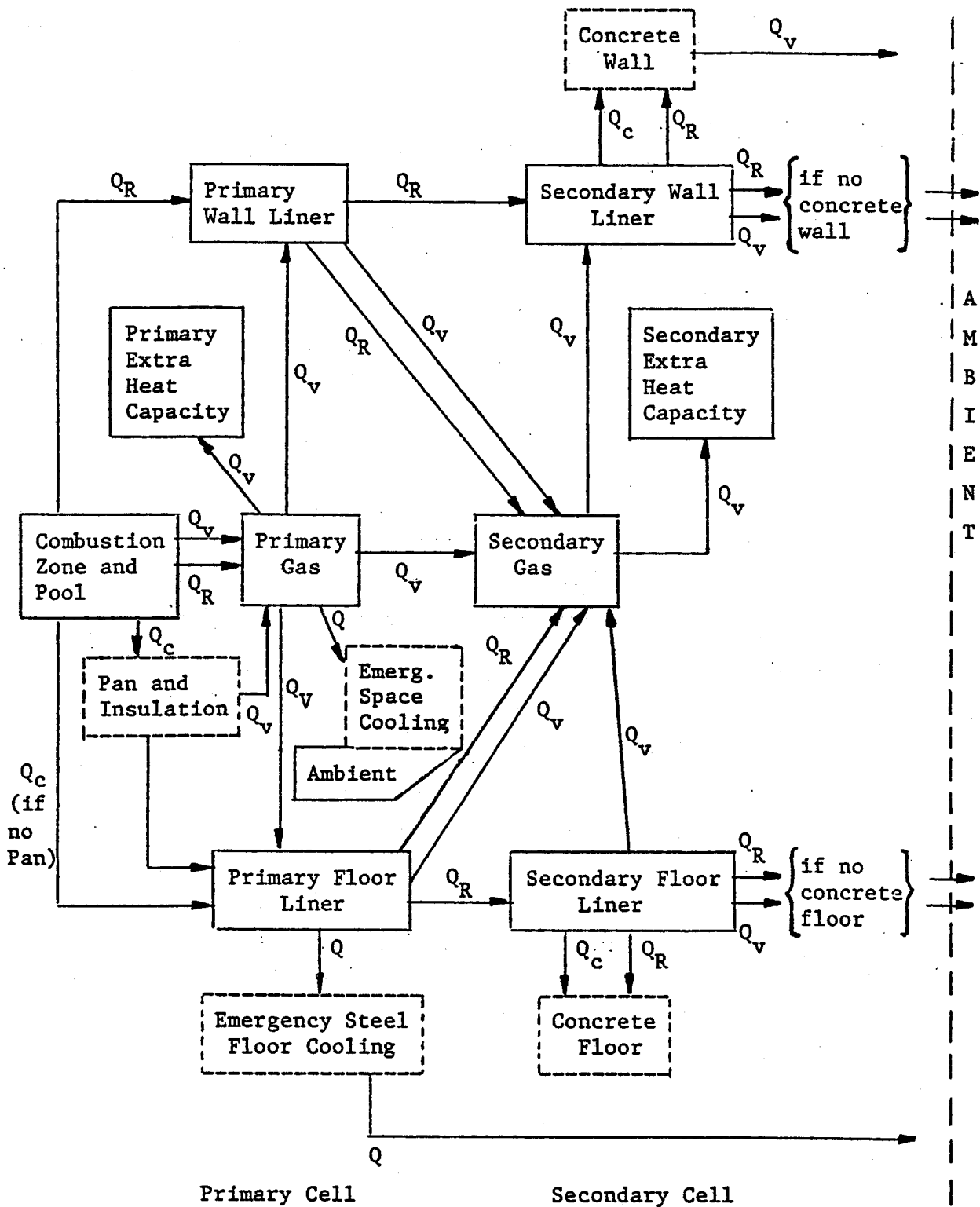


Figure 1.2: Energy flow in two-cell LITFIRE

shown schematically in Figure 1.3. Structural materials are not allowed to participate in the mass flows and are considered stable at any temperature. Therefore, LITFIRE is not capable of predicting the effects of volatilization or melting of structural components and the user should be aware that the predictions of LITFIRE will be inaccurate in this regime. More detailed descriptions of the mass flows are given in chapters 3 (two cell exchange) and 4 (combustion zone-pool transport).

The time history in LITFIRE is determined by a set of simultaneous coupled differential equations. For each thermal element in the model the temperature history is calculated by a set of numerical integration subroutines that use the methods of finite differences in the spatial regime and either Simpson's rule or a fourth-order Runge-Kutta method in the time domain [1]. The actual integration is of the form

$$Y(t) = Y(t_0) + \int_{t_0}^t dt' \frac{dY}{dt'} \quad (1.4)$$

where the time rates of change (dY/dt') are calculated in the main LITFIRE program for each node by finite differencing. The program solves for each node simultaneously during each time step and has a capacity of 100 separate nodes. The numerical stability during each time step determined from the fractional temperature change at certain nodes during a single time step (different from integration time step). LITFIRE uses the most sensitive nodes to determine the stability criteria, but it is still possible that under certain regimes the code may produce nonphysical results. Experience has shown that this can happen when a node is given too thin a thickness or too high a conductivity. Recommended values are listed in the user's guide [11] and were used in the present calculations. Another numerical instability can occur if there is an oscillatory solution to a given node that has a period of the same magnitude of the time step. In LITFIRE, this has been found to occur on occasion when an orifice is used in the two cell option. This phenomena is discussed in more detail in chapter 3.

The program flow has been reorganized to promote clarity and facilitate modification to the existing coding as well as reduce computation time. Nine subroutines have been added to the body of the program that represent options available with LITFIRE. Specifically, these are two cell, LiPb combustion, pan geometry, concrete wall, concrete floor, concrete combustion, gas injection, and SI units subroutines. (Appendix D contains a listing of the version of LITFIRE used in the present calculations.) In addition, many of the variable names and intermediate program calculations have been changed for greater clarity. Appendix F contains a glossary of all variables presently used in LITFIRE.

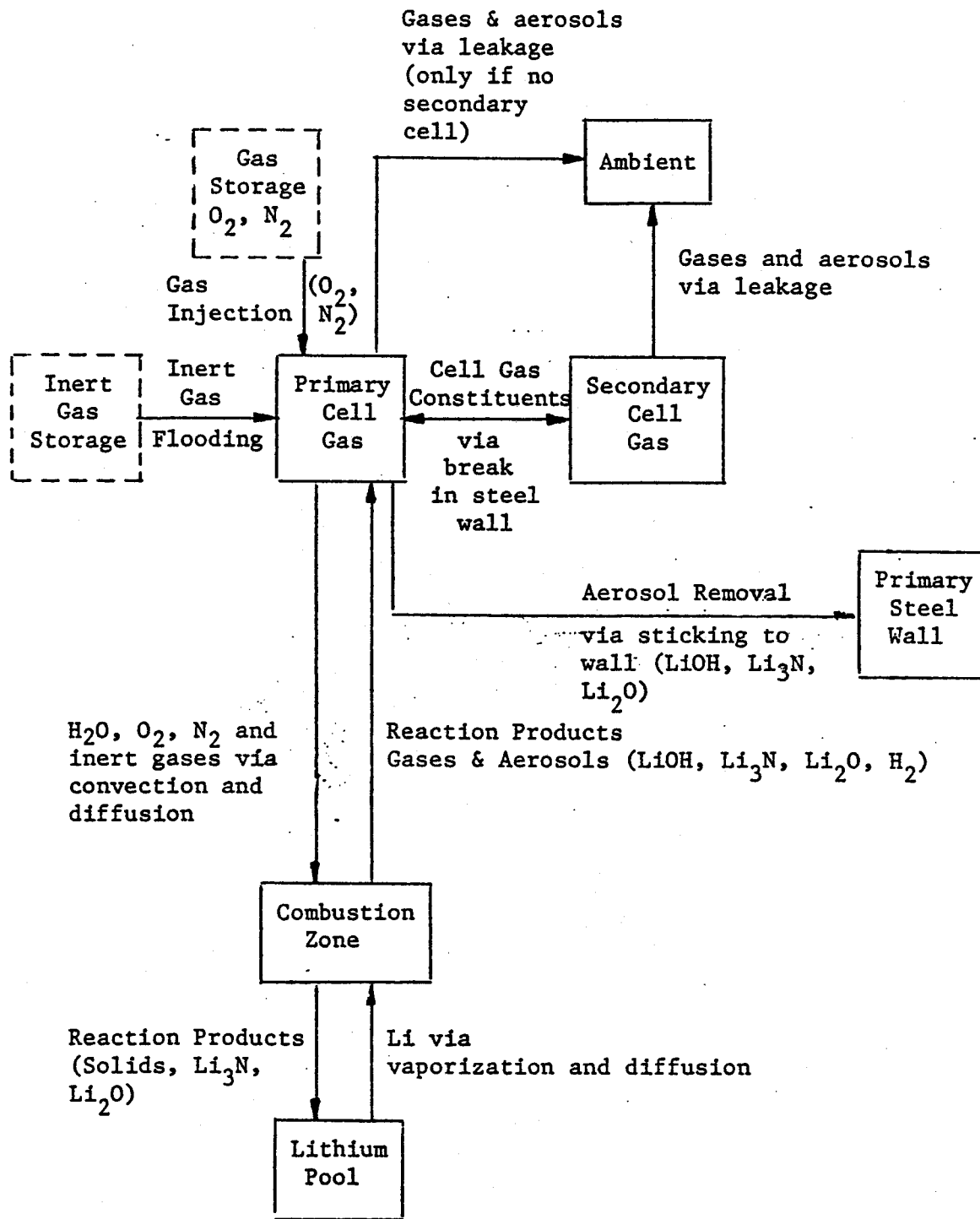


Figure 1.3: Mass flows in LITFIRE

1.4. Scope of Present Work

The purpose of the present work is three-fold. First, to compare predictions from the most recent version of LITFIRE with the latest experimental data available. There are several significant differences between the present modeling in LITFIRE and the modeling in the version that was used for the earlier comparison with the HEDL experiments. [12] In Chapter 2, these differences are discussed and analyzed and the comparison between LITFIRE and experiment is brought up to date.

Second, to study the effects of pure lithium fires in multi-compartment systems. In this case the system approximates those of a commercial scale tokamak torus and containment building. This application of LITFIRE uses the two cell formalism and is described in detail in chapter 3.

The third part of this thesis is to incorporate LiPb-air reactions into the present structure of LITFIRE so that safety comparisons between alternate coolants and/or breeders may be made. This extension of the model required several important changes in the treatment of the pool node and transport of Lithium to the combustion zone. These changes are documented in Chapter 4 as are the results from preliminary comparisons of various LiPb compounds.

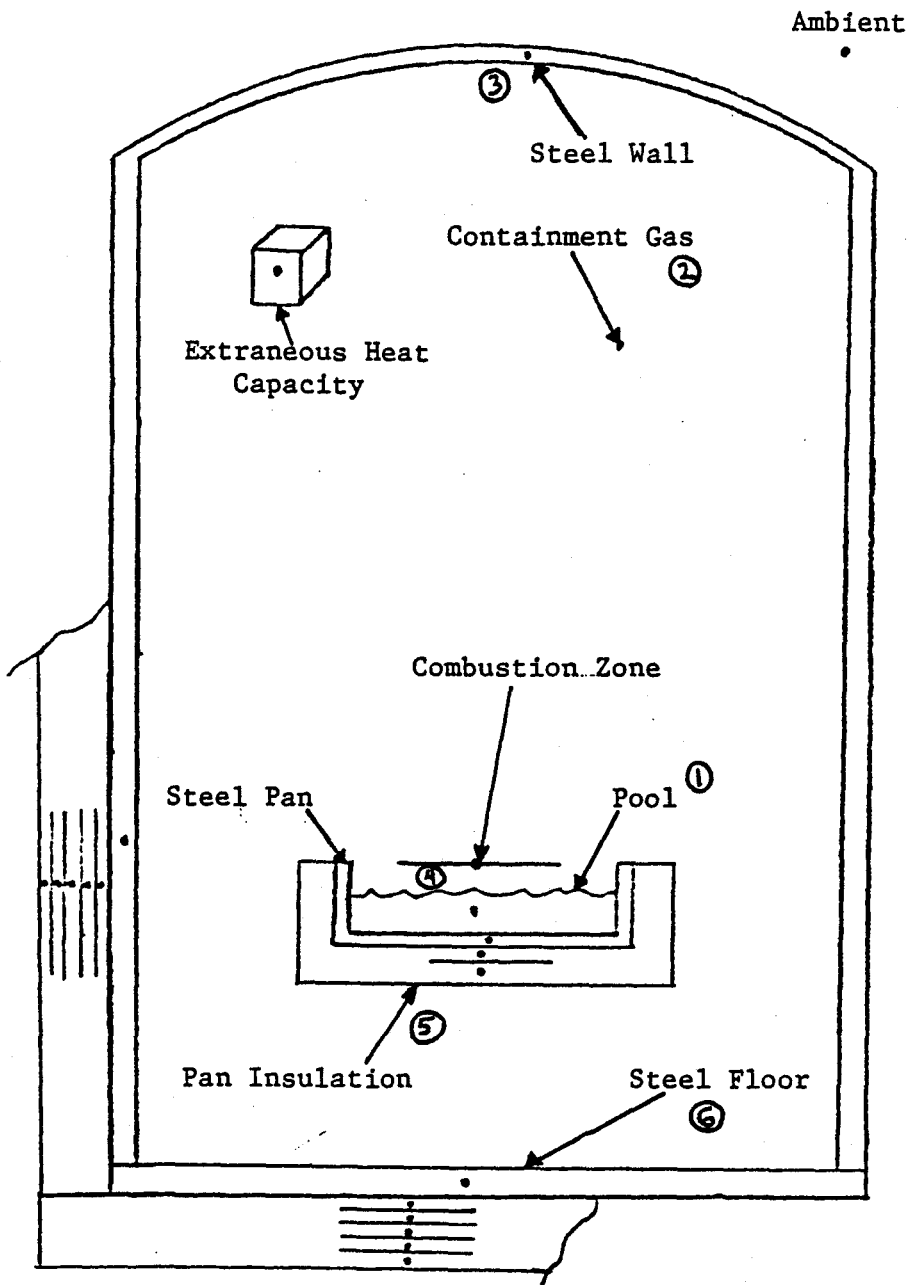
2. DEVELOPMENT AND APPLICATION OF SINGLE-CELL LITFIRE

LITFIRE has been in various stages of development at MIT over the past five years. Results of LITFIRE calculations using intermediate versions of the code have been published by Dube [1] (1978) and Tillack [10] (1980). The comparison to experiment by Tillack [10] did not use the LITFIRE version that incorporated many of the changes made since Dube's publication. Therefore, it is the purpose of the following section to summarize the important changes made since Tillack [10] and the purpose of the remainder of the chapter to compare the most recent version of LITFIRE with experiment and previous calculations.

2.1. Recent Changes to the LITFIRE Model

The major changes to the LITFIRE single-cell model since it was described by Tillack [10] are summarized below and are also indicated pictorially in Figure 2.1.

- **Radiation from pool to cell wall and cell gas.** Originally, only the combustion zone was radiating to the cell wall and containment gas. At present, the pool surface is also radiating heat to the cell wall and gas. This change is based on the assumption that the combustion zone is too thin to absorb all of the radiation emitted at the pool surface. Incorporating this pathway into the model required the addition of a combustion zone transmissivity that allowed greater flexibility in coupling the radiative interchange between the combustion zone and pool nodes. The changes were made in order to bring the pool temperature closer to the combustion zone temperature and at the same time minimize the effect on the cell gas temperature. Appropriate values for the transmissivity are the subject of Section 2.3.2.
- **Cell gas emissivity.** The correlation for the emissivity of the primary cell gas was altered in order to bring the cell gas temperatures in agreement with experimental observations. The upper limit of the emissivity was reduced from 1.0 to 0.04 in order to reduce the radiation heat absorption by the gas. The emissivity of the secondary cell gas was not altered and may still reach a maximum of unity (although this is very unlikely since there usually is very little aerosol present in the secondary gas). These changes were documented by Tillack [10] but were not used in his comparisons with experiment nor did they appear in previous versions of LITFIRE that are still available.
- **Aerosol removal from primary cell gas.** An optional mechanism for the removal of aerosols from the primary cell gas has been included in the code. This can have



1. Radiation From Pool to Gas and Wall
2. Containment Gas Emissivity
3. Aerosol Removal
4. Film Conductivity
5. Radiation From Pan to Containment Gas
6. Convection from Steel Floor to Containment Gas

Figure 2.1: Diagram of Changes to LITFIRE Single Cell

a significant effect on the cell gas emissivity since

$$\text{gas emissivity} = C_1(1 - \exp(-\text{aerosol} \times C_2)) \quad (2.1)$$

where C_1 is a user defined constant between zero and one, C_2 is a function of the cell geometry, and 'aerosol' is the combined volume (mass/density) of all aerosols present in the primary gas. The net effect of aerosol removal will be to reduce the cell gas emissivity. The magnitude of this effect as well as its relation to cell gas temperature is discussed in Section 2.3.1.

- Thermal conductivity between combustion zone and pool. The region between the combustion zone and lithium pool was originally assumed to be composed only of unreacted nitrogen vapor. This assumption was inconsistent with the assumed transport of Lithium through this region by vapor diffusion. As a result, the conductivity of the film region is now calculated using a pressure weighted mean average of nitrogen and lithium vapors. The partial pressure of lithium is a known function of the pool temperature and the partial pressure of nitrogen is assumed to be equal to the cell gas pressure. The resulting conductivity of the film region is higher (due to lithium's high conductivity) and as a result, more heat is transferred from the combustion zone to heating the pool. Unfortunately, the present modeling does not permit calculation of the diffusion *rate* of lithium through this region. Therefore, the combustion rate of lithium is still assumed to be gas (O_2, N_2) limited and is one of the weakest assumptions in LITFIRE. (This has been changed slightly in the LiPb combustion model and is discussed in detail in chapter 4.)
- Radiation from pan insulation to cell gas. This had already been documented as part of LITFIRE but did not appear in the fortran listing. The effect on the cell gas temperature was negligible due to the low emissivity of the insulation.
- Convection between steel floor liner and primary cell gas. This is only allowed when the pan geometry is being used since the floor is no longer in direct contact with the lithium pool. This was included because "suspended" position of the pan allowed communication between the steel floor and cell gas. In addition, the size of the steel floor was made independent of the area of the lithium pool or spill pan. Before the change, the floor area was assumed equal to that of the lithium pool area, regardless of geometry, since it was assumed that axial conduction in the floor would be negligible. However, use of the two-cell code emphasized the importance of the floor area in heat transfer to the secondary cell.

2.2. Application of LITFIRE to Experiment

In the past year, additional lithium combustion experiments have been performed at HEDL. [6] These tests include lithium combustion in air, carbon dioxide, and water, and were larger in scale than the tests reported by Tillack [10]. The two most recent air tests (LA-4 :25 kg.-Li, LA-5:100 kg.-Li) were significantly larger than earlier tests (10 kg.-Li) and provide data to check LITFIRE predictions for somewhat larger fires than the present correlations were obtained from. This serves as a partial check on the applicability of using LITFIRE for modeling the large scale lithium fires that are possible in commercial size fusion reactors.

2.2.1. Description of HEDL Experiment

The basic geometry of the test facility described below is shown in Figure 2.2 and a summary of the important test parameters appears in Table 2.1. The lithium pool-air reaction tests were performed in a carbon steel containment vessel measuring 20.4 meters in height and 7.6 meters in diameter with standard dished top and bottom heads. This containment formed the primary pressure and aerosol boundary within which each test was carried out. Inner surfaces were coated with a modified phenolic paint and the interior of the vessel was essentially void. However, a platform and structural supports provided a 50% increase in horizontal surface area for aerosol particle settling.

Lithium supply to the vessel was through a preheated pipeline (2.5 cm. in diameter) from a heated lithium storage tank to the lithium spill pan. The reaction catch pan was made of 316ss. Temperatures (measured in 49 separate locations), pressure, oxygen concentrations, and hydrogen concentrations were monitored continuously. The gas samples from which the average gas concentrations were determined, were taken from six locations within the containment.

The initiating procedures for both experiments were the same, however, the LA-5 reaction was terminated after 65 minutes, while the LA-4 reaction was allowed to go to completion unhindered. A lid was provided in test LA-5 which terminated aerosol generation and the reaction as well, 3900 seconds after the reaction was initiated. LITFIRE is not capable of modeling a reaction termination by such a procedure and (as will be seen in Section 2.2.3) the predictions of LITFIRE after this time are not valid for test LA-5. In test LA-4, a weld in the spill pan corroded 3300 seconds after the reaction began, and the remaining lithium spilled into the steel catch pan where it formed a shallow pool and burned to completion in ten minutes. This change in reaction configuration was not modeled by LITFIRE so again, the predictions by LITFIRE are not valid after leakage from the spill pan begins. (LITFIRE is only capable of modeling a single user specified configuration for each lithium spill, and there is no allowance for changing the spill condition or cell geometry

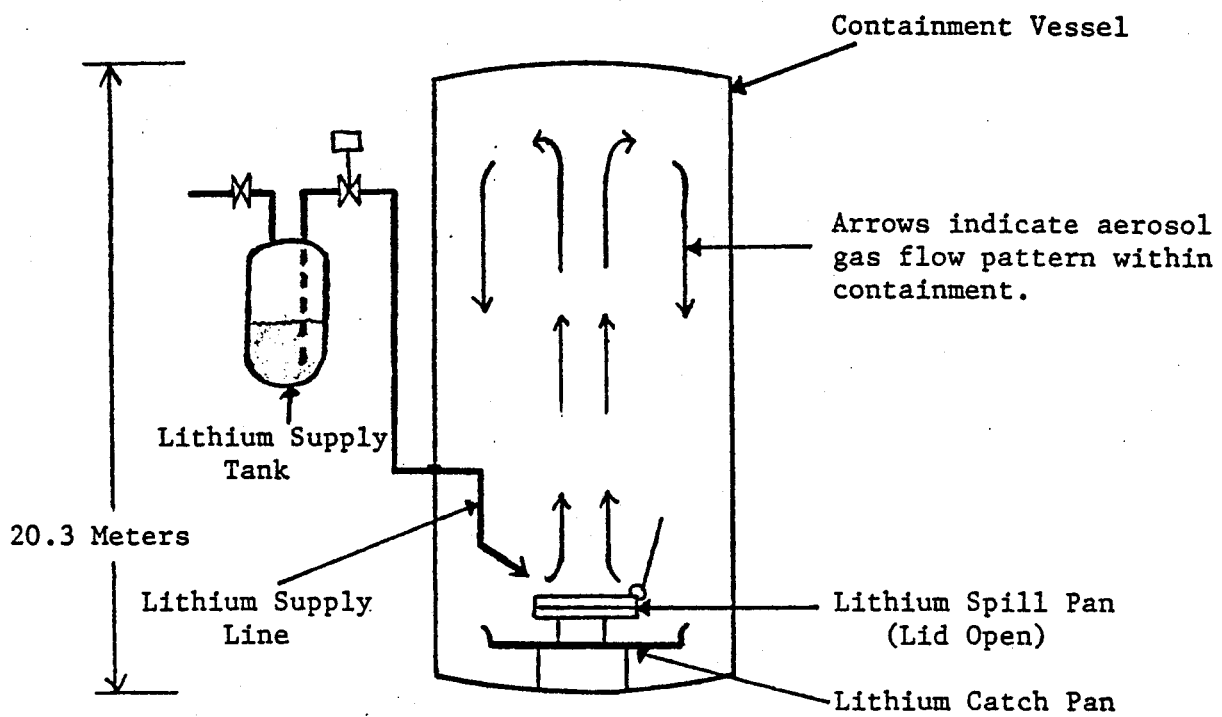


Figure 2.2: HEDL Test Facility

TABLE 2.1

Summary of HEDL Test Conditions

	LA-4	LA-5
<u>Containment Vessel</u>		
Diameter (m)	7.62	7.62
Overall Height (m)	20.3	20.3
Volume (m ³)	850.0	850.0
Total Horizontal Surface (m ²)	88.0	88.0
Wall Surface (m ²)	520.0	520.0
Vessel Mass (Rg)	103,000	103,000
<u>Lithium</u>		
Mass of Lithium Spilled (kg)	26.7	100.0
Lithium Reaction Pan Surface (m ²)	0.124	2.0
Initial Lithium Temperature (°C)	600.0	500.0
Depth of Lithium Pool (m)	0.46	0.10
<u>Containment Atmosphere</u>		
Initial Oxygen (mole %)	20.9	20.8
Initial Gas Temperature (°C)	31.0	31.8
Initial Pressure (MPa, absolute)	0.116	0.113
Maximum Temperature (°C)	68	83
Maximum Pressure (MPa, absolute)	0.127	0.127
Final Oxygen Concentration (mole %)	20.0	19.1

Comments

LA-4 Reaction: As a deep pool for ~3300 sec when the pan integrity failed and all lithium spilled to the floor and reacted within 10 mins. LA-5 Reaction Terminated after 3900 seconds.

as a function of time or temperature. More detailed descriptions of the test facility along with a description of earlier test procedures appears in [6,10,12] and will not be repeated here.

2.2.2. LITFIRE Geometry Used to Model Experiment

Several of the options available in LITFIRE were used to model the HEDL test. These were the pan geometry, gas injection, and aerosol removal options within a single containment cell. In test LA-5 insulation surrounding the outer cell was modeled by specifying the appropriate properties in the concrete nodes. In test LA-4 the containment was not insulated and the concrete nodes were not used. The geometry used in the LITFIRE calculation is indicated in Figure 2.3 and the input data corresponding to the HEDL test conditions is listed in Appendix A.

Some of the input variables to LITFIRE are the coefficients (C_{ij}) for the convective heat transfer coefficients which are calculated according to

$$h_{ij} = \frac{C_{ij} D_i}{k_i} (Pr Gr)^{\frac{1}{4}} \quad (2.2)$$

Recommended values for the various coefficients (C_{ij}) were obtained by Tillack [10] through trial and error in an attempt to match all the HEDL test data with a consistent set of coefficients. Since the geometry of the earlier tests was very similar to the present experimental setup, the recommended values for the C_{ij} 's will be used. In addition, several new coefficients were required due to the addition of the cell gas convective contact with the steel floor and the insulated pan. Values for these parameters were chosen to be consistent with the values indicated by Tillack [10].

There are three parameters that must be input to the code that have not been precisely determined as yet. These are the aerosol sticking coefficient ("BETA"), the combustion zone emissivity ("EMCZ"), and the combustion zone transmissivity ("TAUCZ"). The importance of these parameters in LITFIRE is discussed in section 2.3 of this report and recommended values determined in that section were used in the present calculation.

The remainder of the input values (geometric and physical properties) for LITFIRE were obtained from a listing of LITFIRE used at HEDL before the tests to predict the consequences of the tests. Data received after the test indicates that these values were properly specified beforehand and no changes were made.

2.2.3. Comparison of LITFIRE Predictions with Experimental Observations

The comparisons between experiment LA-5 and LITFIRE are shown in Figures 2.4a through 2.4d. These comparisons are for the the average cell gas temperature, the lithium pool temperature, and the primary steel wall temperature. In addition, the primary cell gas pressure is plotted since it

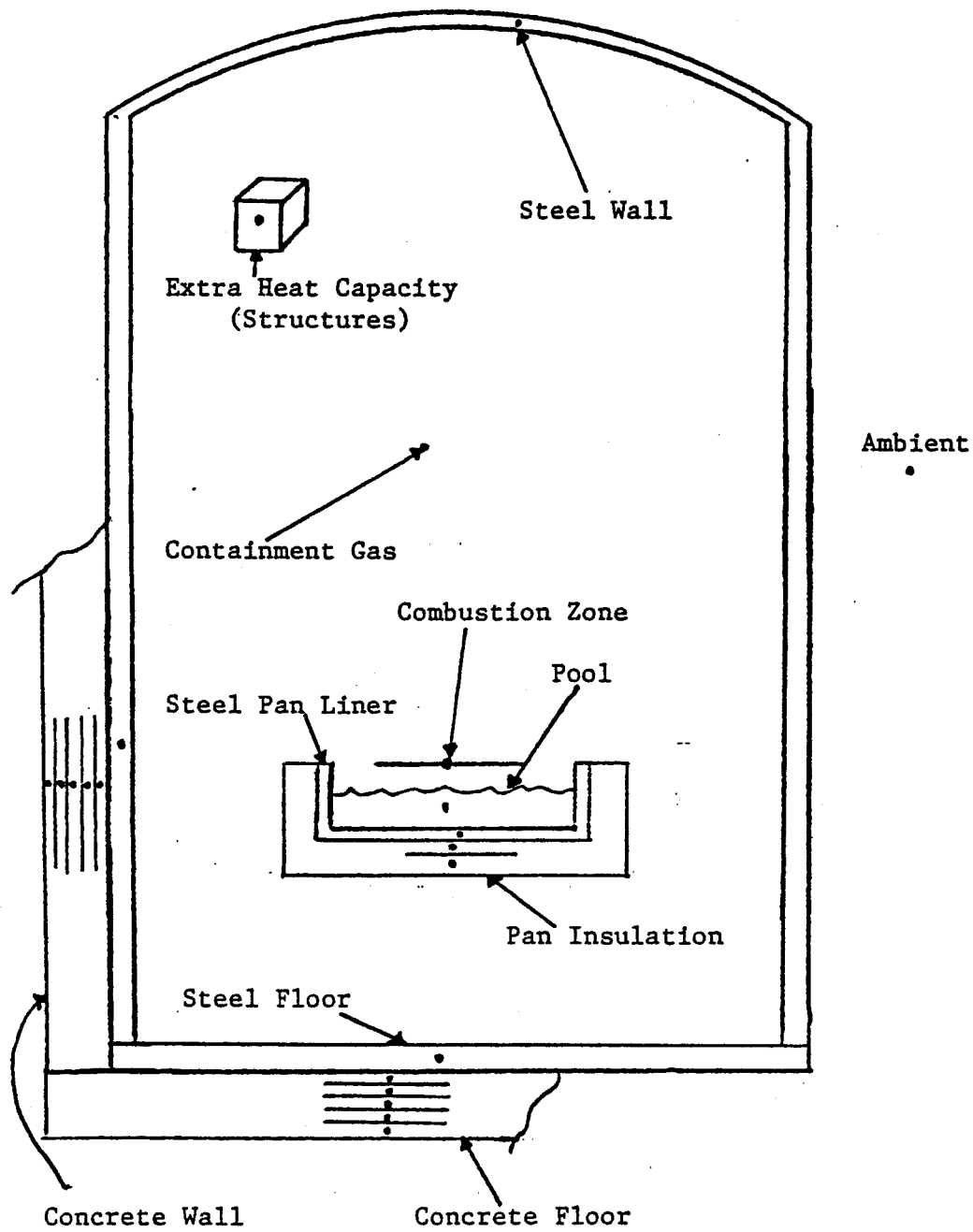


Figure 2.3: LITFIRE Geometry for HEDL Comparison

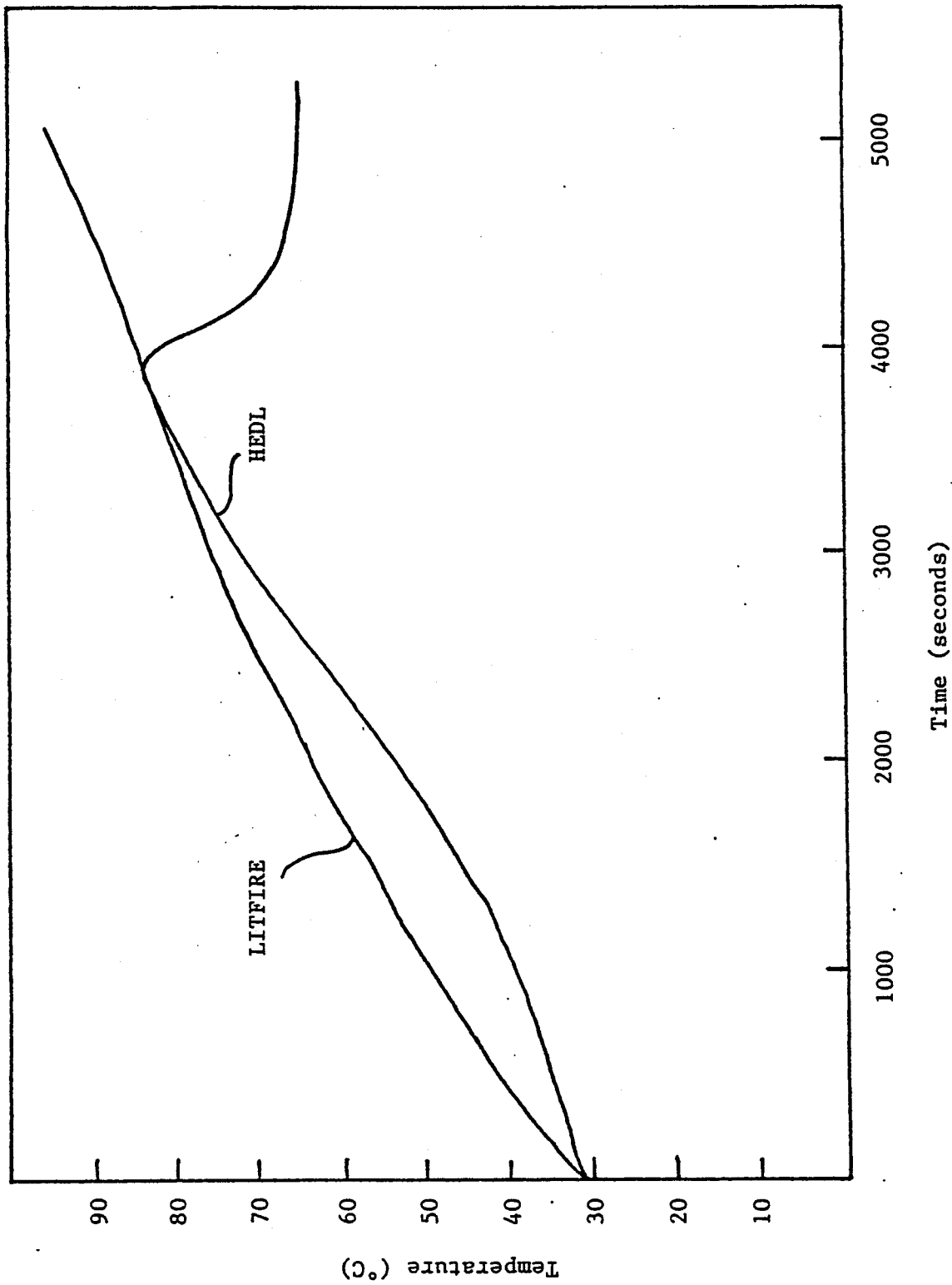


Figure 2.4a: LA-5 Cell Gas Temperature

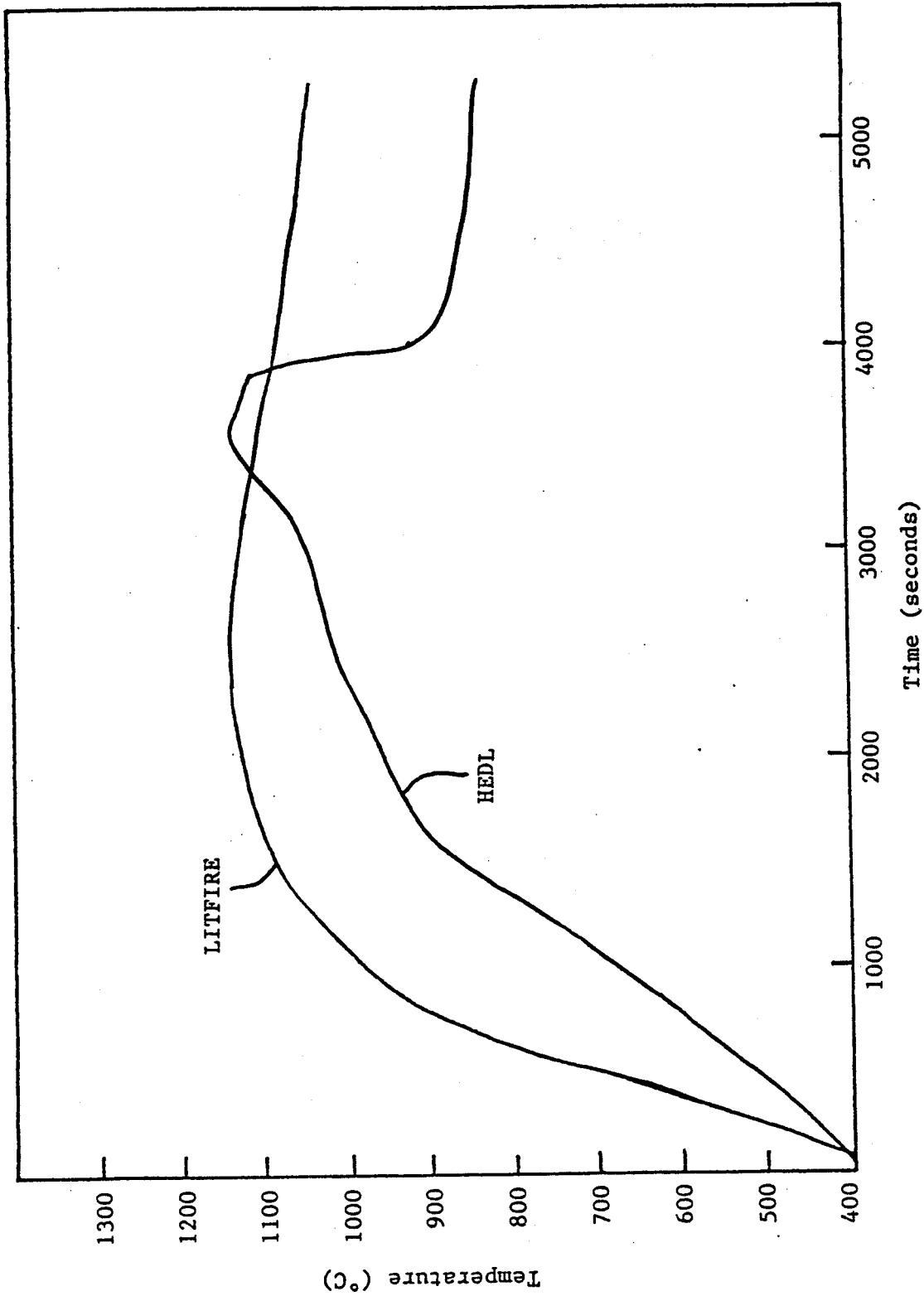


Figure 2.4b: LA-5 Lithium Pool Temperature

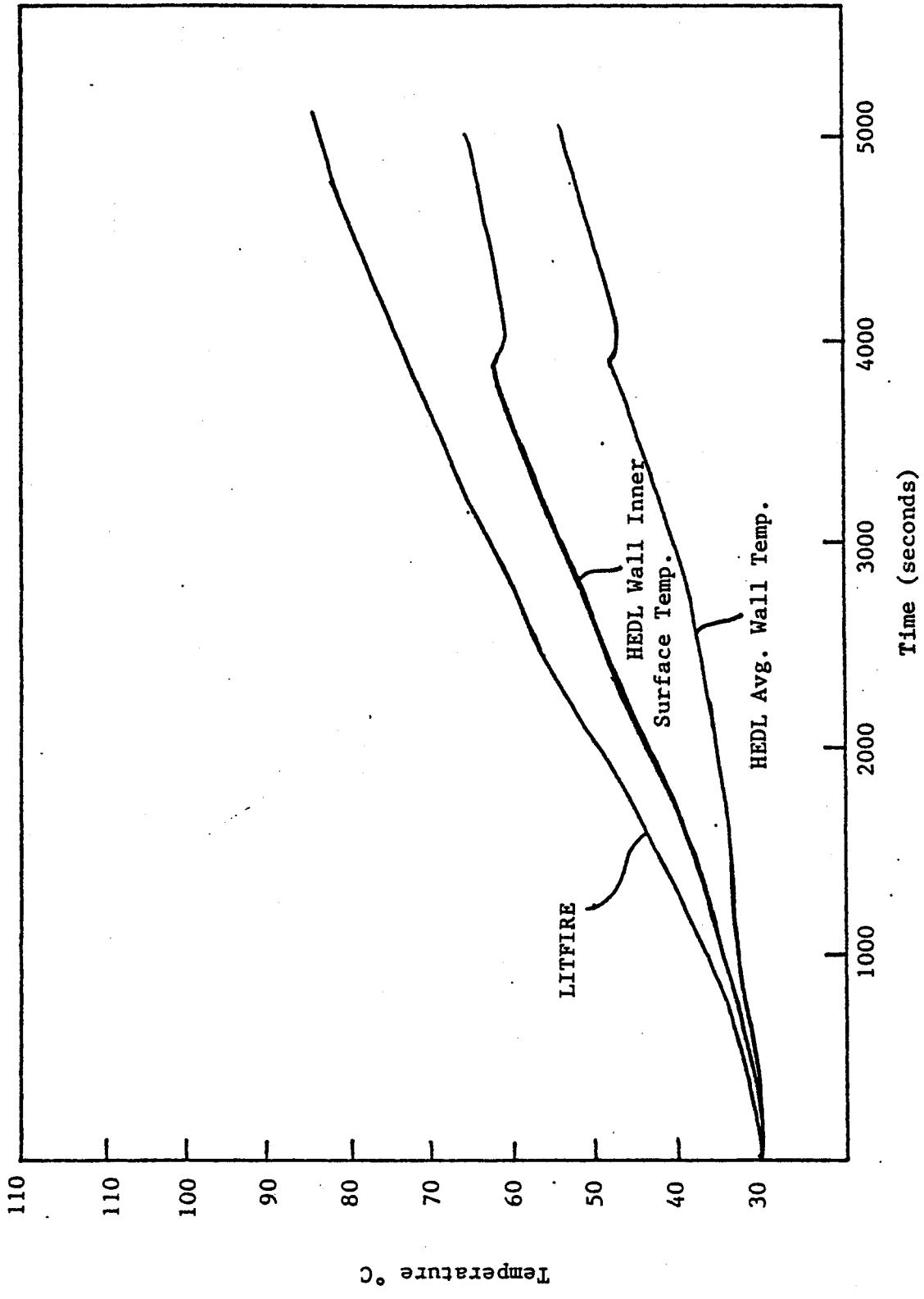


Figure 2.4c: LA-5 Containment Vessel Wall Temperature

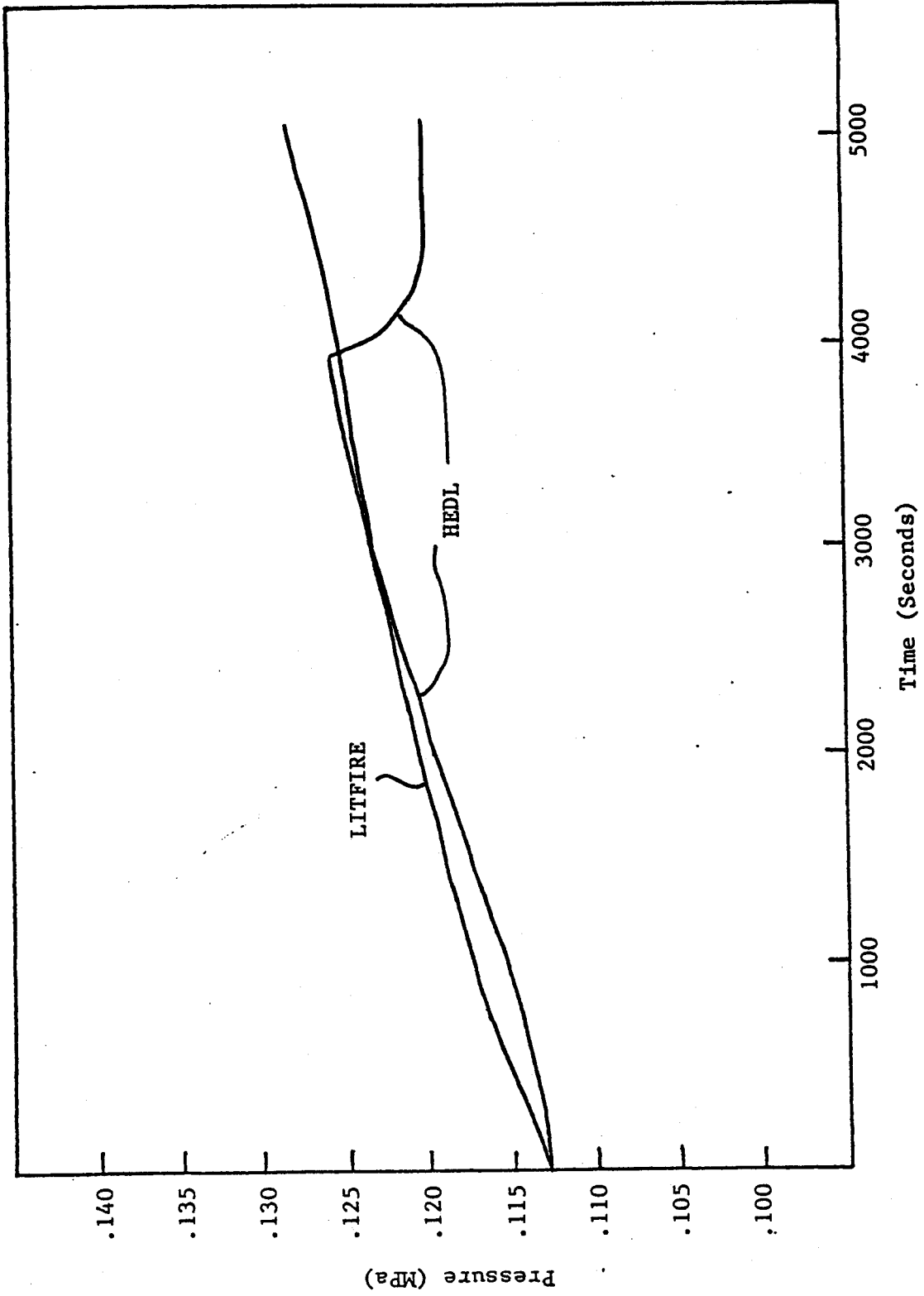


Figure 2.4d: LA-5 Cell Gas Pressure

is dependent on both the cell gas temperature and the mass of the gases present. The temperature and pressure profiles together can provide a check on the combustion rate since this is the dominant pathway for mass transfer from the gas. The reaction at HEDL was terminated after 3900 seconds and this is indicated in the figures by a vertical dashed line.

In the comparisons of the mixed species combustion experiments with LITFIRE by Tillack [10], several areas of importance were recommended for observation. These include: the nitrogen reaction rate as a function of temperature and oxygen concentration; the film conductance between the pool and combustion zone; the thickness of the pool; the cell gas emissivity; and the pool/combustion zone coupling. The experimental data obtained from HEDL indicated that the temperature differential through the lithium pool was a maximum of about 50°C for a pool thickness of 0.46 meters. However, the bottom thermocouple in the pool (which recorded the lowest temperatures) was affected by the buildup of Li_3N and Li_2O solids. These reaction products are formed at the pool surface but tend to fall through the pool and collect at the bottom as the reaction proceeds. The other thermocouples recorded temperature variations of less than 10°C during the time that the lithium was contained in the pan. Therefore, the single node representation of the pool node is probably a reasonable representation and should not add major inaccuracy to the the LITFIRE predictions, even for larger spills.

The reaction rate of lithium with nitrogen and oxygen was not measured directly but must be inferred from the data on gas composition and cell temperature and pressure. This can be done by applying the ideal gas law

$$PV = nRT \quad (2.3)$$

to the experimentally determined profiles of average cell temperature and pressure. The mole percent concentration of oxygen in the cell gas was measured at various points in the cell and an average of these was used in the present calculation. The reaction rate is extrapolated from the change in moles of O_2 and N_2 at specific intervals and is considered constant between those intervals. Table 2.2 lists the results of these calculations and Table 2.3 compares them to the reaction rates calculated by LITFIRE.

The combustion rate of oxygen predicted by LITFIRE is, on average, higher than the experimentally inferred values by a factor of two and a half. However, the actual oxygen consumption rate in the HEDL experiment is probably larger than estimated here since the present analysis used an average oxygen concentration over the entire cell volume, while the actual concentration of oxygen near and in the combustion zone will be much less due to its uninhibited reaction with lithium. This effect should be larger when the lithium fire is in its early or late stages

TABLE 2.2

Experimental Gas Composition During LA-5(using $PV = n_M RT$ with $V = 850 \text{ m}^3$, $R = 8.314 \times 10^{-6} \text{ m}^3 \text{ MPa/gmole K}$)

Time (Secs.)	Temp. (°K)	Pressure (MPa)	O ₂ (mole fraction)	N _{O₂}	N _{N₂}
0	304.8	.113	.208	7884	29282
200	306	.113(4)	.208	7881	29270
400	308	.114	.208	7871	29233
600	311	.115	.207(5)	7844	29224
1000	316	.116	.207	7769	29024
2000	333	.120	.204	7515	28590
3000	346	.123	.200	7269	28369
3900	356	.126	.196	7092	28356

TABLE 2.3

Comparison of LITFIRE and Experimental Combustion Rates

(Based on Values in Table 2.2)

Time (Secs.)	Lithium Reaction Rate with Nitrogen (kg-Li/hr-m ²)		Lithium Reaction Rate with Oxygen (kg-Li/hr-m ²)	
	HEDL	LITFIRE	HEDL	LITFIRE
100	4.5	10.9	1.4	16.9
300	13.9	14.05	2.4	23.6
500	3.4	23.56	6.8	26.4
800	37.5	5.22	9.4	27.4
1500	32.5	0.0	12.8	27.0
2500	16.6	0.0	12.4	24.9
3450	1.1	0.0	9.8	22.5
Average During 3900 secs.	17.8	3.6	10.2	25.3

(i.e. when the combustion rate is lower than average) since the combustion zone volume is inversely proportional to combustion rate. Indeed, the discrepancy between LITFIRE and experiment is larger when the expected combustion rates are lower.

The agreement for the nitrogen reaction rate is worse than that for oxygen. LITFIRE predicts no nitrogen combustion will take place above a pool and combustion zone "mean" temperature of 1300 Kelvin or above oxygen concentrations of 0.28 by weight. If the experimental extrapolation is to be believed, and the LITFIRE temperature predictions are accurate, nitrogen is indeed reacting under these conditions. A possible explanation for this may be a difference between the actual combustion zone temperature and the combustion zone temperature predicted by LITFIRE. Unfortunately, direct measurements of an appropriate "combustion zone" were not made during the latest HEDL tests. However, LITFIRE does predict fairly well the cell gas and lithium pool temperature profiles. Since these two nodes bound the combustion zone, the major inaccuracy in the combustion zone temperature would most likely be due to errors in calculating the heat capacity of the combustion zone node itself, and not in the conductivity of the film region or the radiative heat transfer to the pool and cell gas. The present form of the combustion zone heat capacity is based on a quasi-steady state analysis and may not be appropriate for the transients encountered in lithium fires. Further tests are needed to clarify the correct combustion zone temperatures for comparison with LITFIRE.

There is no direct means of checking the predicted film conductance in LITFIRE with the experiment. However, the relative magnitude of the combustion zone and pool temperature coupling provides a check on both the film conductivity and the combustion zone emissivity (and transmissivity as well). In test LA-4 several thermocouples were positioned at various heights above the lithium-air reaction interface, the closest one being 5.08cm above the lithium pool. The temperatures measured at each of these thermocouples was lower than that of the lithium pool, so there is reason to believe that the reaction took place very close to the pool surface. An estimate of the combustion zone temperature might have been made by extrapolating the temperature gradient from these three positions to the pool surface, but the resulting temperatures are very much dependent on the form of the gradient assumed and yield temperatures below that of the lithium pool. However, there is a period during the reaction when the temperatures above the pool have stabilized while the pool temperature continues to rise. This observation is probably due to the leveling off of the combustion zone temperature near its maximum. Previous tests have measured the maximum combustion zone temperature to be in the vicinity of 1260°C [12] and this value is used as the limit in the present comparison. The above approximation is very crude, yet it serves as a partial guide to the degree of heat transfer coupling within the combustion zone-lithium pool system. The results of this estimation are listed in Table 2.4 and a graph of

the combustion zone/pool temperature difference for both the HEDL experiment and LITFIRE prediction is presented in Figure 2.5.

The temperature differences predicted by LITFIRE using a combustion zone emissivity of 0.9 are higher than those estimated from the HEDL experiments. After the reaction rate has peaked (approximately 200 seconds from ignition) the temperature difference begins to decrease, with the predicted and measured slopes of this decrease nearly the same. In order to reduce LITFIRE's temperature difference, the film conductivity should be increased. However, the uncertainty associated with this estimation is quite large and no firm conclusions about conductivity can be drawn. Comparisons using LITFIRE with a combustion zone emissivity of 0.5 or less resulted in very high combustion zone temperatures and temperature differences in excess of 1200°C for the duration of combustion, and eventually lead to bulk pool temperatures above vaporization. The lithium pool emissivity can also have a large effect on the degree of pool and combustion zone coupling, but this parameter is calculated within LITFIRE and is based in part on the buildup of reaction products at the pool surface. The temperature difference between the pool and combustion zone was fairly insensitive to changes in the cell gas emissivity which was already limited to a maximum value of 0.04 as previously indicated. Therefore this comparison is another indication that the combustion zone emissivity should be higher than values recommended earlier.

An additional area of concern is the generation and removal of aerosols in the test containment. The generation of aerosols is determined by the reaction rate and by the fraction of reaction products formed that become suspended in the containment atmosphere. Measurements at HEDL indicate that a maximum aerosol concentration of ~8 grams per cubic meter was achieved 65 minutes after combustion began. An estimate for the fraction of suspended particles may be made using the predicted combustion rate and knowledge of the containment volume, if aerosol removal is neglected. These estimated values range from one to six percent of reaction products evolved into the containment atmosphere. The removal rate of aerosols from the gas is a strong function of the internal geometry of the containment structure. A value for the HEDL test condition may be inferred from the observation that the aerosol concentration decreased to less than 0.001 grams per cubic meter after four days. This yields values of "BETA" that lie between 10^2 and 10^3 seconds. A sensitivity analysis of aerosol removal appears in the next section.

2.3. Sensitivity of LITFIRE to New Modeling

2.3.1. Sensitivity to Aerosol Removal

In LITFIRE, the mechanism for aerosol removal from the primary containment is an optional, highly idealized model and is a function of a single parameter for a given geometry. This parameter,

TABLE 2.4

Estimation of LA-4 "Combustion Zone" Temperatures

(Temperatures are approximate)

Time (Seconds)	Lithium Pool Aug. Temp. (°C)	Air Reaction Interface @5.08 cm 15.24 cm 30.48 cm (above Pool) (°C)	Estimated "C.Z." Temperature (°C)
0	(200 - 600)	165 150 125	~
600	650	400 350 200	> 800
1200	750	745 600 300	> 900
1800	900	780 630 315	~ 1200 - 1300
2400	975	780 620 310	~ 1200 - 1300
3000	1020	770 610 310	~ 1200 - 1300

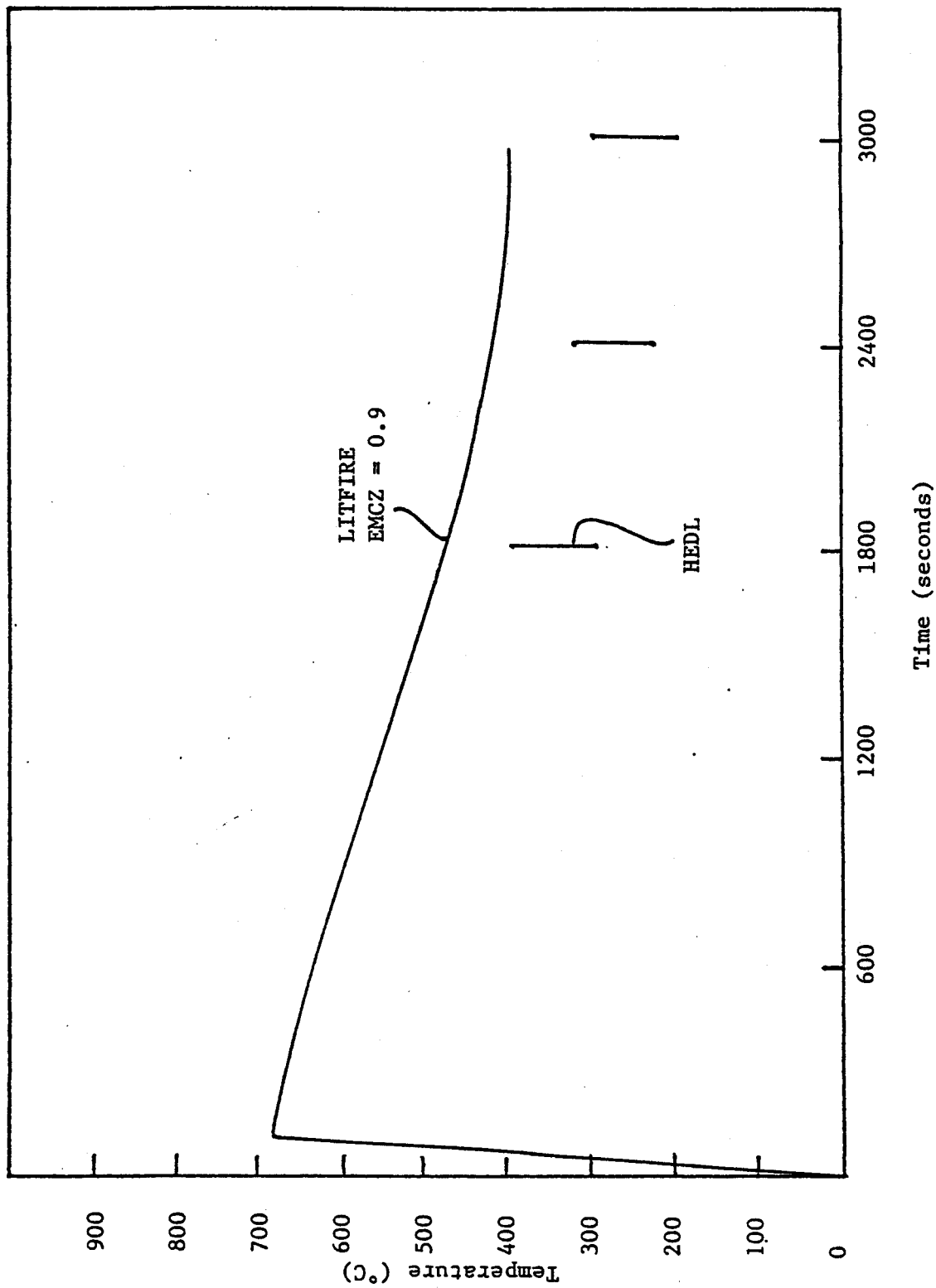


Figure 2.5: LA-4 "Combustion Zone" - Lithium Pool Temperature Difference

(BETA), is an input variable that represents the "sticking time" of the aerosol in containment. The sticking time is defined as the average time it takes for an aerosol particle near a wall to be removed from the cell gas. In LITFIRE, "near the wall" is assumed to be one inch. Therefore, the fraction of aerosols removed per second is equal to the fraction of aerosols within one inch of the wall divided by the sticking time. The removal of aerosols is assumed to take place in the primary cell only, since the concentration of aerosols in the secondary cell should be very small.

The major effect of aerosol removal is in the calculation of the primary cell gas emissivity, since

$$\text{gas emissivity} = C_1(1 - \exp(-C_2 \text{ aerosol})) \quad (2.4)$$

where C_1 is a user defined constant, and C_2 is a function of geometry, particle size, and path length.

It is possible that for sufficiently low values of BETA, a large fraction (or even all) of the aerosol in containment would be removed in a single time step. LITFIRE checks for this condition and reduces the time step accordingly, in order to insure numerical stability. In addition, program execution is terminated if the aerosol removal fraction is greater than unity.

Figures 2.6 and 2.7 show the sensitivity of the cell gas temperature and emissivity respectively, as a function of BETA. In these tests the maximum emissivity allowed was 0.04, a value recommended by Tillack [10] as best fitting the experimental data. The minimum value of the cell gas emissivity is 0.005 in order to insure numerical stability as well as allow some amount of radiative heat transfer to the cell gas. Although variations in BETA have a pronounced effect on the cell gas emissivity, the calculated effect on the cell gas temperature was negligible. This is due to the restricted maximum value that the cell gas emissivity was allowed to reach. To first order the heat transfer to the gas through the radiation channel is proportional to the cell gas emissivity. Therefore, it is possible that in cases where radiative heat transfer to the gas is the dominating heat transfer mechanism the temperature of the cell gas might be substantially more sensitive to changes in the aerosol removal rate.

2.3.2. Sensitivity to Combustion Zone Transmissivity

LITFIRE currently allows for the selection of combustion zone emissivity (EMCZ) and transmissivity (TAUCZ) separately. In allowing finite transmission through the combustion zone, Tillack [10] rederived the radiative interchange factors for the pool to the wall, cell gas, and combustion zone. In that work the value of $EMCZ \leq 0.1$ was recommended as best fitting the experimental data then available. Previously, Dube [1] indicated that the probable values for

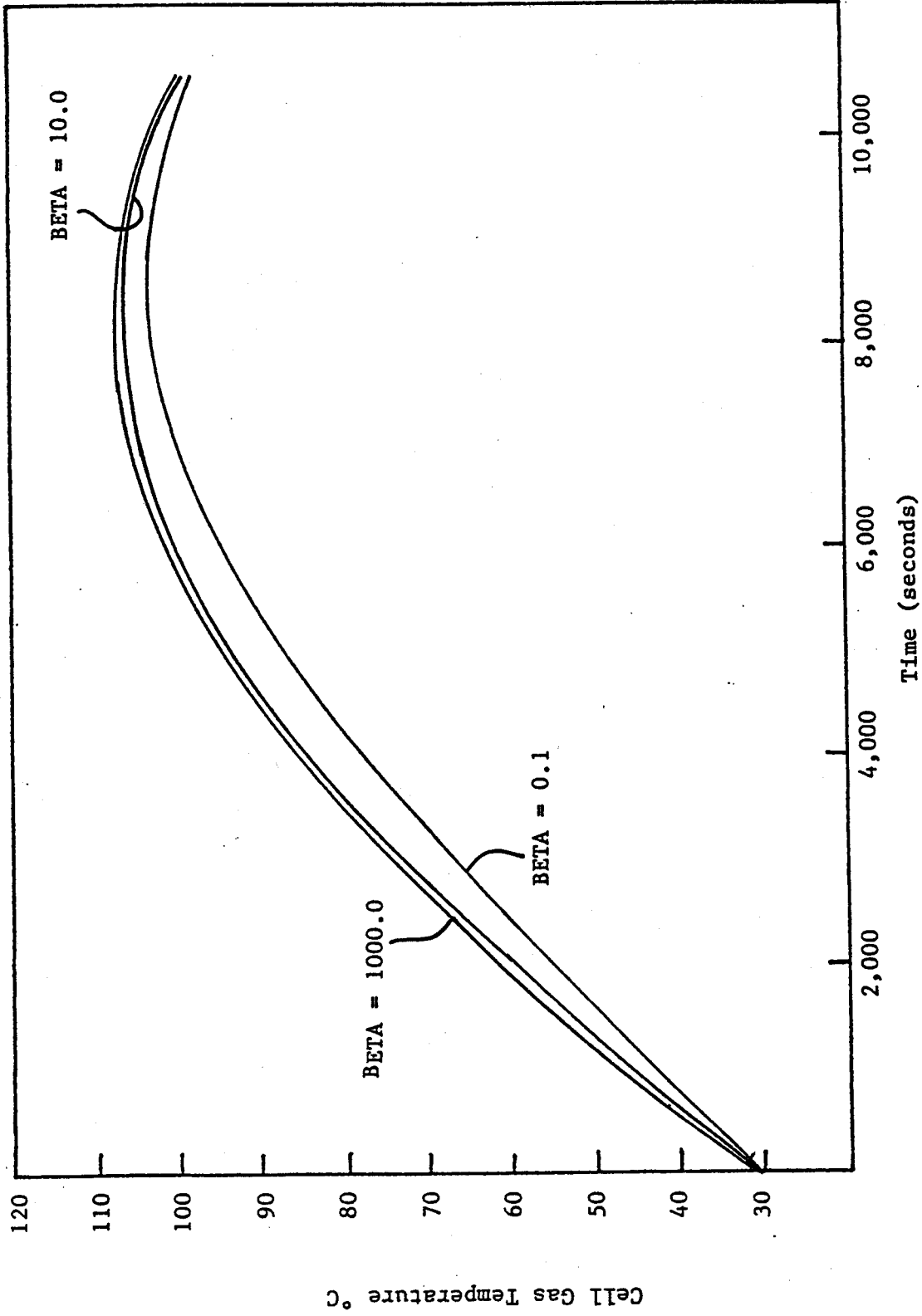


Figure 2.6: Cell Gas Temperature Sensitivity to Aerosol Removal

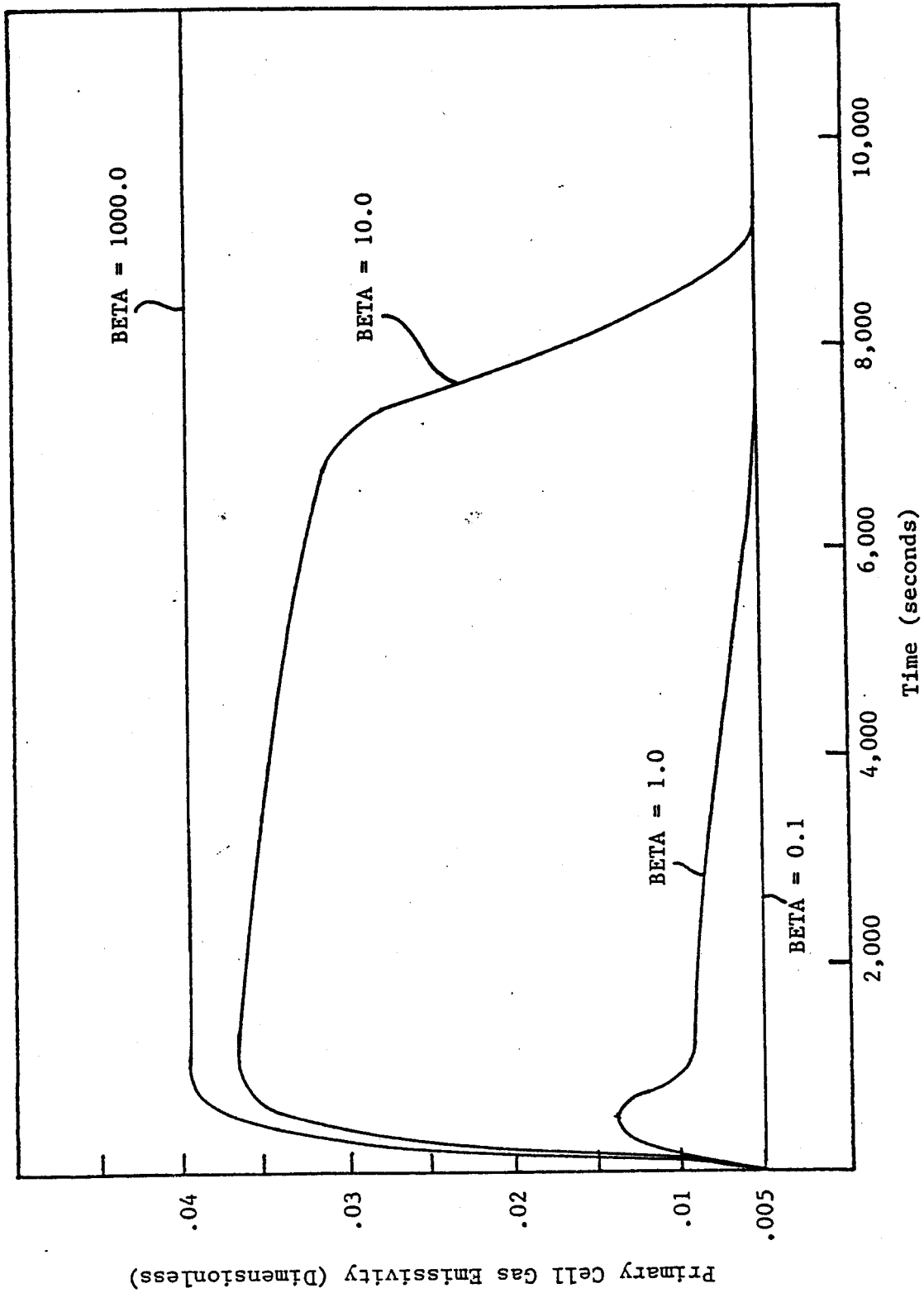


Figure 2.7: Cell Gas Emissivity Sensitivity to Aerosol Removal

EMCZ would lie in the range of 0.5 to 0.9. No mention was made of the appropriate value for TAUCZ except for the condition that, in general, $TAUCZ \leq 1-EMCZ$.

The bases for the comparison are the lithium pool and cell gas temperature profiles, since these are the two nodes that are most sensitive to a change in combustion zone transmissivity and emissivity. (Actually, the combustion zone itself is the most sensitive, but accurate temperature profiles for this node were not made during the HEDL tests.) Since the temperature profiles are more sensitive to changes in the emissivity than changes in transmissivity, the accompanying Figures (2.8 and 2.9) are given for the complete range of emissivities and only the maximum and minimum transmissivity that corresponds to each emissivity. At a given emissivity, the effect of increasing the transmissivity is to decrease the lithium pool temperature. This is due to the larger radiative interchange that is allowed between the pool surface and the gas and steel wall. This trend is seen to be valid at any value of the combustion zone emissivity. However, since the maximum allowed change in the transmissivity decreases as the emissivity is increased, the sensitivity to transmissivity at the higher emissivities is necessarily reduced. Increasing the transmissivity tends to increase the cell gas temperature at lower emissivities, and slightly reduced the cell gas temperature at higher emissivities. Since increasing the transmissivity always increases the radiative interchange between the pool and cell gas regardless of the combustion zone emissivity, the reduction in cell gas temperature must be a second order effect and is probably associated with lower radiative heat transfer from a slightly cooler combustion zone.

The figures indicate that higher emissivities fit the experimental data best. Therefore, the effect of variations in transmissivity are relatively small. The "best guess" values chosen for the present study are an emissivity of 0.9 and a transmissivity of 0.1. Several combinations of values brought the LITFIRE predictions within close agreement to experiment. An additional criterion in choosing the present set was an upper limit applied to the maximum combustion zone temperature. This had been measured in earlier experiments to be about 1260°C.

The results of these comparisons are in disagreement with the recommendations put forth by Tillack [10], and more in agreement with the original indications made by Dube [1]. Tillack's suggestion was based on the expected increased coupling between the pool and combustion zone temperatures after the combustion zone transmissivity model was incorporated into LITFIRE. In point of fact, this coupling did not occur in the LITFIRE calculations because the net effect of reducing the emissivity was to reduce the radiative heat transfer between the pool and combustion zone. This heat transfer pathway is proportional to the temperature difference to the fourth power while that of conduction varies linearly with temperature difference. Even with the higher conductance to the pool, the net effect of lowering the emissivity of the combustion zone is

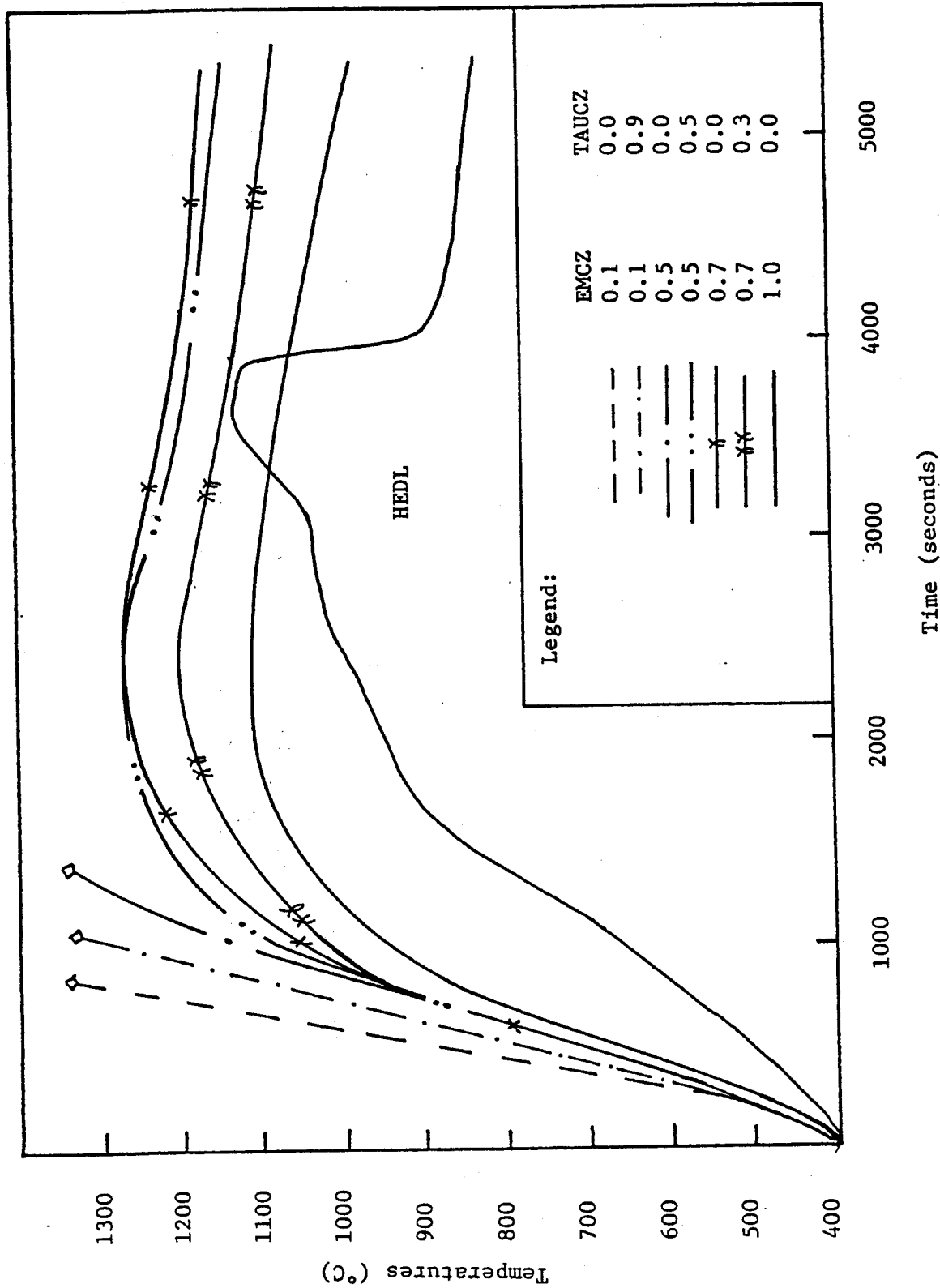


Figure 2.8: Lithium Pool Temperatures LA-5 for Various EMCZs

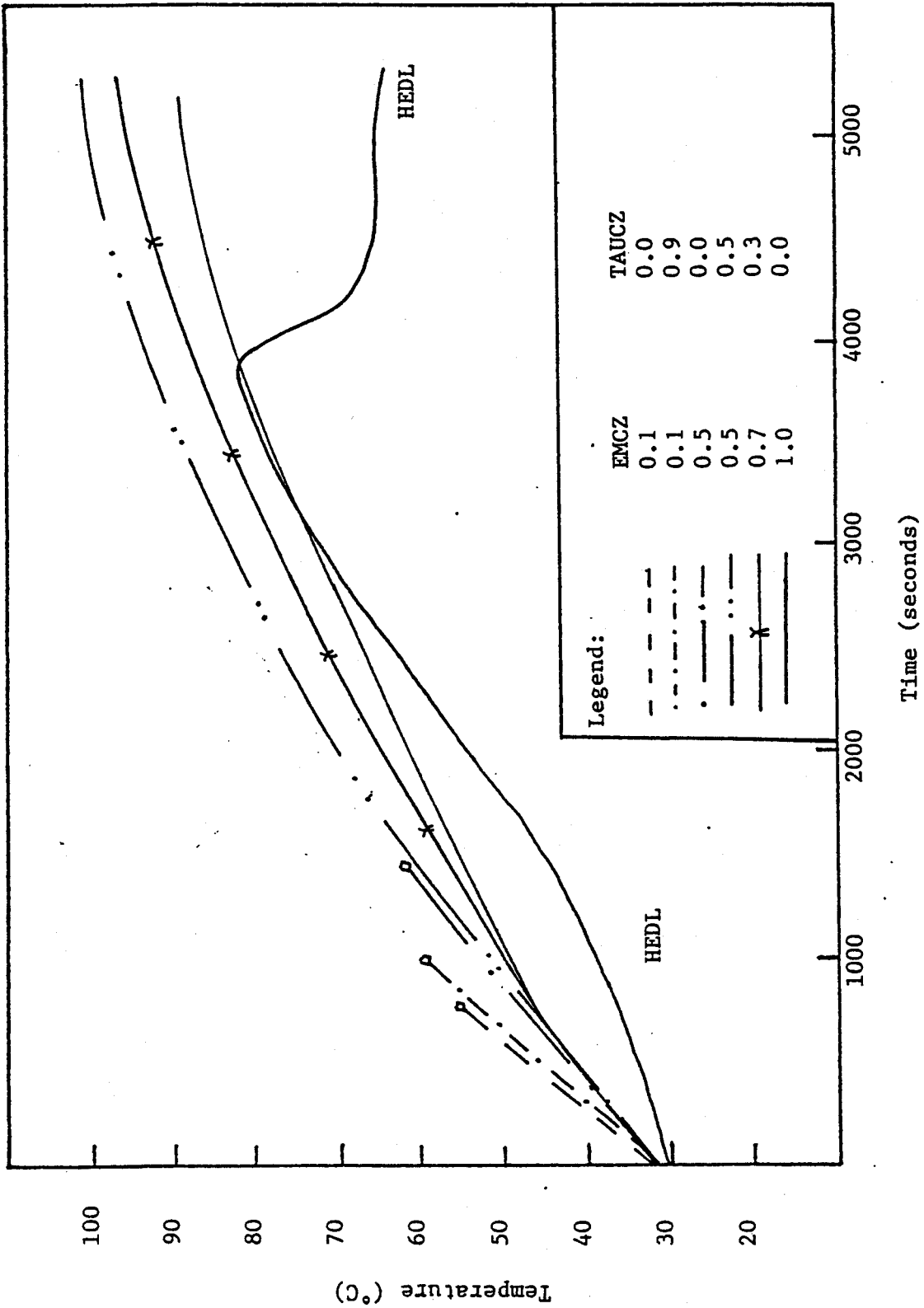


Figure 2.9: LA-5 Cell Gas Temperature Sensitivity to EMCZ

to dramatically increase the combustion zone temperature. Figure 2.10 shows the maximum temperature difference between the pool and combustion zone generated by LITFIRE, for various values of the combustion zone emissivity.

The recommendations of Tillack [10] were also based on fitting LITFIRE predictions to experimentally obtained data so a comparison between that data and the present predictions of LITFIRE might indicate the magnitude of the discrepancy. This comparison is shown in Figures 2.11 and 2.12 and includes data from HEDL test LA-2 which is described in detail by Tillack [10]. Also included are the predictions by LITFIRE using values for emissivities and transmissivities recommended above and also those suggested by Tillack [10].

2.4. Analysis of a Lithium Spill in UWMAK-III

The original purpose of LITFIRE was to predict the consequences of lithium fires in commercial size reactor containments. The agreement between LITFIRE and small scale experiments is encouraging but should not be used as concrete evidence that larger spills and fires will be accurately modeled.

2.4.1. Description of UWMAK and LITFIRE Geometries

The prototypical fusion reactor chosen by Dube [1] for his analysis was the UWMAK- III design of which the containment building is shown in Figure 2.13. Dube [1] published a sensitivity analysis of the relevant parameters for modeling large fires and proposed a base set of parameters as a best guess at predicting the consequences of large fires. This base case is retained for the present modeling with notable exceptions being the concrete nodal distribution and the presence of an extraneous heat capacity. In addition, the coefficients for convective heat transfer were obtained from Tillack's [10] recommendations. The value of the combustion zone emissivity (EMCZ) is 0.9, representing the best guess of the present study. The aerosol removal option (including BETA) was not used in these test cases. None of the options for mitigating the effects of lithium fires were employed in order to make a conservative best estimate. These safety features were found to have significant affects and are discussed in detail in reference [1].

2.4.2. Prediction of Lithium Fire Consequences

The results of this calculation are plotted in Figure 2.14. The reaction stopped ~3850 seconds after ignition because the lithium pool was depleted. Although there should not be any lithium left after this time, LITFIRE requires that a certain amount of lithium exist in the pool node in order to have a finite thickness and insure numerical stability. Thus, LITFIRE artificially constructs a pool node after this time but "knows" that there is no combustible lithium remaining. Therefore, the primary steel floor is still "covered" by the lithium pool and does not interact thermally with

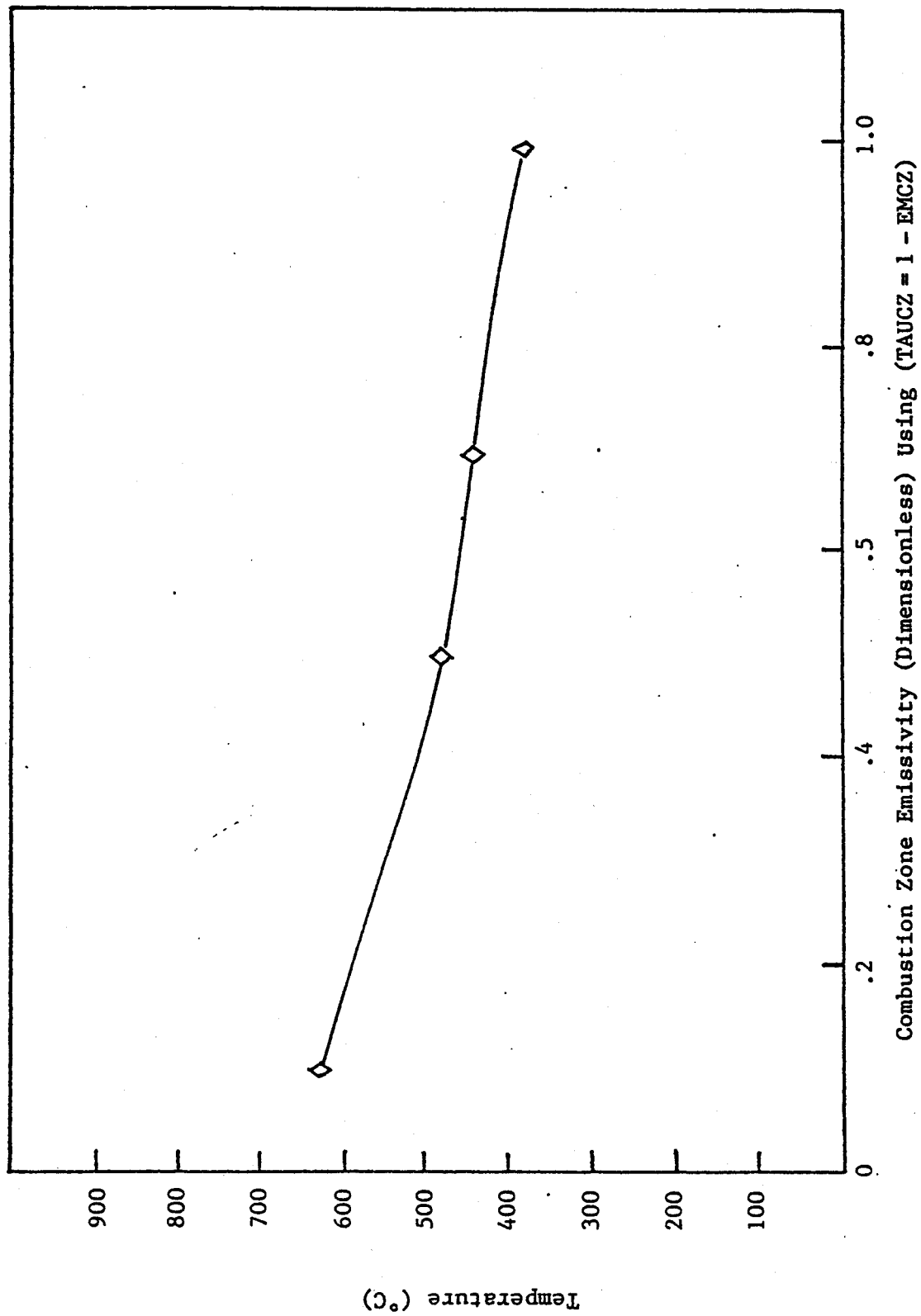


Figure 2.10: LA-5 Maximum Pool-Combustion Zone Temperature Difference

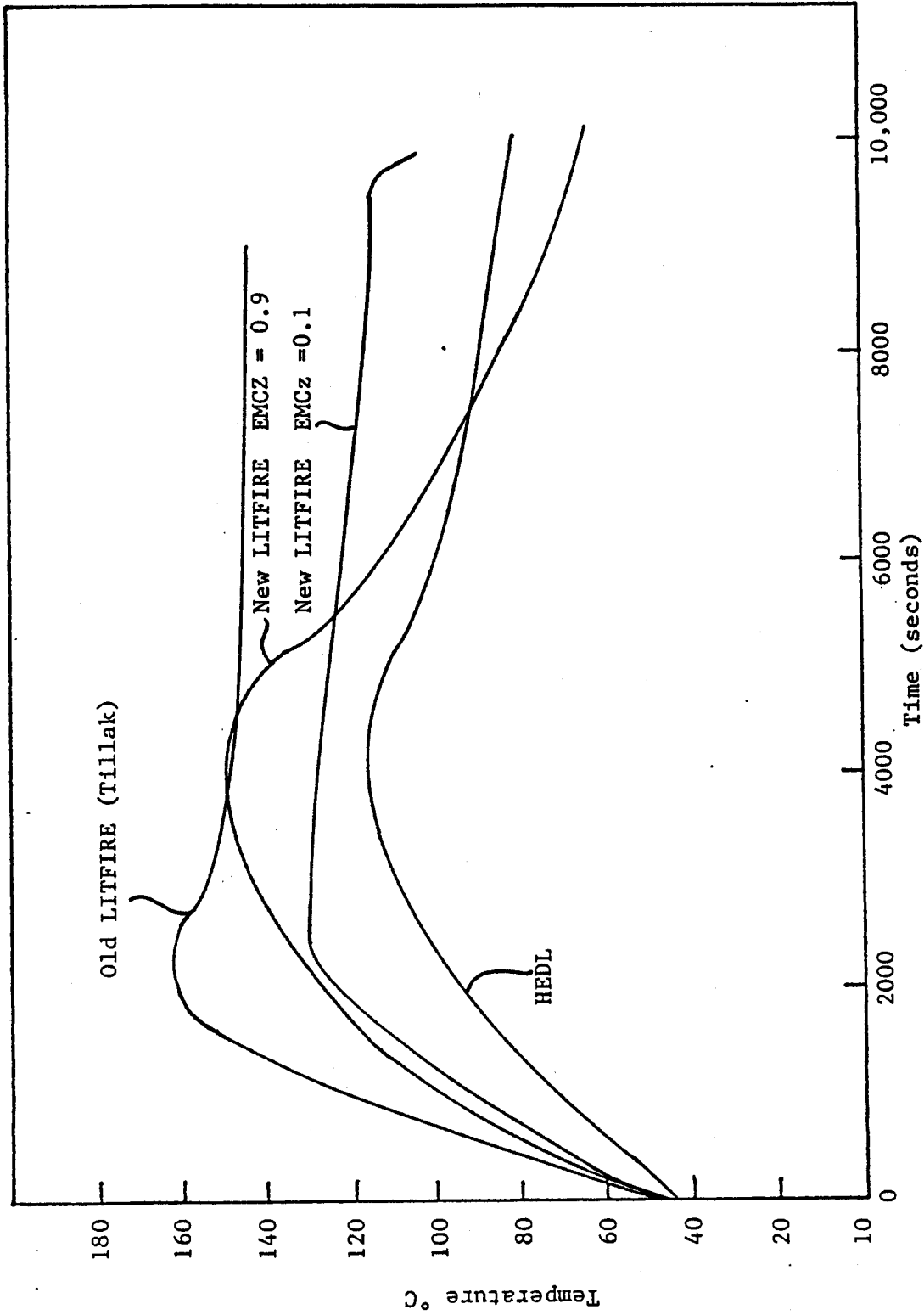


Figure 2.11: LA-2 Comparison between Present and Tillack Cell Gas Temperature

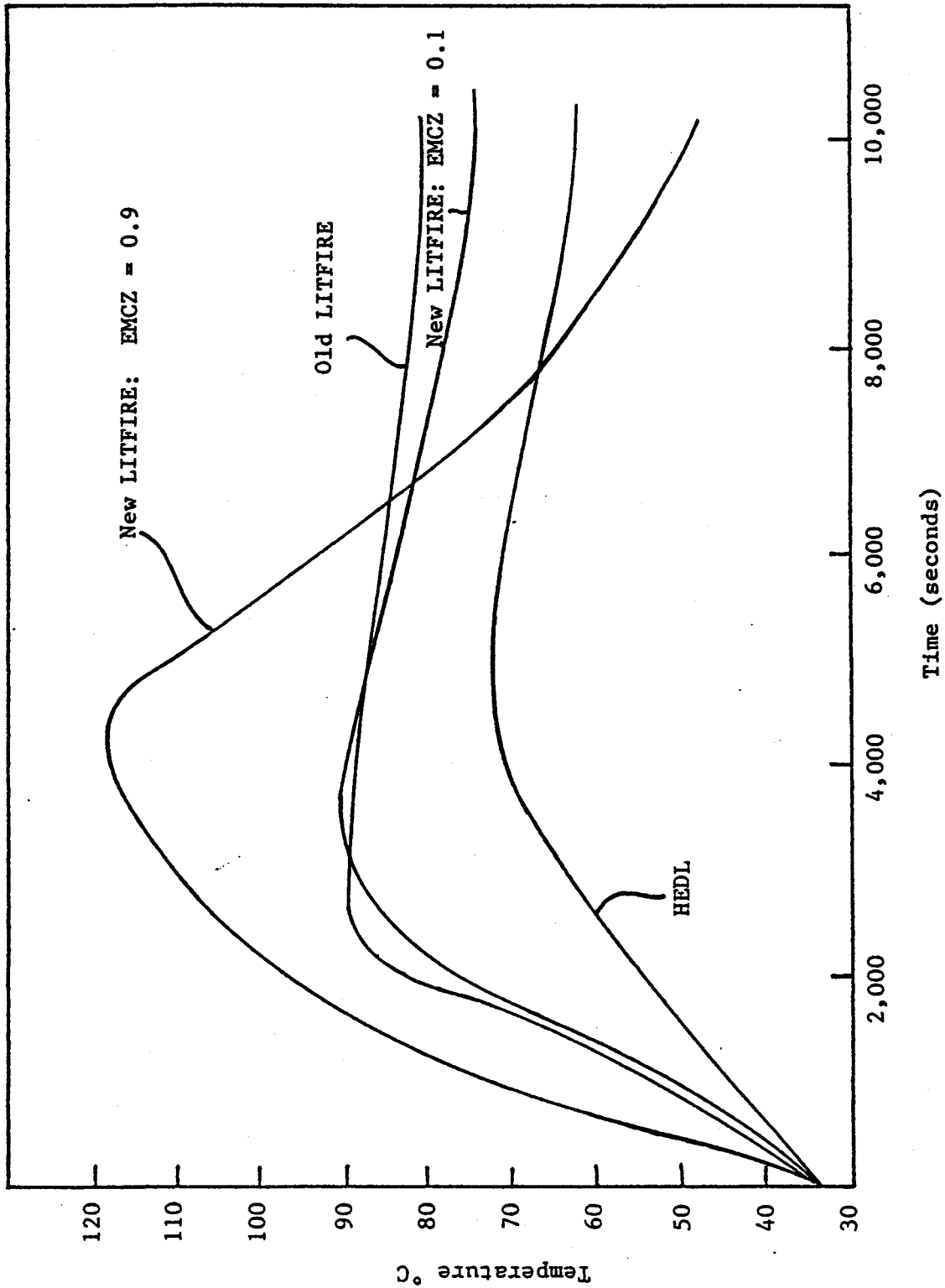
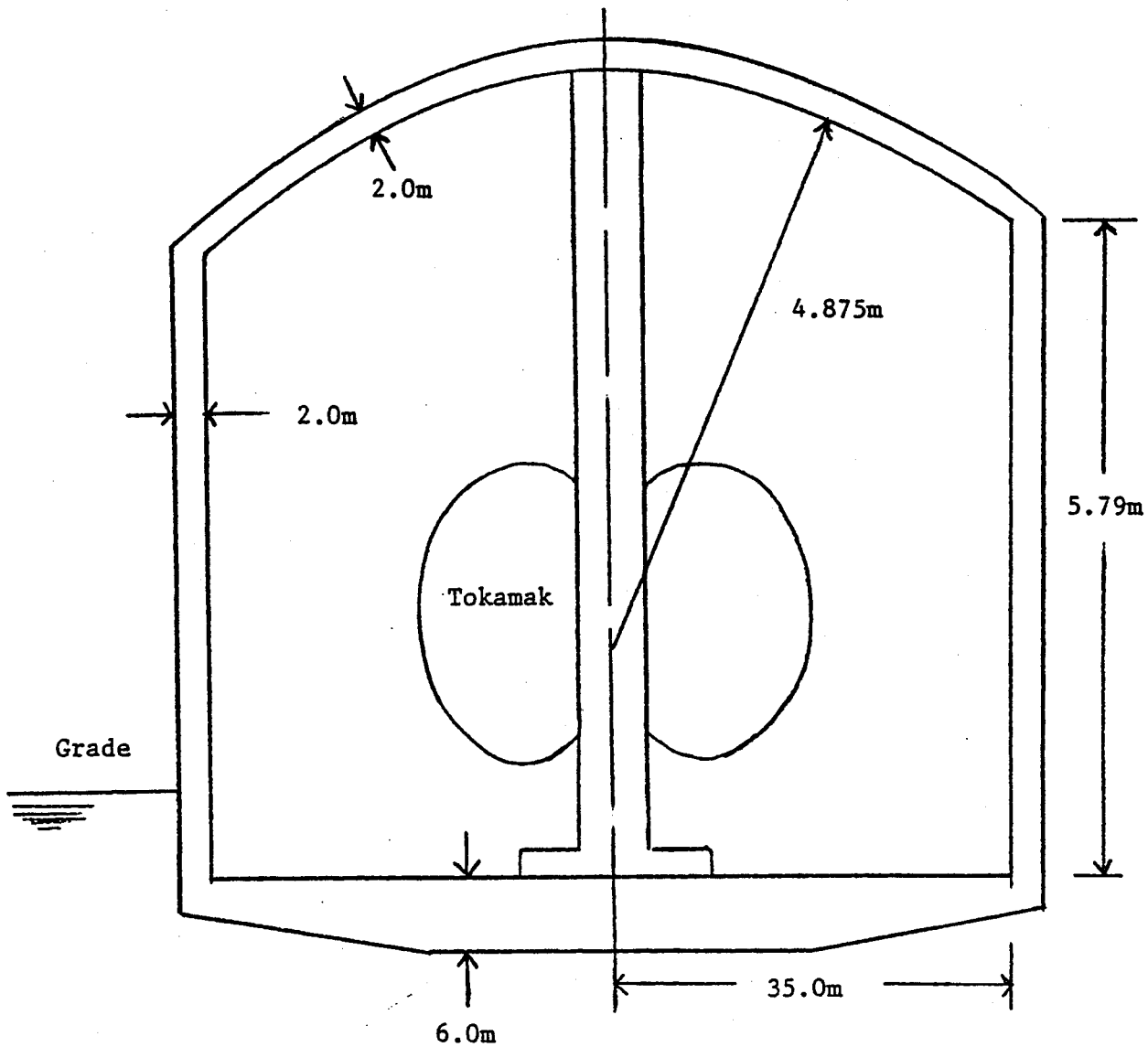


Figure 2.12: LA-2 Steel Vessel Temperature



Total Floor Area	3860m ²
Total Volume	250725m ³
Wall Area	17050m ²
Total Lithium Mass	396000kg
Lithium Spilled	22000kg
Ambient Temperature	25.9 °C
Initial Pressure	.101 MPa

Figure 2.13: Cross Section of UWMAK-III Primary Containment Building

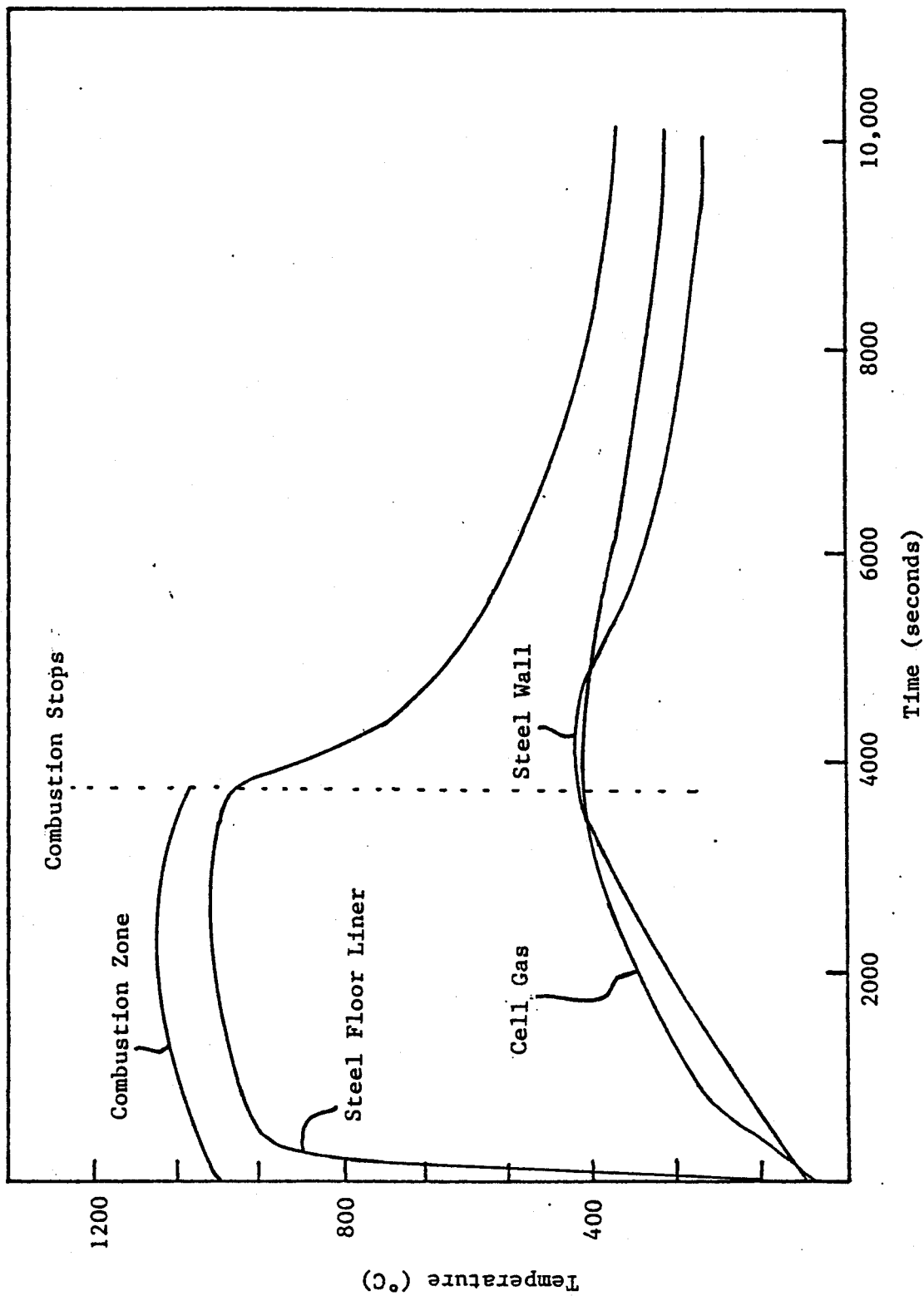


Figure 2.14: UWMK-III Containment Thermal History Using Present Version

the primary cell gas directly. This should not radically alter the primary cell gas since the thermal conductivity of the lithium is very high and the thickness of the phantom pool node is small.

Even though the containment atmosphere and structures are much larger than in the HEDL experiments, the predicted consequences are much more severe. This is primarily due to the large surface area of the lithium pool in the UWMAK prediction. Since the reaction rate is proportional to surface area, the reaction burned to completion in about one hour, during which time very little heat was transferred to ambient. Lithium fires with smaller surface areas (and smaller primary containment volumes as well) are discussed in the next chapter.

2.4.3. Comparison with Previous Predictions

The consequences of large scale lithium fires were predicted by Dube using a version of LITFIRE that is different than the one used here. Figures 2.15 and 2.16 give the current LITFIRE prediction using the parameters suggested by Dube. The dashed lines are the combustion zone and cell gas temperature profiles that were published in 1978. This has been included to show the direction that the "improved" model has taken with respect to consequences as well as to gain a feel for the sensitivity of LITFIRE to all of the recent changes simultaneously. There is a discrepancy between the heat of vaporization of lithium that was used by Dube and the known value. The one used in the present LITFIRE calculation is correct. One important observation from these comparisons is that the severity of the predicted consequences is not a strong function of the combustion zone emissivity. The range in combustion zone emissivity was from 0.1 to 0.9 while the maximum combustion zone temperature varied from 1120°C to 1265°C. This indicates that very large spills are less sensitive to this parameter than the predicted sensitivity for the smaller tests at HEDL (see Section 2.3.2).

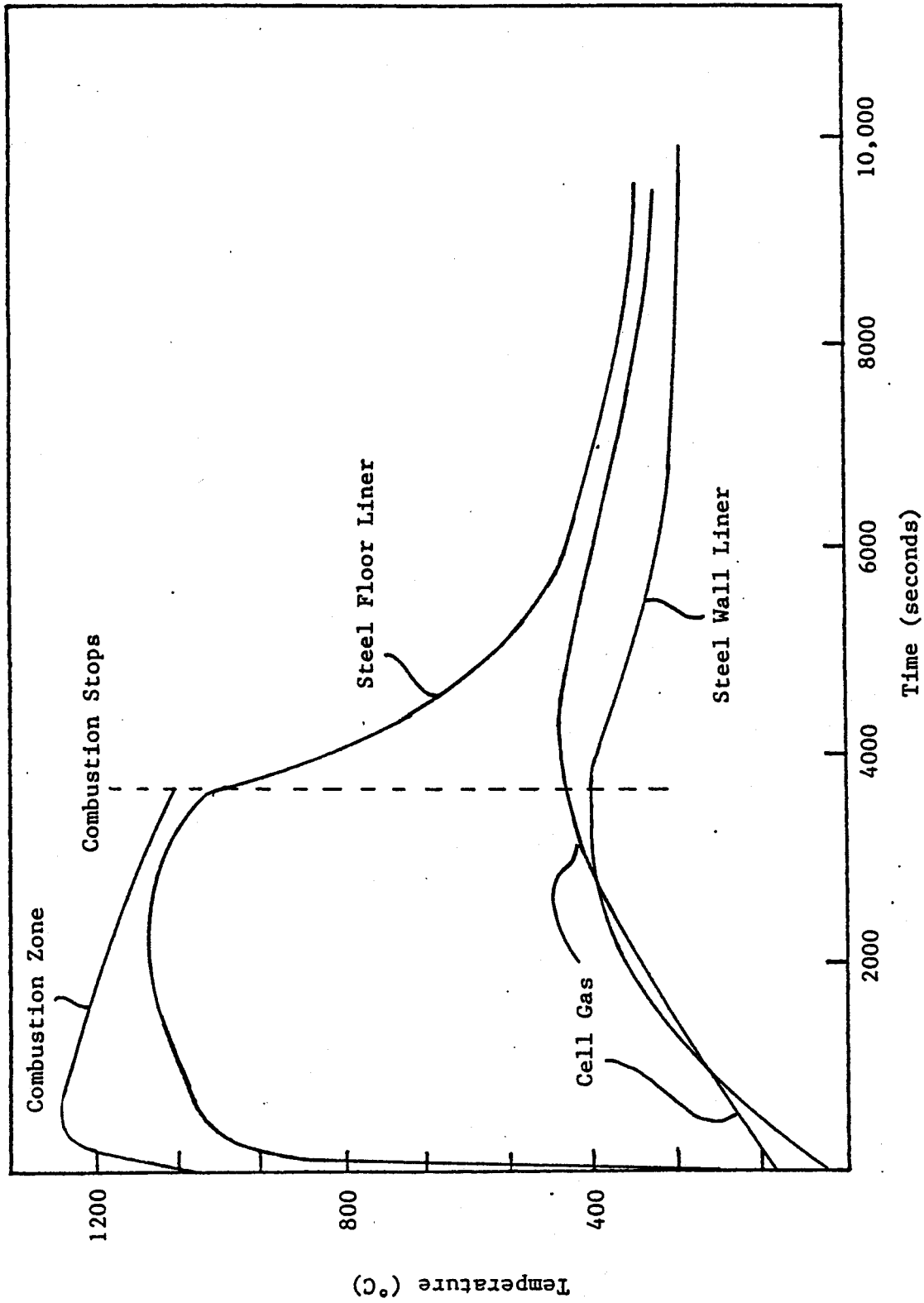


Figure 2.15: UWMK-III Predictions Based on Dube's Parameters

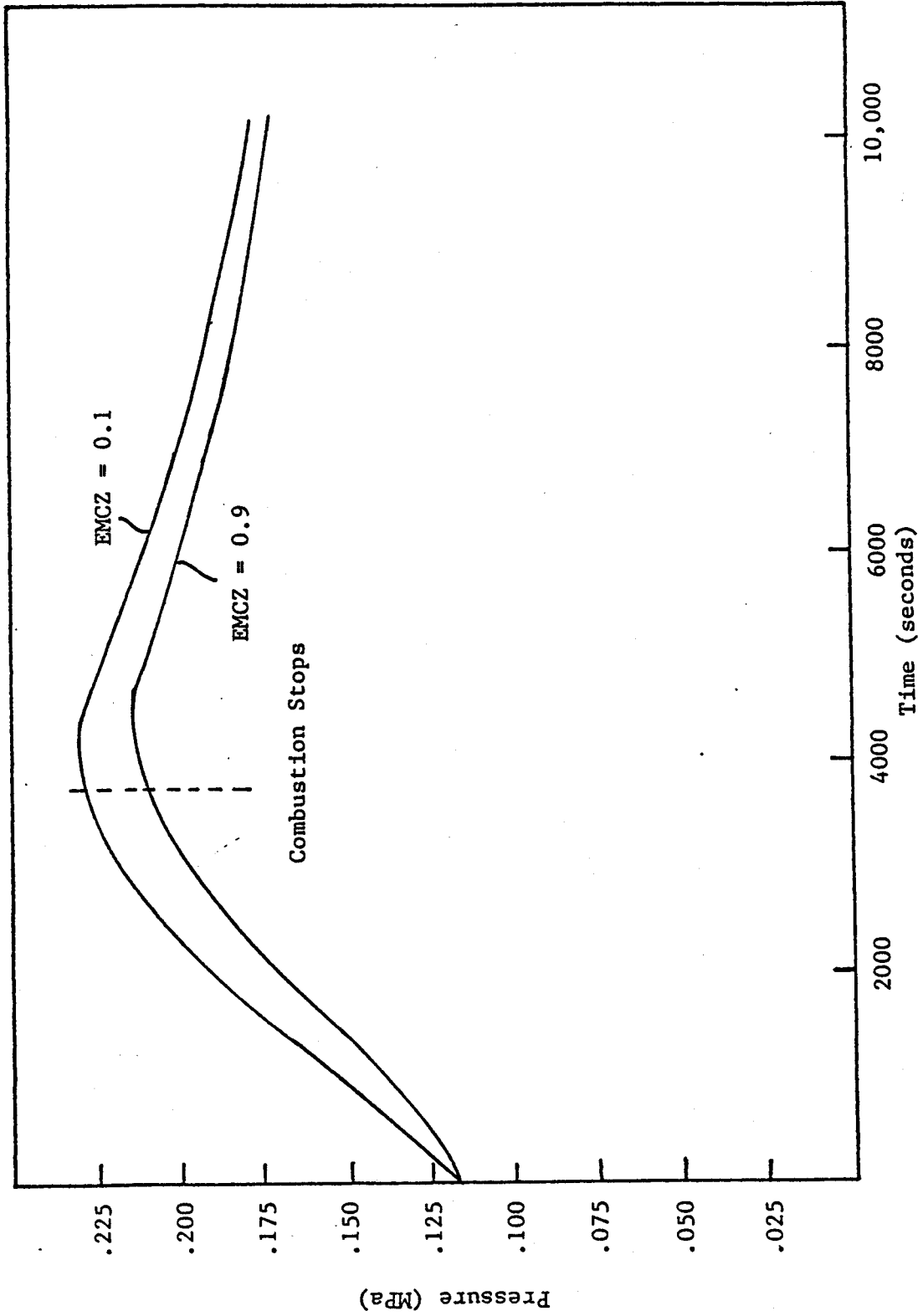


Figure 2.16: UWMK-III Cell Gas Pressurization History

3. DEVELOPMENT AND APPLICATION OF TWO-CELL LITFIRE

3.1. Motivation for Development of Two-Cell LITFIRE

The optional two cell formalism in LITFIRE was developed in order to more accurately model fusion related components and geometries. Typically the code could be used to model lithium fires contained in one cell, with mass and heat transfer allowed between the two cells. Such configurations could represent a fire in a torus (of a tokamak), in a coolant pipe, or in the inner cell of a double containment. Limiting the combustion to a smaller cell might reduce the consequences of lithium combustion because less combustible gas would be immediately available for reaction with the lithium. However, significant changes in the combustion time history might occur if a breach of the primary containment occurred.

The two-cell LITFIRE geometry was designed to be compatible with the existing one-cell model and is shown in Figure 3.1. No new heat transfer mechanisms within the primary containment were added and the only new mass transfer mechanism is the allowance for the breach of the primary steel liner (herein referred to as "crack") permitting exchange of the cell gases.

It should be noted that several changes to the LITFIRE program that are especially important in two cell applications have been made since the two cell formalism was introduced by Tillack [10]. Principally these are:

- Incorporation of separate floor nodes for the primary and secondary cells.
- Removal of the concrete nodes attached to the primary steel floor.
- Allowance for different properties in each wall and floor node of inner and outer cells.
- Allowance for different emissivities for each wall and floor node.
- Inclusion of radiative and convective heat transfer from primary containment to secondary as well as separate gas convection coefficients for the wall and floor nodes.
- Allowance of gas flow through crack to cease during run if pressures equate in order to reduce computation time.

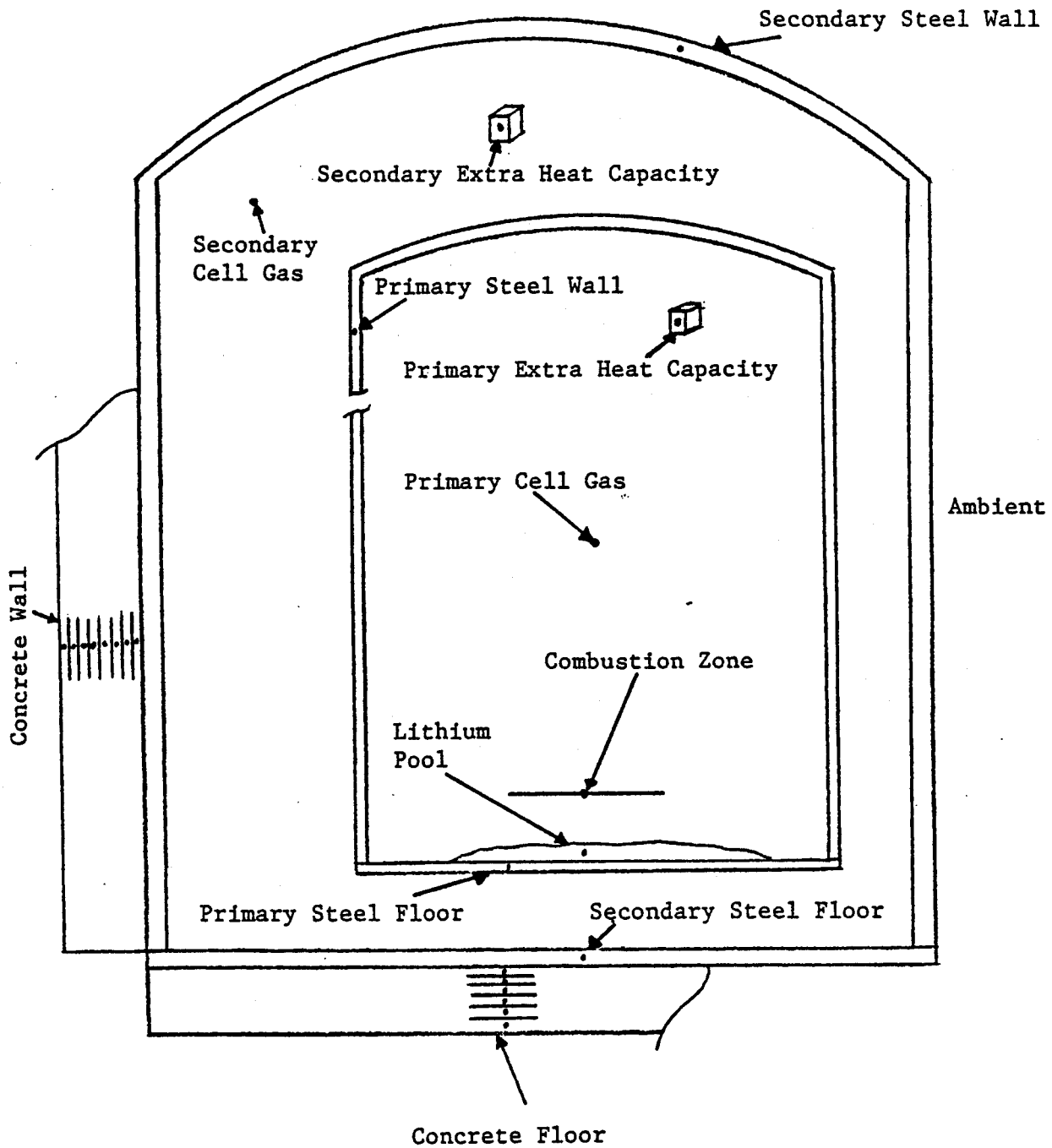


Figure 3.1: Litfire Two Cell Geometry and Nodal Structure

3.2. Model Description

3.2.1. Two-Cell Geometry

The geometry of the two cell LITFIRE model is an extension of the one cell model. All options and nodes present in the one cell version of LITFIRE are incorporated in the two cell formalism. In the idealized description of the two cell geometry (Figure 3.1) it can be seen that the combustion zone and pool are not directly affected by the presence of an outer containment cell. There are new radiative and convective heat transfer pathways between the primary wall and floor nodes to the secondary gas, floor, and wall nodes. The concrete is only permitted around the outer cell steel wall and floor. No allowance was made for concrete around the primary cell wall since the conductivity of concrete is relatively low. Therefore heat transfer between the concrete and ambient or a secondary cell gas would be expected to be very much the same and this setup can be adequately modeled by the existing one cell version of LITFIRE. An important consequence of this exclusion is that there is only a single structural node between the primary and secondary cell gases which can be an important limitation in modeling real systems.

In order to increase the flexibility of the two cell calculation without adding nodes to the present structure, each of the existing structural nodes is allowed to have unique physical properties, thicknesses, emissivities, and convection coefficients. (This is not true for the concrete nodes which are only allowed to vary in their relative thickness.) Since these are all user defined parameters, LITFIRE can mock simple heat flows with various sinks and/or obstructions. For example, the primary steel floor can be "insulated" from the secondary cell (but not the primary) by choosing appropriately low emissivity and convective coefficients.

Another interesting feature allowed by the addition of the secondary cell is the ability to have different atmospheres (and pressures) in the primary and secondary cells. One application of this would be an inert inner cell enclosed in a larger containment of air (or any gas mixture of nitrogen, oxygen, water vapor, and inert gases) at a higher pressure. Such a setup has been proposed for the main containment of the STARFIRE reactor. Another obvious application is the modeling of two cells at different pressures, e.g., a vacuum torus enclosed by a pressurized containment. This application of LITFIRE is discussed in Section 3.4.

The simplicity of LITFIRE is characterized by the single node allotted to each of the secondary cell components. The secondary cell gas, like the primary gas, is assumed well mixed and uniform in temperature. All the internal temperature gradients of the secondary cell structural materials are neglected. This can be a rather crude set of assumptions but the actual temperature gradients that might be generated in the secondary cell will most likely be much smaller than those in the primary cell, which is already characterized by a single, one-dimensional nodal structure.

3.2.2. Explanation of Two-Cell Gas Exchange

The geometry of LITFIRE includes an idealized orifice in the sense that the crack between the two cells has no length and there are no associated pressure and friction losses due to the flow. The inertia of any gas that would be inside a real orifice is neglected and as a result the flow can change directions instantaneously. The flow rate is obtained by using the relation for simple orifices,

$$\frac{dm}{dt} = C_d A \sqrt{2 g_c \rho \Delta P} \quad (3.1)$$

where

$\frac{dm}{dt}$ = mass flow rate

C_d = coefficient of discharge (unity in LITFIRE)

A = area of orifice .

g_c = dimensional constant $(32.2 \frac{\text{lb}_m \text{ ft}}{\text{lb}_f \text{ sec}^2})$

ρ = gas density

ΔP = pressure drop between cells

The validity of Eq. (3.1) is subject to the following restriction,

$$\frac{P_{\text{high}}}{P_{\text{low}}} \leq \left(\frac{\gamma + 1}{2} \right)^{\frac{2}{\gamma - 1}} \quad (3.2)$$

$$\leq 1.89 \text{ for air,}$$

where the constant γ is the ratio of specific heats C_p/C_v . For larger pressure drops the flow becomes sonic, and the flow rate is calculated according to

$$\frac{dm}{dt} = C_d A \sqrt{0.94 g_c \rho P} \quad (3.3)$$

where P is the higher of the two cell pressures. Therefore, LITFIRE can track sonic or subsonic flow, into or out of, the primary cell.

The mass that is transferred between the cells represents the same homogeneous mixture (if more than one constituent is present) of gases that characterizes the cell of the higher pressure. It is therefore possible, given high enough exchange rates, to have a significant alteration of the cell gas compositions if they were initially different. This also permits aerosols generated by the combustion of lithium to appear in the outer cell gas. Since these aerosols are corrosive, structural damage to the outer containment cell may occur if they appear in sufficient quantities. LITFIRE

monitors the individual aerosol species in both cell gases. A major assumption implicit in the flow calculation is that mass transfer by diffusion due to a concentration gradient is negligible and is ignored. This assumption may not be valid for large crack sizes when the cell pressures are nearly equal and are of significantly different composition. As a result, the mass transfer through large cracks may not be accurately modeled by LITFIRE. Although there is no correlation indicating what may constitute a "large" crack, Section (3.2.3) describes a limit to the usable crack size due to numerical considerations.

The temperatures of both cell gases will change as a result of the flow due to the convection of the gases at different temperatures. In addition, the associated expansion (or compression) of the cell gas due to the flow will give rise to a temperature change. Using the method of forward differencing, Tillack [10] performed an energy balance on the system shown in Figure 3.2 which is reproduced below:

$$\text{Let } \frac{dT}{dt} = \frac{T_{n+1} - T_n}{\Delta t} \quad (3.4)$$

Applying conservation of energy yields

$$\text{final energy} = \text{initial energy} + \text{energy added} \quad (3.5)$$

$$m_{n+1}U_{n+1} = m_nU_n + (\chi\Delta t)h_n \quad (3.6)$$

where the variables are as indicated in Figure 3.2. Applying this condition to each cell,

$$(m_n^{(1)} - \chi\Delta t)C_vT_{n+1}^{(1)} = m_n^{(1)}C_vT_n^{(1)} - (\chi\Delta t)C_pT_n^{(1)} \quad (3.7)$$

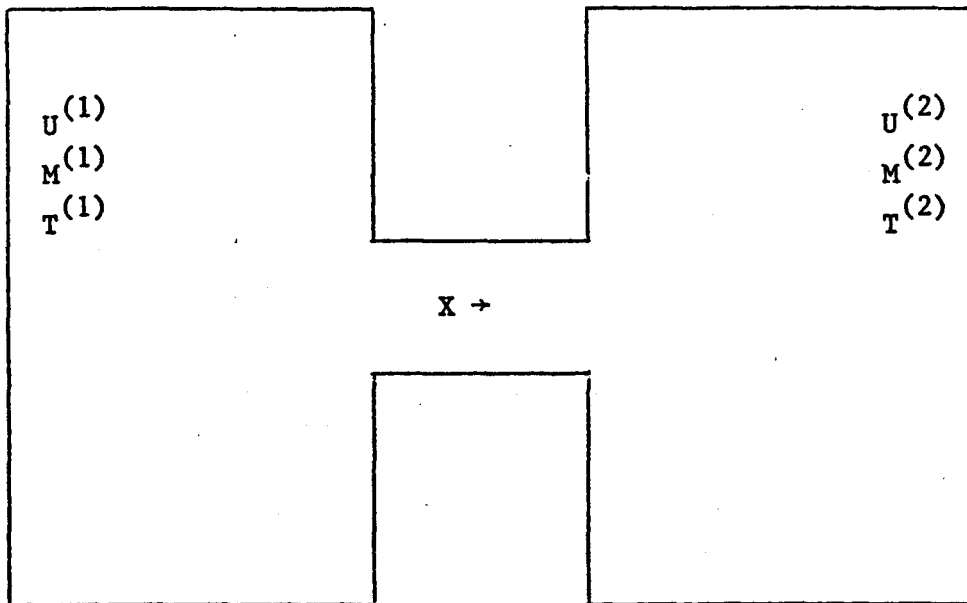
$$(m_n^{(2)} + \chi\Delta t)C_vT_{n+1}^{(2)} = m_n^{(2)}C_vT_n^{(2)} + (\chi\Delta t)C_pT_n^{(1)} \quad (3.8)$$

using $\gamma = C_p/C_v$ (assumed independent of temperature) and some algebraic manipulation, the following expressions for the temperature change result

$$\frac{dT^{(1)}}{dt} = \frac{\chi(1 - \gamma)T_n^{(1)}}{m_n^{(1)} - \chi\Delta t} \quad (3.9)$$

$$\frac{dT^{(2)}}{dt} = \frac{\chi(\gamma T_n^{(1)} - T_n^{(2)})}{m_n^{(2)} + \chi\Delta t} \quad (3.10)$$

These expressions are compatible with the LITFIRE integration method since they refer only to the values for the temperature ($T_n^{(i)}$), and mass ($m_n^{(i)}$) at the previous time step.



$U_n^{(i)}$ = internal energy of cell i at time t_n .

$M_n^{(i)}$ = Mass of all gases and aerosols in cell i at time t_n .

$T_n^{(i)}$ = Temperature of gas in cell i at time t_n .

X = Mass flow rate

Δt = integration time step.

(Note: mass flow rate is assumed constant during a single time step.)

$$h_n = T_n c_p$$

Figure 3.2: Two Cell Energy and Mass Balance Diagram

3.2.3. Coding Changes Required for Numerical Stability

In order to insure numerical stability in the calculation of mass exchange between the primary and secondary cells, several checks have been incorporated into LITFIRE. One numerical instability is due to the possibility of an oscillatory solution to the flow rate calculation having a period of the same magnitude as the integration time step. This can cause a discrepancy between the indicated flow direction and the mass buildup of the cell gases. For example, a test case was run where the flow was continually out of the primary yet the mass of nitrogen in the primary cell was increasing in time. The inconsistency is due to the fact that within the integration looping itself, the flow is changing directions with each integration time step. Since there are an even number of integration time steps per "real" time step the flow always appears in the same direction. For such a mechanism to occur the change in pressure drop ΔP in a single time step must be equal to the pressure drop. Applying the equations developed in Section 3.2.2 above, as well as the ideal gas relations

$$P^{(1)}V^{(1)} = m^{(1)}RT^{(1)}, \quad P^{(2)}V^{(2)} = m^{(2)}RT^{(2)} \quad (3.11)$$

results in the following restriction on the integration time step (Δt),

$$\Delta t \leq \frac{C_1 V^{(1)} \sqrt{\Delta P}}{A \sqrt{P^{(1)}}} \quad (3.12)$$

by requiring that the change in the pressure difference $\Delta(\Delta P)$ across a single integration time step must be equal to the pressure difference (ΔP) itself.

$$\frac{\Delta(\Delta P)}{\Delta t} = \Delta P \quad (3.13)$$

C_1 is a constant for a given geometry and small variation in the temperature over a single time step and A is the area of the orifice.

There are two regimes of interest for Δt . The first is when the cell pressures are nearly equal requiring Δt to be small in order to insure stability. The second regime is in the presence of a "large" orifice, A , which also requires that Δt be small. In principle Δt can be made arbitrarily small, but in practical terms a lower limit on Δt is necessary in order to consume finite computational time. Fortunately both these regimes are not critical for modeling flow calculations in the sense that cell gas dynamics will be relatively unaffected at low pressure differentials and large cracks almost imply that a single cell calculation would be just as applicable. As a result, LITFIRE now has the user specified option of closing the orifice after a predetermined amount of "real" time if the cell pressures equilibrate to within one part in ten thousand.

3.3. Comparison of One and Two Cell Results for HEDL Test LA-4

Figure 3.3 shows the predicted steel wall temperature for HEDL test LA-4, for both a one cell and two cell geometry. No orifice existed between the cells and the secondary volume was very large to approximate the infinite ambient environment implicit in the LITFIRE code. This node was found to be the most sensitive to this change in geometry due to its direct contact with ambient in the one cell version. The agreement between the two versions is within four percent (up to about 10,000 seconds after ignition). The discrepancy is probably due to a small amount of heating of the secondary cell gas, thus reducing slightly the convective heat transfer to that node from the steel wall.

3.4. Effect of Crack Size on Lithium Fires in a Two-Cell Geometry

A study was performed on the sensitivity of lithium fire consequences in a full scale reactor to the crack size in the steel wall separating the two cells. Since UWMAK-III had been the basis for earlier studies (see Section 2.4) it was retained as the reactor of interest in the present calculation. The major change for this comparison is that the lithium fire is contained in the torus of the reactor (inner cell of LITFIRE) and the secondary containment in UWMAK has become the outer cell for LITFIRE. The spill sizes are approximately the same (~22,000 kg. Li) though the thickness of the pool in the torus is much greater due to the smaller surface area available.

Both cells were initially at atmospheric pressure and contained identical concentrations of oxygen and nitrogen. The volume of the inner cell was approximately three percent of the volume of the outer containment cell. The crack size was varied between 0.0 and 100.0 square centimeters. Above 100 square centimeters the two cells act as one large cell since the communication between the cells limits the maximum pressure difference to less than a few percent. Table 3.1 lists the main combustion characteristics for various crack sizes. Figures 3.4 and 3.5 show the temperature and pressure history for a typical two cell calculation (crack size = 1.0 cm²) and give an idea of the dynamic effect of a breach of containment. Figure 3.6 gives the temperature profiles for structural components in the inner cell and the lithium pool. The first and second maxima in the temperature and pressure plots (Figures 3.7 and 3.8) were taken at the points indicated by the arrows in Figures 3.4 and 3.5. In this application the outer cell was large enough that the maximum change in pressure was less than eight per cent regardless of the crack size. However, the temperature rise in the outer cell was substantial (up to 90°C) for the larger crack sizes. The maximum outer cell temperature as a function of crack size is plotted in Figure 3.9.

For crack sizes below 1.0 cm² the flow was almost always into the inner cell due to the underpressure from gas consumption in combustion. Therefore there was no buildup of reaction

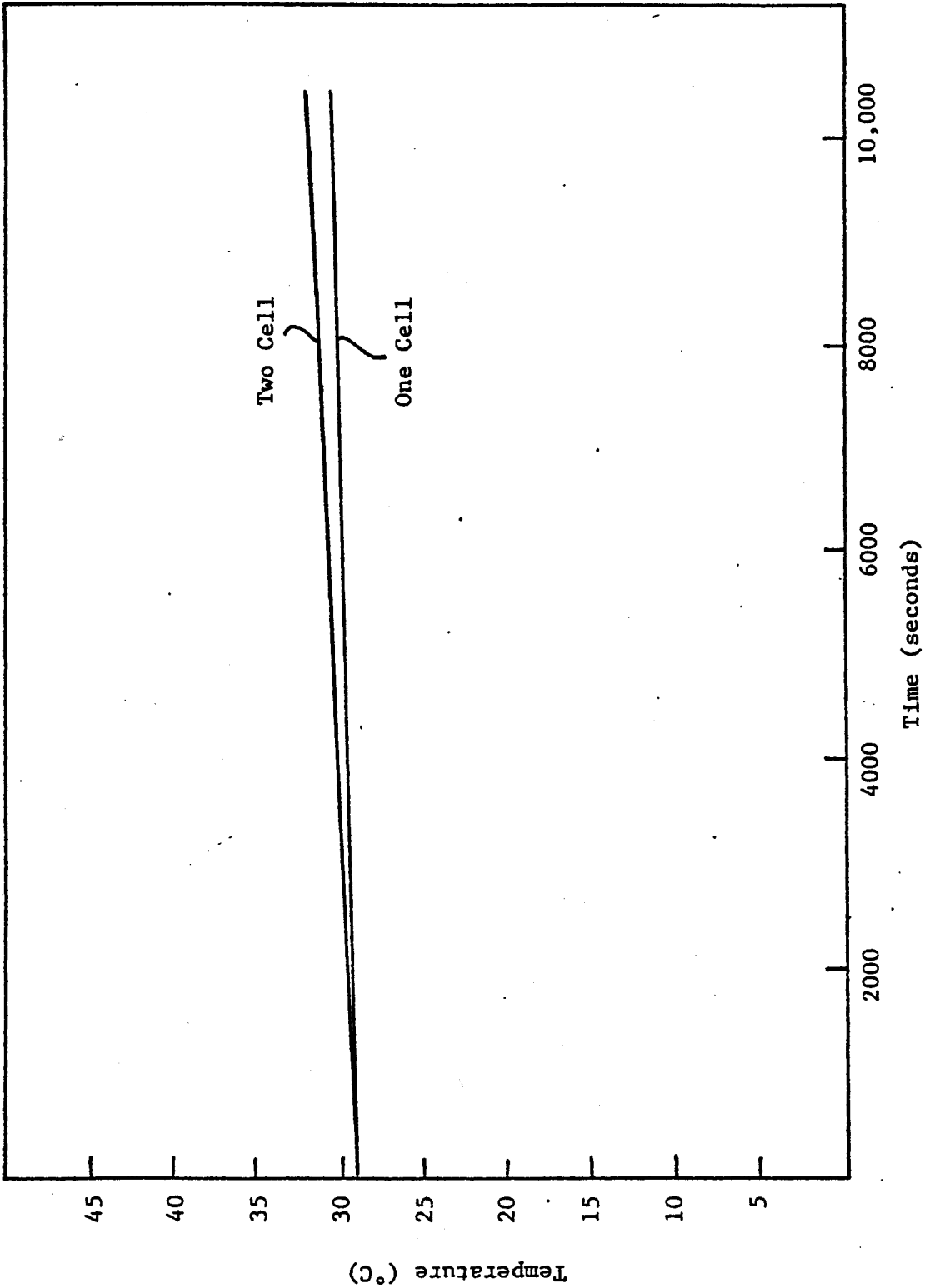


Figure 3.3: Comparison of One Cell and Two Cell Predictions for LA-4 Steel Wall Liner

TABLE 3.1

Combustion Characteristics for Various Crack Sizes

Crack Size (cm ²)	Lithium Consumed in Fire (kg)	Duration of Fire (secs.)	Peak Structural Temperature (°C)
.0000	487.6	3750 ^t	318
.0001	487.7	3750 ^t	318
.0100	488.9	3800 ^t	318
1.0000	930.5	11,000 ^t	576
10.0000	22,000.	41,000 ⁱ	576
100.0000	22,000.	19,400 ⁱ	716

t - Temperature of lithium pool dropped to lithium's melting point.

i - Reaction was limited by amount of lithium spilled (22,000 kg.)

Crack Size = 1.0cm²

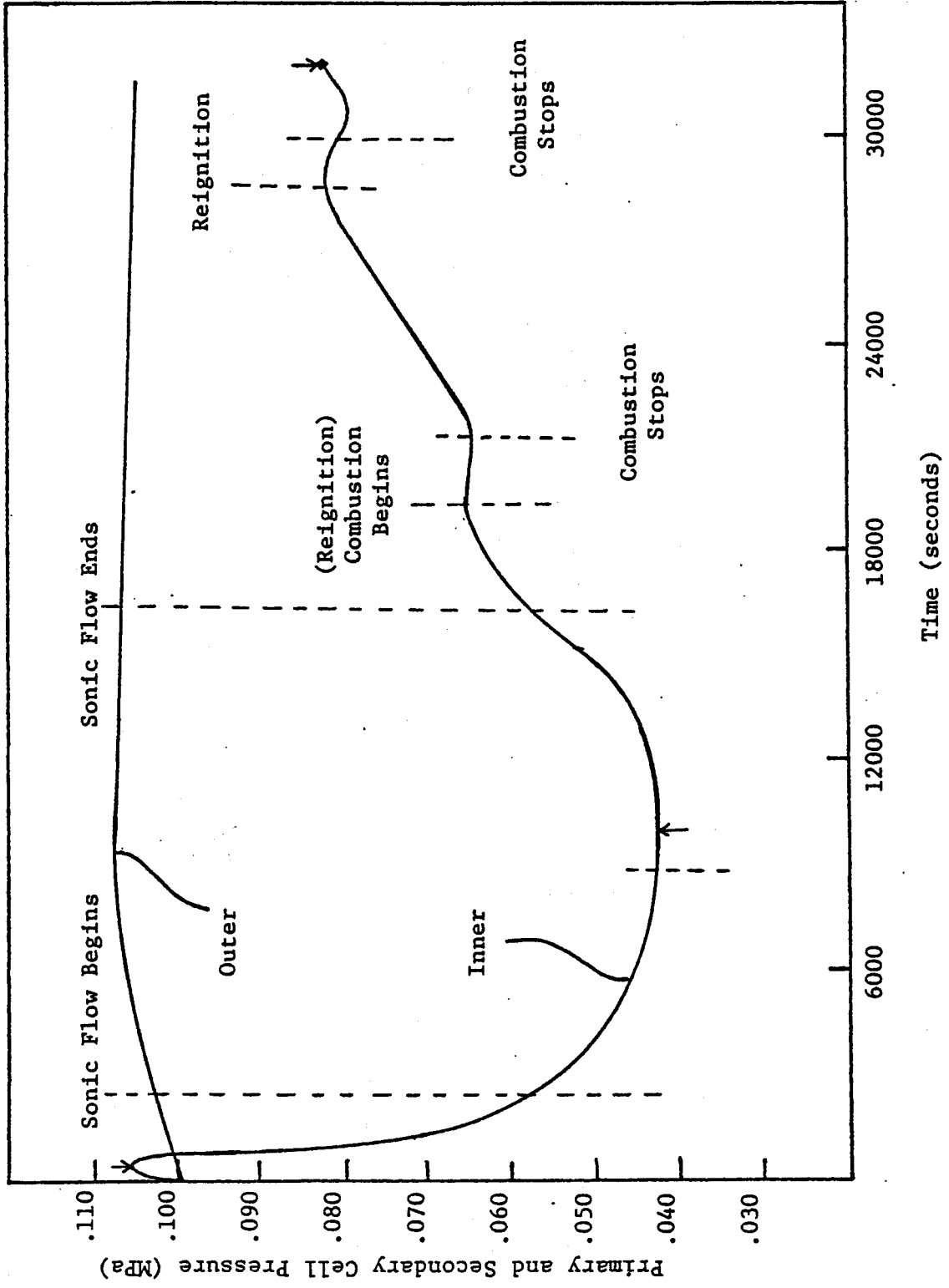


Figure 3.4: Typical Pressurization History for UMMAK-III Two Cell Geometry

Crack Size = 1.0cm²

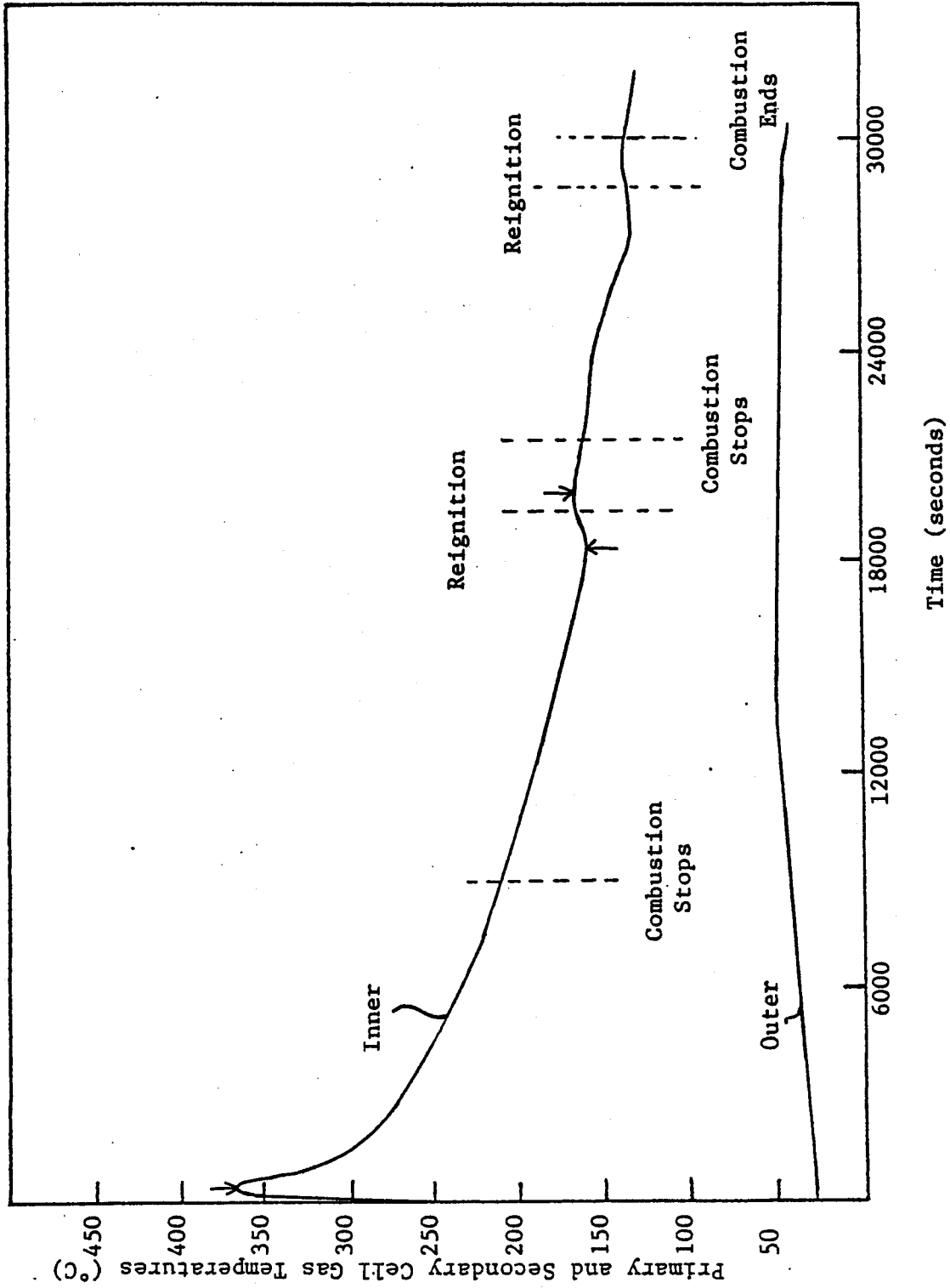


Figure 3.5: Typical Temperature History for UWMK-III Two Cell Geometry

Crack Size = 1.0cm²

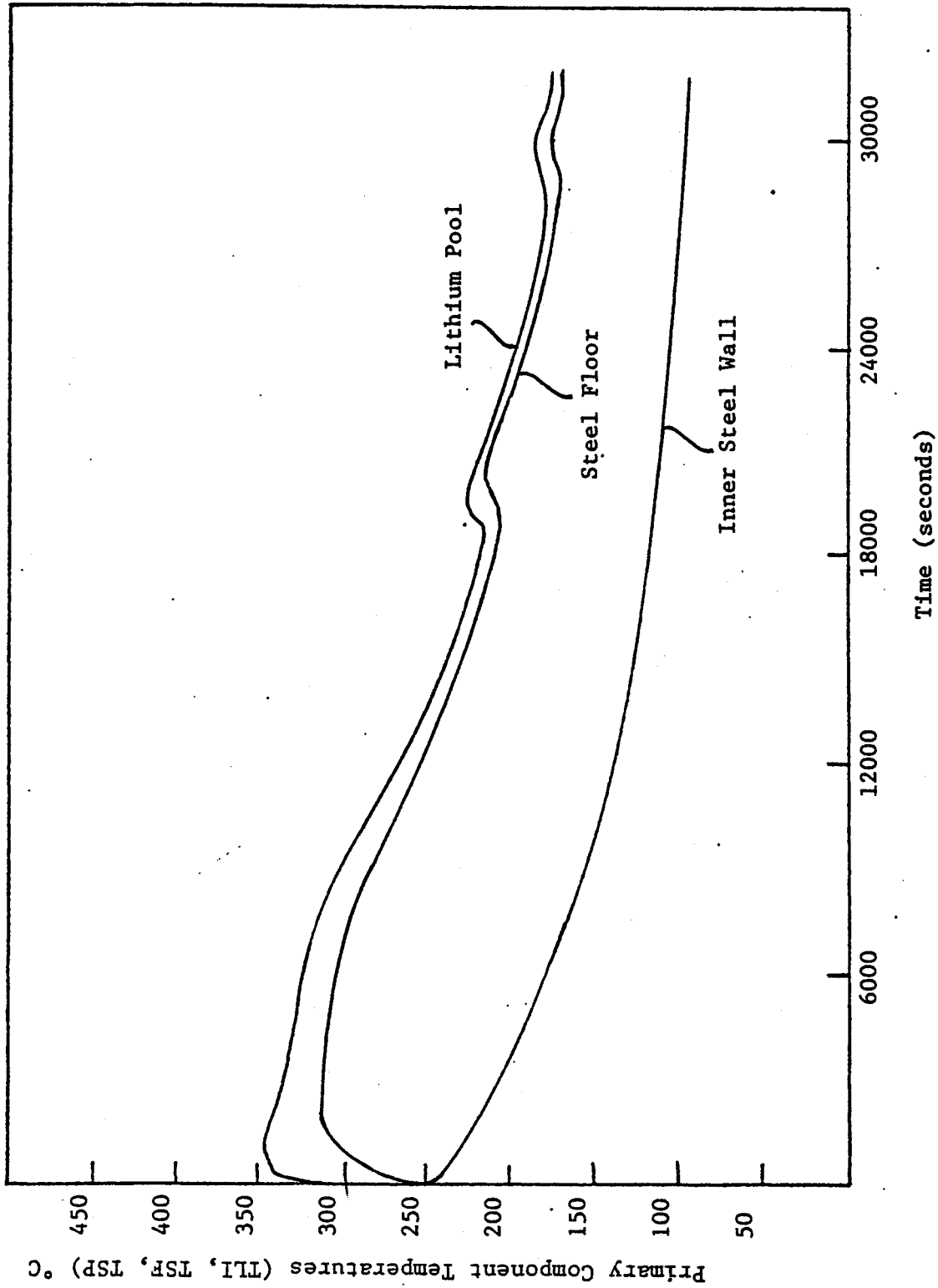


Figure 3.6: Typical Component Temperatures for UWMK-III Two Cell Geometry

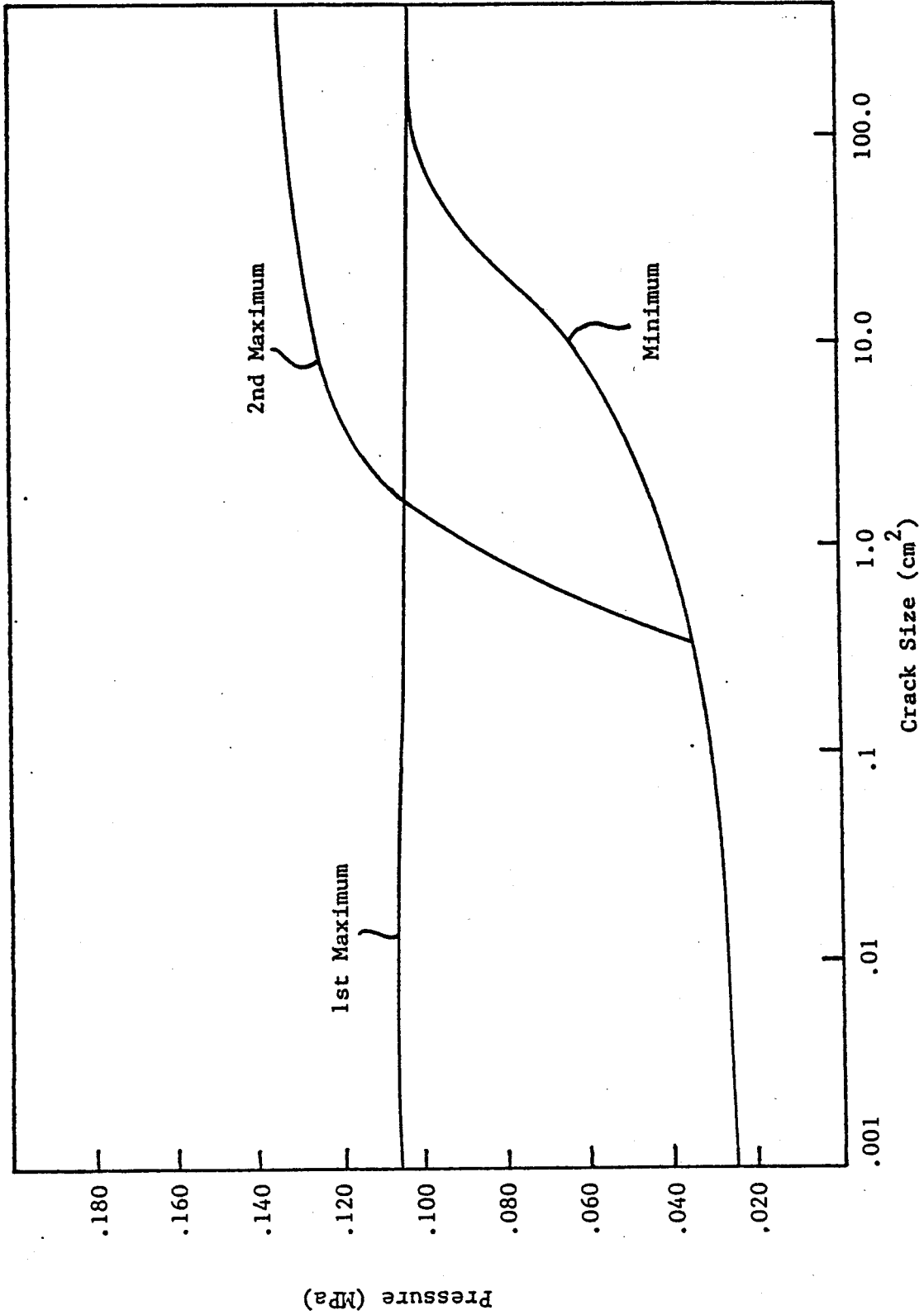


Figure 3.7: Minimum and Maximum Cell Pressure in UWMK-III
Two Cell Geometry (Smoothed)

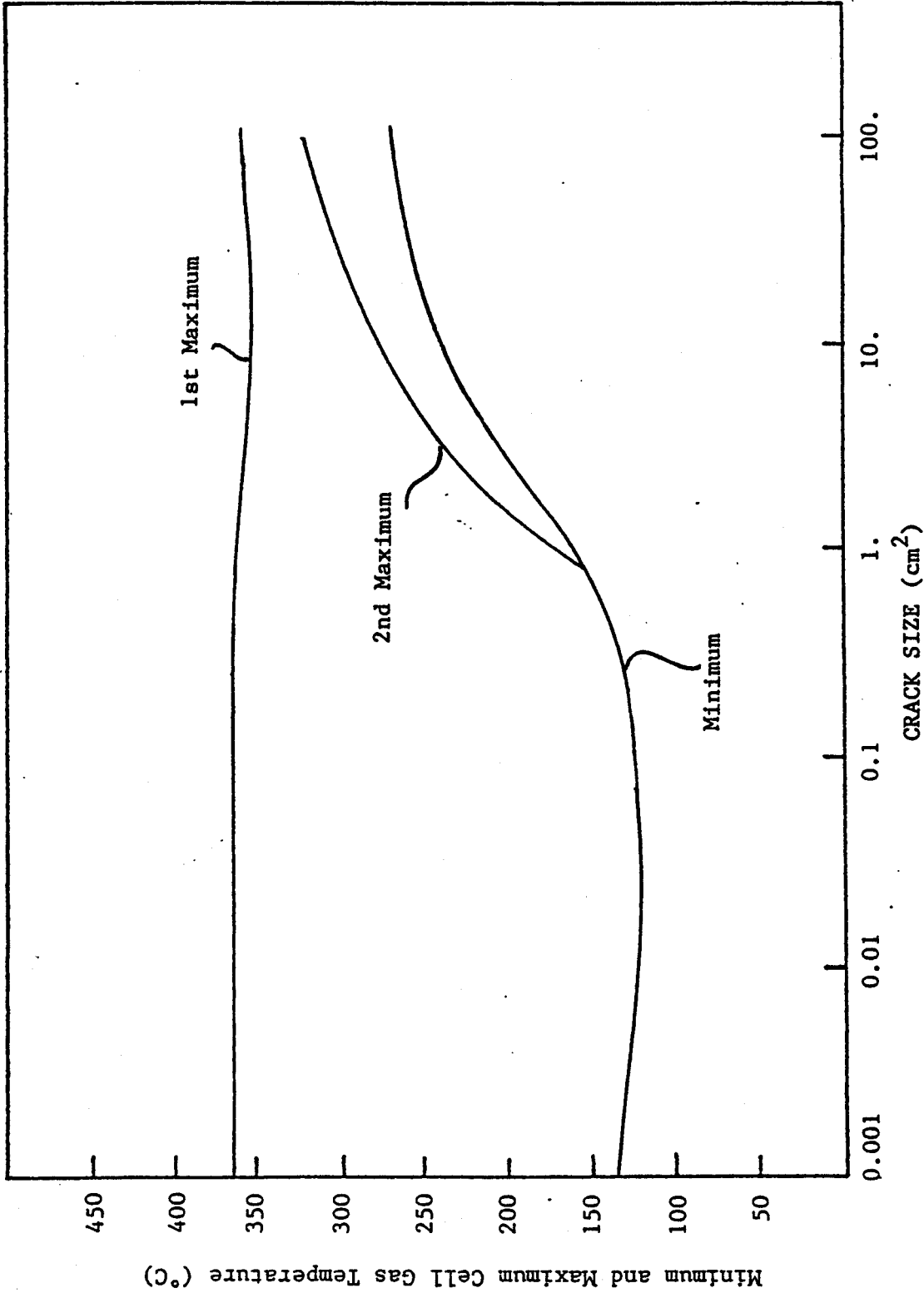


Figure 3.8: Minimum and Maximum Cell Gas Temperature for UWMak-III Two Cell Geometry.

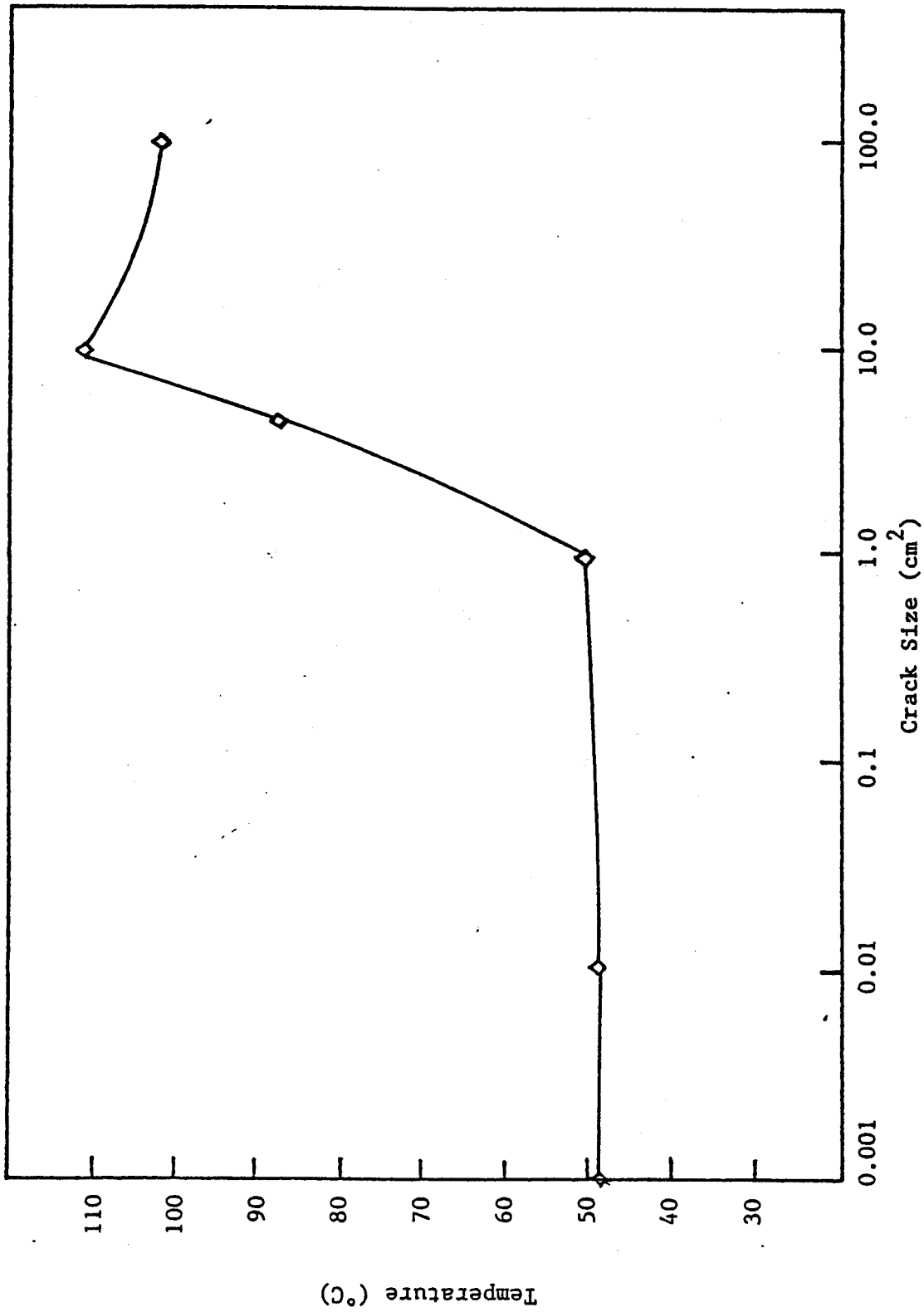


Figure 3.9: Maximum Secondary Cell Temperature (Initial Temperature = 27 °C)

products in the outer cell. However, lithium fires with larger crack sizes did generate inner cell pressures greater than those in the outer cell, causing the flow to go from the inner into the outer cell. For the maximum crack size used (100 cm^2) the maximum reaction product concentration in the outer cell was $4.5 \times 10^{-3} \text{ kg/m}^3$. The maximum concentration of Li_2O and Li_3N in the inner cell was 66.7 kg/m^3 . Aerosol removal by particle settling was not allowed in these tests (when permitted removal is assumed to be effective in the inner cell only).

3.5. Application of LITFIRE to a Lithium Spill in a Vacuum Torus

In this section a test case using the UWMAK-III geometry described above was run, but with the inner cell initially at a pressure of 0.001 megapascals. This was done in order to test the ability of LITFIRE to model high velocity flows as well as to see the effect lithium fires might have on the rapid pressurization of the torus and vice versa. Since the reaction rate is determined by the convection of gas to the combustion zone, low pressures can limit and even fail to ignite, the lithium reaction.

The results from this calculation are shown in Figures 3.10 and 3.11 indicate that there is indeed a limitation on the reaction rate due to low pressures, with ignition taking place a little under a thousand seconds after the transient was initiated. In addition, the maximum inner cell pressure attained was limited by the consumption rate of the gases due to combustion. To first order, pressurization is a linear function of crack size, so that larger cracks will reduce the time to ignition and increase the maximum pressure in the inner cell. In these predictions, the initial temperature in the torus components are assumed to be 250°C which is approximately the operating temperature near the first wall of proposed fusion reactors. Also, no spray fire was included in the model since the initial pressure inside the torus was assumed to be negligible.

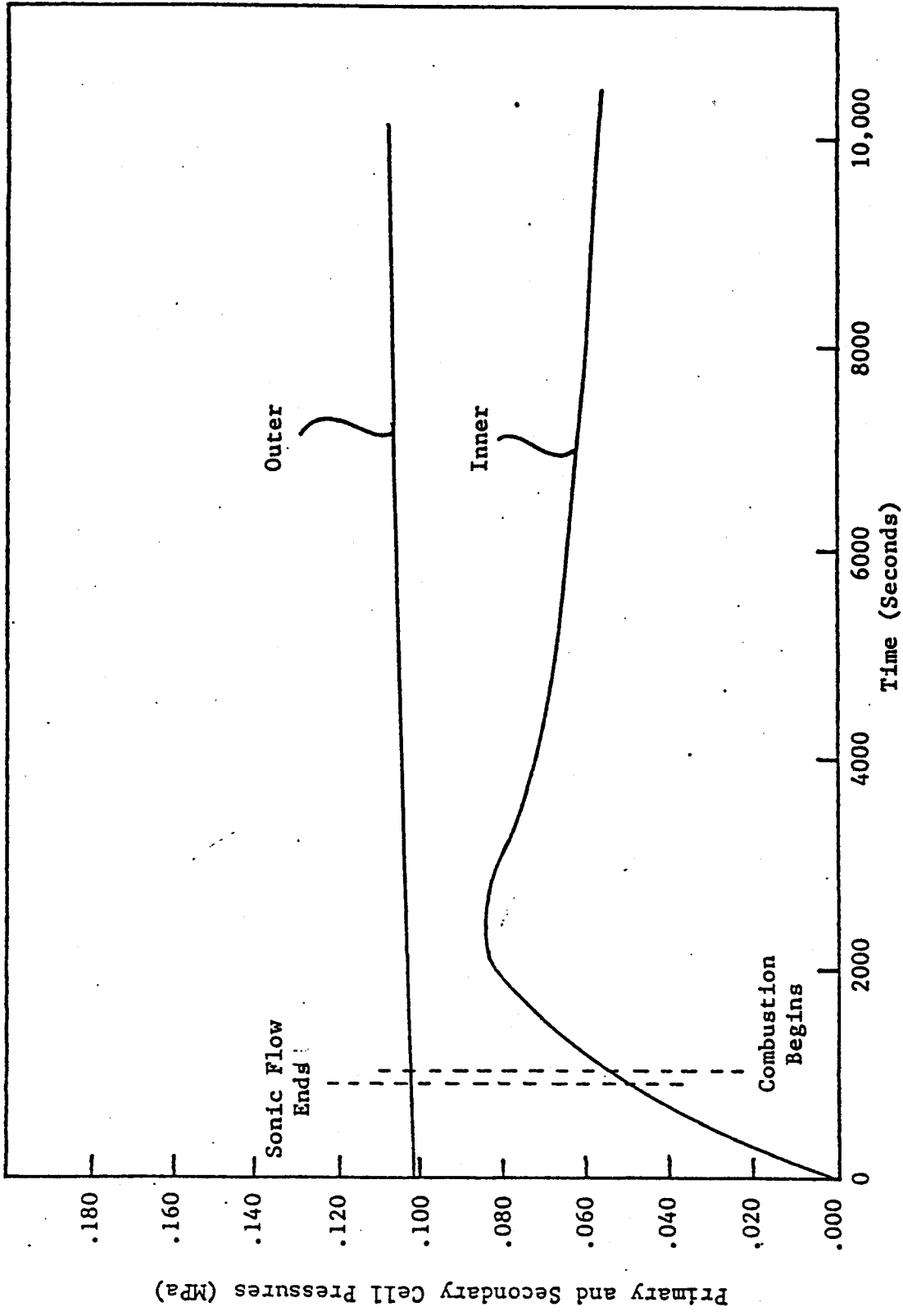


Figure 3.10: Torus Pressurization History, Crack = 10.0 cm²

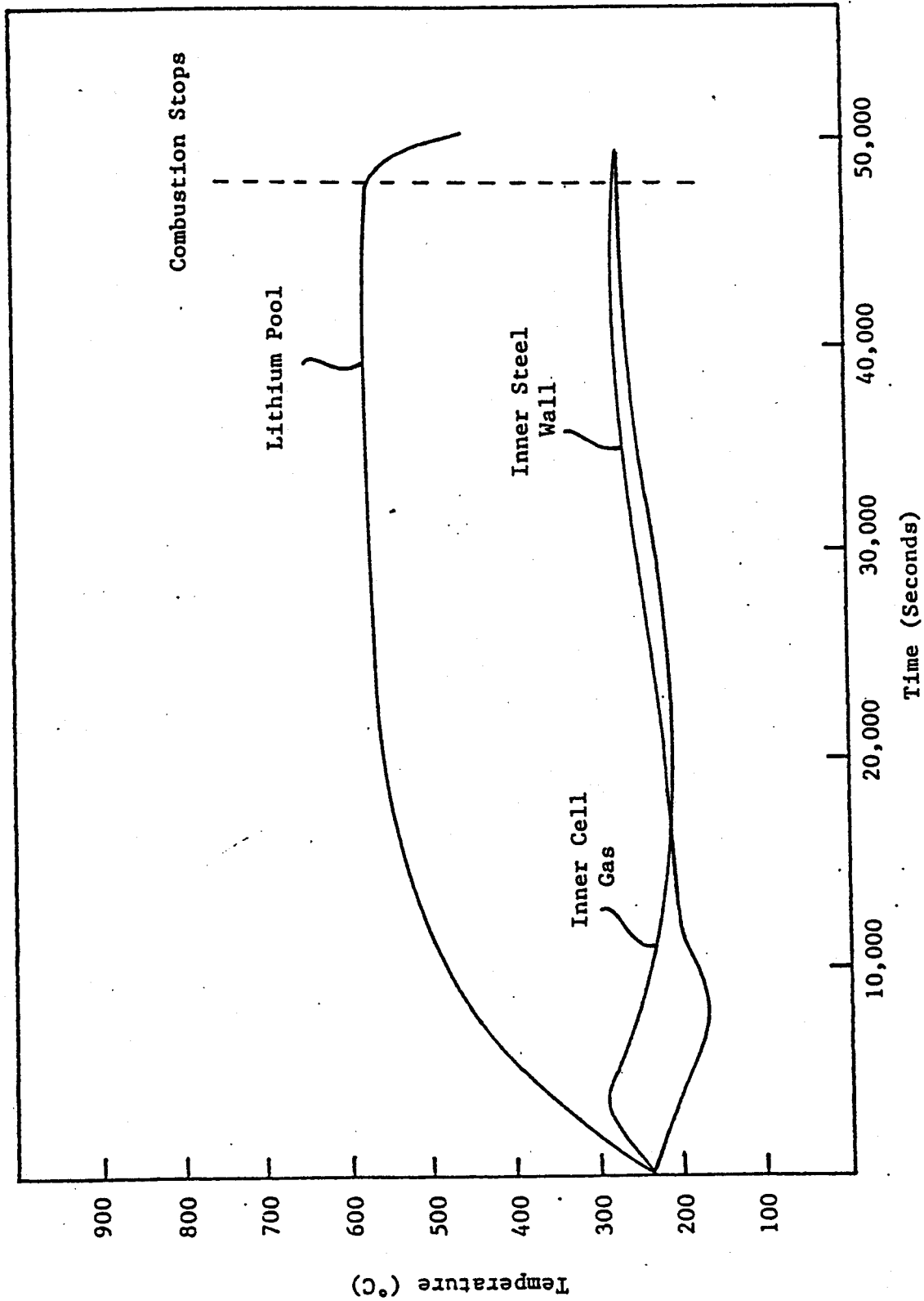


Figure 3.11: Torus Component Temperature History, Crack = 10.0 cm²

4. LITHIUM-LEAD COMBUSTION IN AIR

4.1. Lithium-Lead Use in Fusion Related Systems

Various compositions of lithium-lead (LiPb) alloy have been proposed as a tritium breeder for fusion reactors using the deuterium-tritium fuel cycle. The form of LiPb is unique in that the lithium acts as a tritium breeder and the lead acts as a neutron multiplier. Thus, the lithium inventory in the blanket can be minimized, limiting the total amount of lithium that is available for combustion in the event of an accident. In addition, LiPb compounds with a low melting point may also function as a coolant as well as breeder, further simplifying the reactor blanket design. The potential problems of using lithium lead alloys are associated with proper tritium confinement, structural material compatibility, and chemical reactions with air and water. The last of these concerns is the focus of this chapter, which presents models for lithium-lead pool combustion in an air atmosphere that is allowed to contain some moisture. Lithium-lead reactions with water in a prototypical fusion blanket assembly have been modeled by Krane [2] and are already incorporated in another version of LITFIRE (see Table 1.3).

4.2. Properties of Lithium-Lead

A recent literature search indicates that there is little data available with regard to physical, chemical, and thermodynamic properties for the temperature range of interest in fire modeling. This section summarizes the available data that is important in the present calculations.

4.2.1. Physical Properties

The density as a function of composition is known as is the phase diagram of the lithium-lead system. These are shown in Figures 4.1 and 4.2. The thermal conductivity of lithium-lead is estimated using the correlation

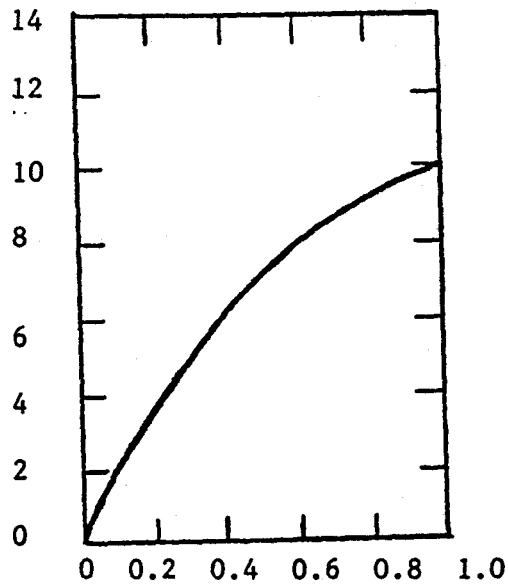
$$k_{LiPb} = k_1 w_1 + k_2 w_2 - 0.72 \times |k_2 - k_1| (w_1 w_2) \quad (4.1)$$

which is appropriate for a binary liquid mixture and where the k 's are the thermal conductivities of the element and the w 's are the weight fraction of each species in the alloy. [13]

The specific heat of the alloy is estimated by using an extrapolation of the specific heats of the pure elements

$$(C_p)_{LiPb} = \chi_{Li}(C_p)_{Li} + \chi_{Pb}(C_p)_{Pb} \quad (4.2)$$

where χ is the atom percent of each species in the alloy, and the C_p 's are the specific heat of each element. [3]



Mole Fraction of Lead

Figure 4.1 Density of LiPb

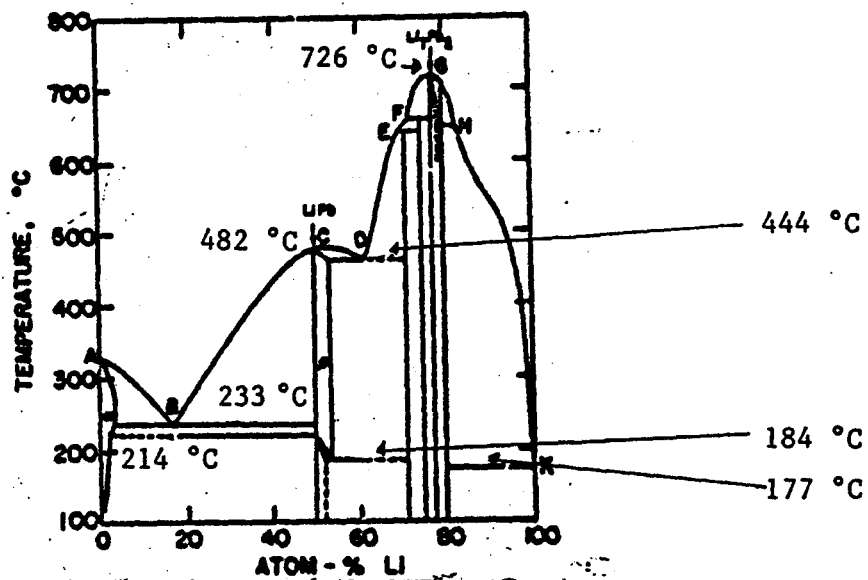


Figure 4.2: LiPb Phase Diagram

The latent heat of melting for a metallic alloy is determined by the correlation

$$\frac{H_{\text{melt}}}{T_{\text{melt}}} \sim 2.2 \quad \begin{array}{l} \text{(H: cal/gm mole)} \\ \text{(T: °Kelvin)} \end{array} \quad (4.3)$$

where T_{melt} is the melting temperature of the alloy. [13]

All of the above correlations are approximations at best and are calculated using lithium properties that vary with temperature and lead properties that are fixed for all temperatures.

4.2.2. Thermodynamic and Chemical Properties

The activity of lithium in the lithium-lead system has been measured at a temperature of 750 Kelvin. It decreases continuously from 4.0×10^{-3} at 61 atom percent lithium to 2.0×10^{-5} at five percent lithium. Figure 4.3 shows the lithium activity over the entire range of lithium concentration in lithium-lead. In addition, the activity of $\text{Li}_{17}\text{Pb}_{83}$ has been measured as a function of temperature [7] and found to follow

$$\ln a_{\text{Li}} = \frac{-6960}{T} + 0.0245 \quad (4.4)$$

where a_{Li} is the activity and T is the alloy temperature in Kelvin. Although the values of activity are quite low for the temperature range of interest, it is expected that the chemical reactivity of LiPb will be dominated by the lithium chemistry, due to the large thermodynamic stability of lithium with oxygen, nitrogen, and hydrogen. A thermodynamic analysis of lithium in lithium-lead performed by Piet [3] indicated that the energetics of a lithium-nitrogen reaction (with lithium from LiPb) is slightly unfavorable from a free energy standpoint at low temperatures (25°C) but is favored at higher temperatures. It is expected that the lithium-oxygen reaction at the lower temperatures would catalyze the reaction with nitrogen. In the present analysis, lithium nitrogen reactions will be allowed at all temperatures of interest even if there are no lithium-oxygen reactions taking place.

The dissociation reaction,



is assumed to precede all lithium chemical reactions, so that the lithium that is reacting is effectively pure lithium and could just as well have come from a pure lithium pool. This simplifies the coding changes required to model LiPb pool fires and is a credible assumption based on the inert behavior of lead. The estimated heat of dissociation is shown in Figure 4.4 for the full range of lithium concentrations.

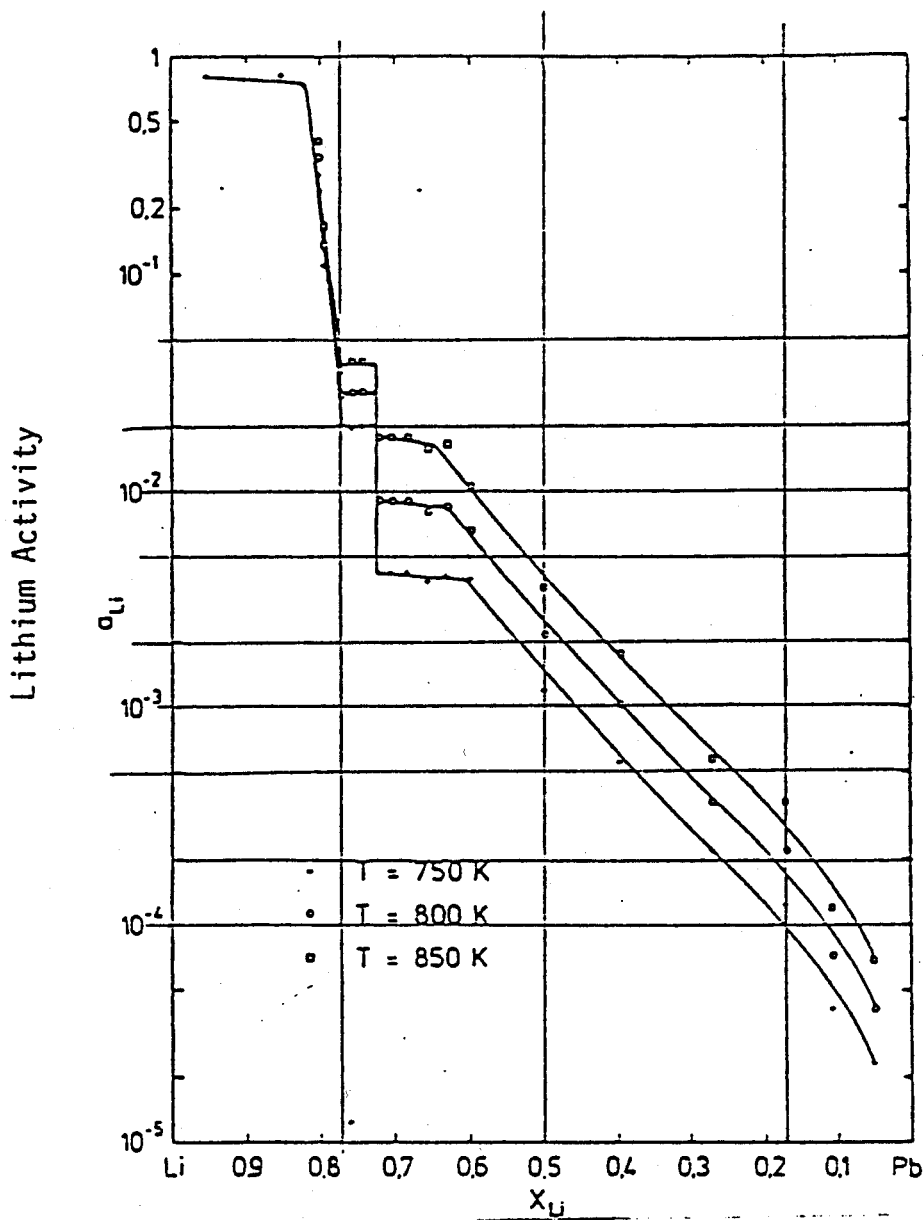


Figure 4.3: Lithium Activity in the LiPb System
As a Function of Lithium Concentration
[14]

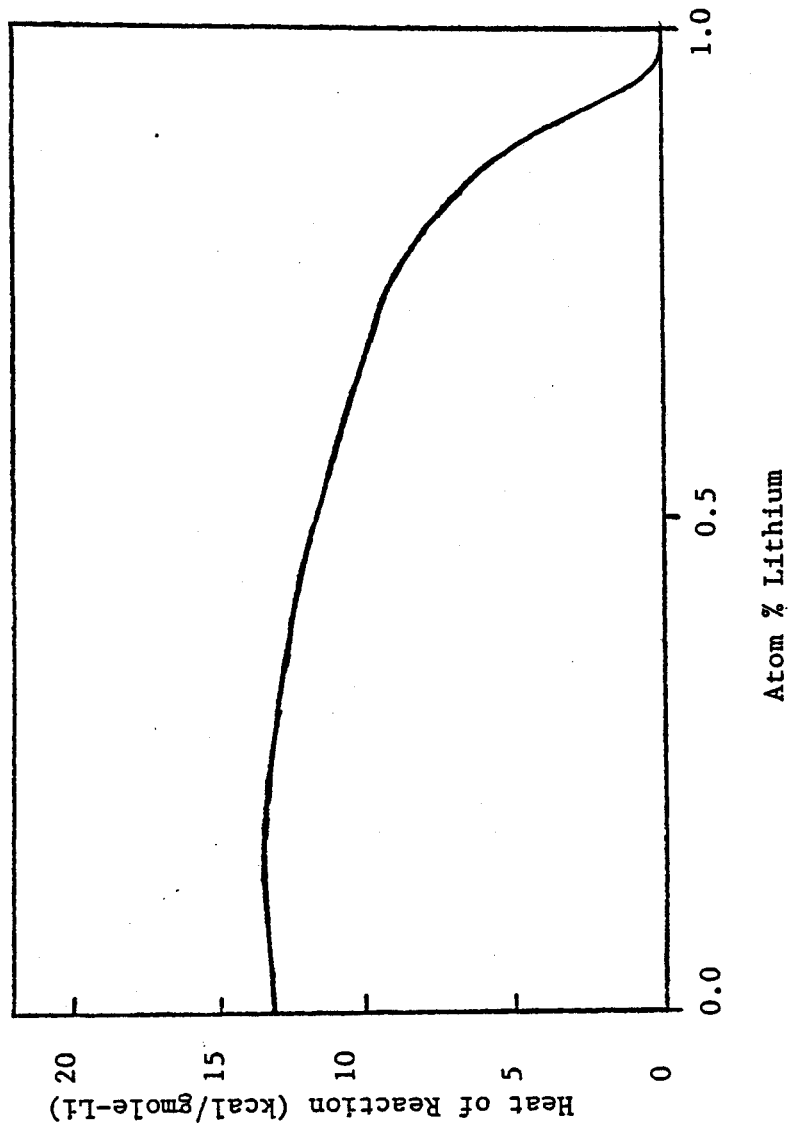


Figure 4.4 Heat of Dissociation for Li From Lithium Lead

The inertness of lead has been demonstrated by one experiment that immersed LiPb in air at 500°C:

"The material melted and smoked vigorously until all of the lithium had escaped as Li_2O or Li_3N and only molten lead was left." [5]

However, in another test it was found that pure lead will ignite in an atmosphere of pure oxygen at temperatures greater than 850°C. It is conceivable that a LiPb pool fire will have two components: the first, a lithium fire with lead inert, and the second, a surface burning reaction of lead and oxygen once the lithium has been depleted. Due to lack of data on lead combustion, no lead reactions are allowed by LITFIRE.

4.3. Models of Lithium Lead Air Reactions

Since the underlying assumption is that once the lithium leaves the LiPb pool its behavior is not influenced by the presence of lead, the lead can only influence lithium transport within the pool itself, in addition to changes in the physical properties of the pool. Data from tests being performed at HEDL reacting LiPb in air are not yet available so there are no quantitative results on which to base a model of LiPb-air combustion. In light of this, the present study proposes two models of LiPb pool dynamics in order to "bound" the problem from conservative and optimistic views.

The first model is conservative in the sense that no inhibition of the lithium reaction takes place. The reaction rate is still limited by the transport of the cell gases to the combustion zone, and the pool uses the physical properties of LiPb. The pool is assumed well mixed and turbulent and of homogeneous concentration, hence it is called the "turbulent pool model", and is represented by a single pool node. The heat and mass transfer pathways important in this modeling are shown in Figures 4.5 and 4.6.

The second model is probably not conservative since it assumes a large inhibition of the reaction due to the presence of a lead layer above the LiPb pool, through which the lithium must diffuse through before it can reach the combustion zone. The thickness of the lead layer increases with the depletion of lithium and is considered semi-stable in that no mixing between the lead layer and the LiPb pool takes place. This model required the addition of one node in the pool to model the two layers and is called the "layered pool model". The important heat and mass transfer pathways for this modeling are indicated in Figures 4.7 and 4.8.

4.3.1. Turbulent Pool Model

The major assumption in this model is that the pool is well mixed and homogeneous. All

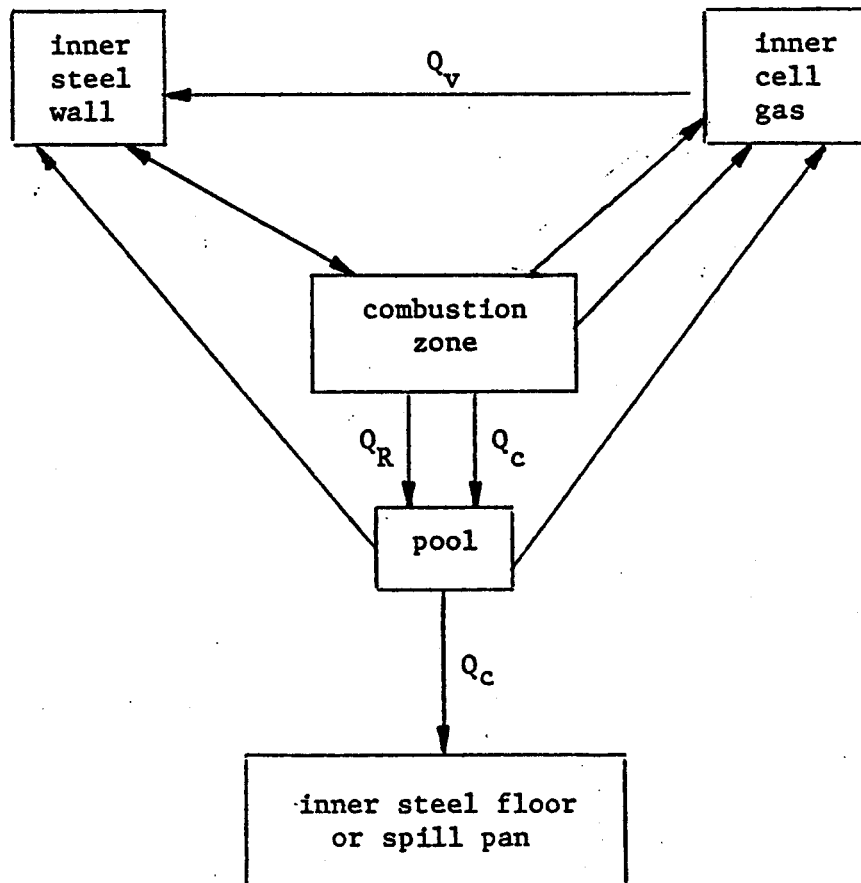


Figure 4.5: Heat Flow in Turbulent Pool Model

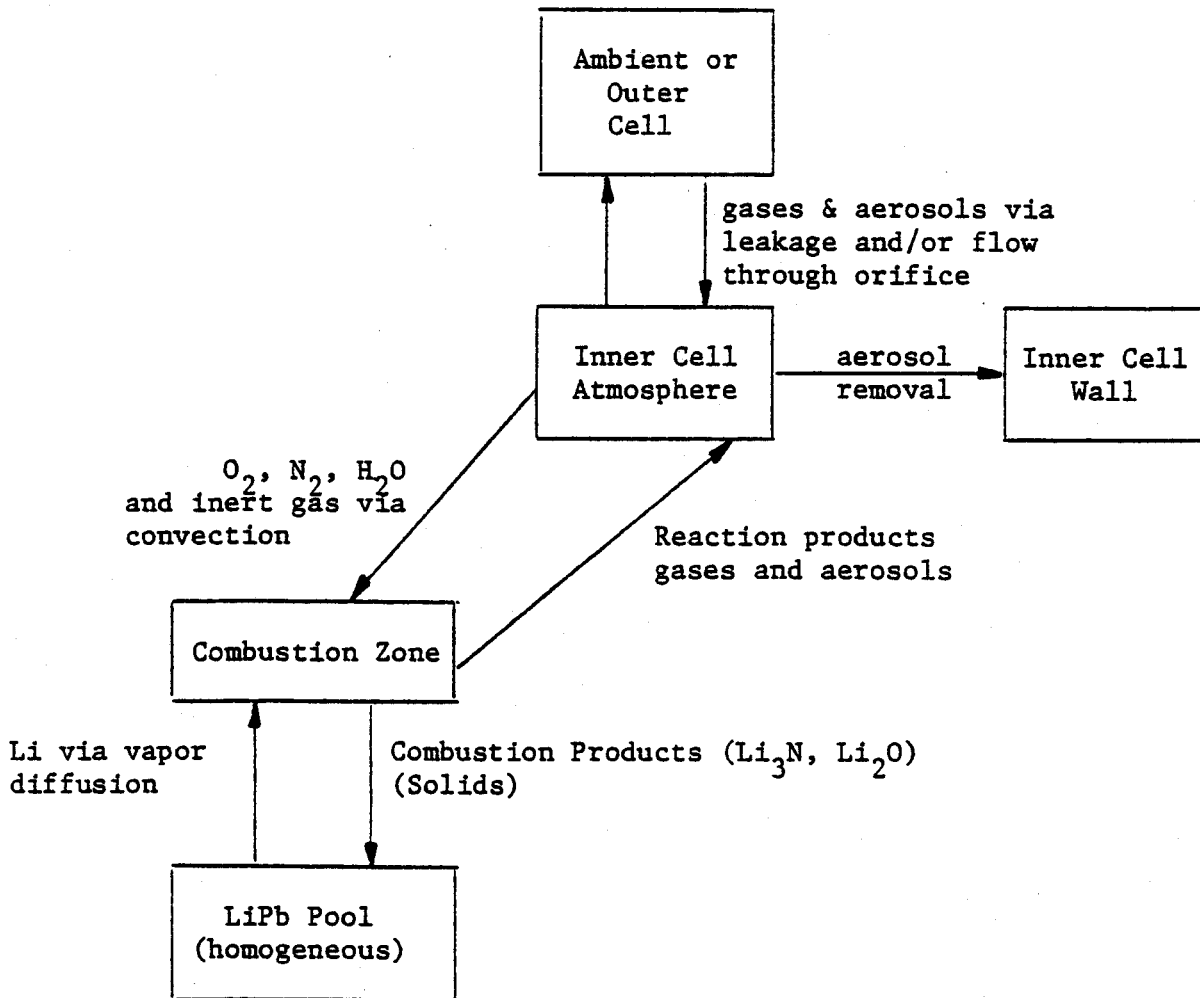


Figure 4.6: Mass Flow in Turbulent Pool Model

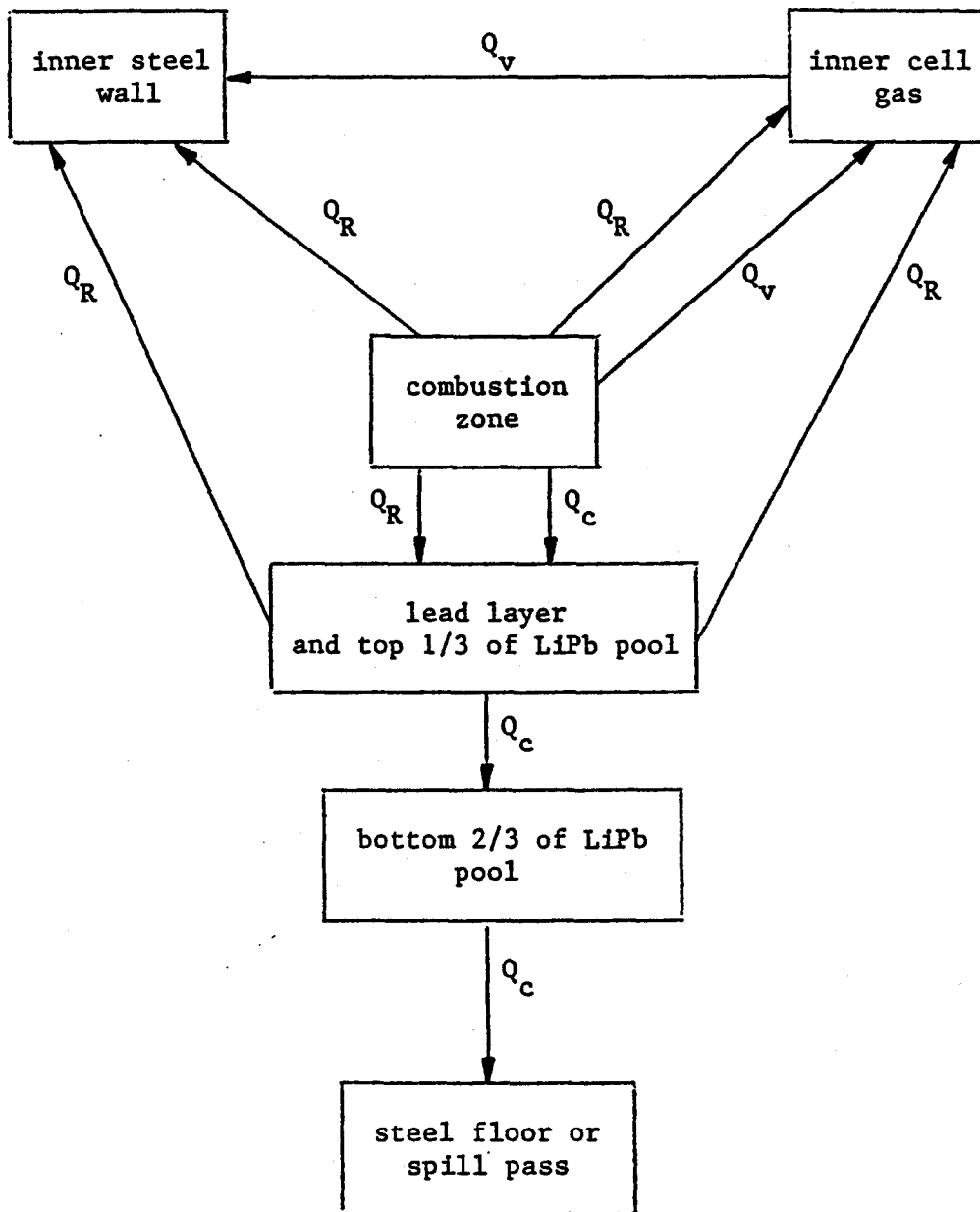


Figure 4.7: Heat Transfer in Layered Pool Model

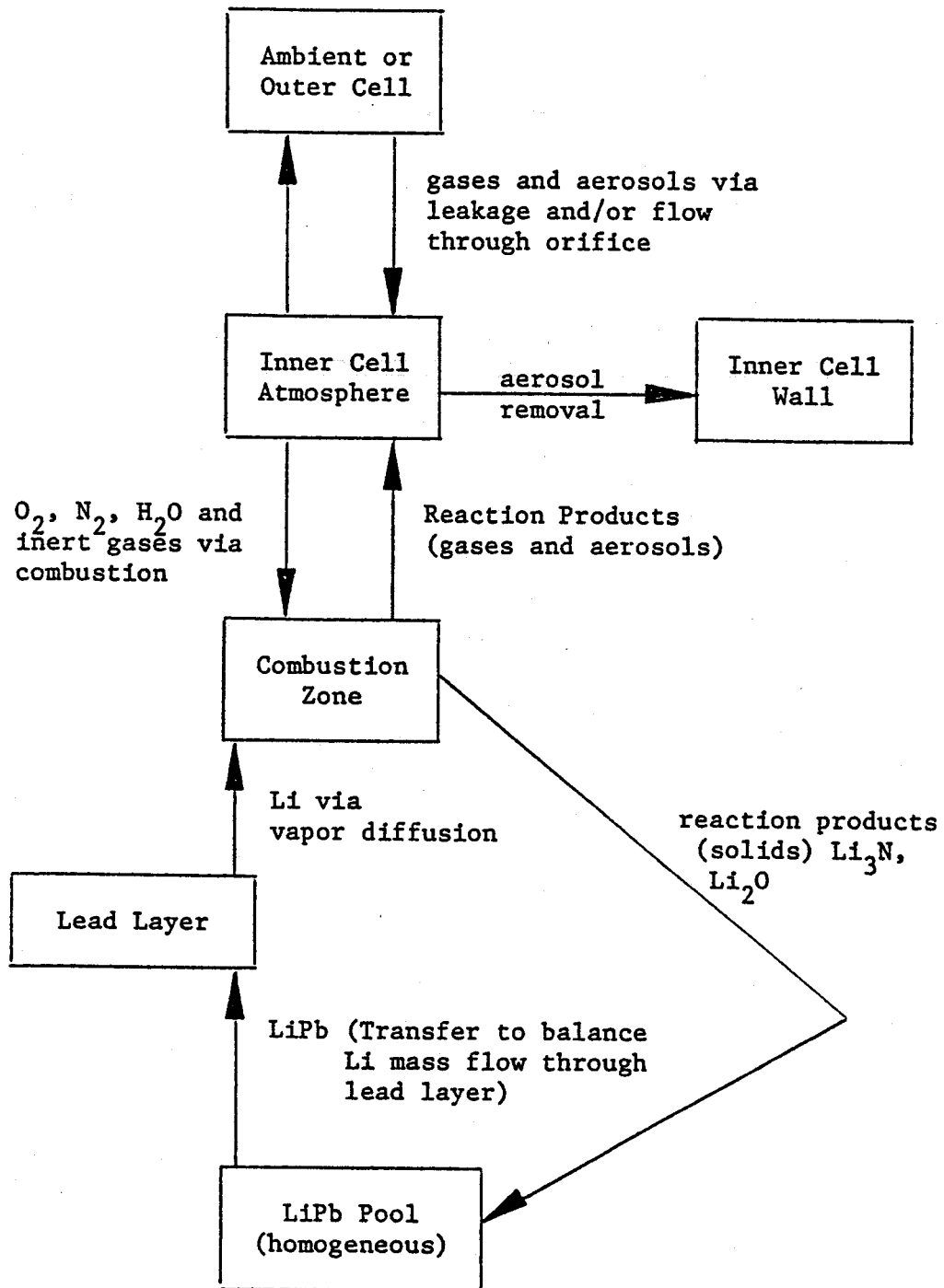


Figure 4.8: Mass Flow in Layered Pool Modeling

the combustion zone and pool modeling remains the same as that of pure lithium pools except for the following changes.

- **Lithium pool properties.** The conductivity, density, and specific heat of the pool are calculated using the correlations presented in section 4.2.1. Since lithium is being depleted by the lithium fire, the concentration of lithium in the pool is decreasing in time. Combustion stops when all the lithium in the pool is depleted or when the pool drops to the pool's melting temperature (which is also a function of concentration).
- **Heat addition to the pool.** The effect of the dissociation reaction is to absorb some of the heat transferred to the pool. The assumption that the dissociation takes place before vaporization and transport to the combustion zone implies that this effect is limited to the pool and does not affect the combustion zone heat balance.
- **Lithium-nitrogen film thickness.** The thickness of the film region between the combustion zone and pool is determined from the diffusion rate of lithium through the region according to the relation

$$d = -D_{Li} \left(\frac{\rho_{cz} - \rho_{Li}}{\left(\frac{dM}{dt}\right)_{Li}} \right) \quad (4.6)$$

where D_{Li} is the diffusion coefficient for lithium in air; $\left(\frac{dM}{dt}\right)_{Li}$ is the mass flow rate of lithium (assumed equal to the combustion rate of lithium); ρ_{cz} is the lithium density in the combustion zone (assumed to be zero); and ρ_{Li} is the density of lithium at the pool surface. This last parameter is affected by the presence of lead in the pool, which reduces the lithium atom density and as a result will reduce the thickness of the film. The net effect is an increase in heat conduction from the combustion zone to the pool due to the smaller thermal resistance of a thinner pool.

The heat of solution (mixing) and "kinetic" energy of the pool are ignored since the latter would reduce the temperature rise by an amount equal to $(\text{kinetic energy}/M_{LiPb}C_{pLiPb})$ and the former is an order of magnitude smaller than the heat of dissociation [15].

4.3.2. Layered Pool Model

The basic assumption of this model is that the LiPb pool is covered by a separate layer of pure lead that inhibits the transport of lithium to the combustion zone. Evidence of layered species within pool mixtures during and after combustion was indicated by [16] when investigating petrochemical fires. Since the density of lead is greater than that of LiPb, the top layer in this

model is unstable and would tend to fall into the pool. However, since lithium is continually being depleted at the pool surface it is expected that there should be some finite layer that is lithium poor with respect to the rest of the pool. The stability of this layer would be a function of the turbulence of the fire as well as the lithium depletion rate. Lithium dissociation from lead would also be higher in this region since it is at a higher temperature than the rest of the pool although this effect should be secondary because of the high thermal conductivity of the pool.

The simplest (and least conservative) model incorporating the important effects is to allow lithium diffusion through a pure lead layer since this top layer is no longer a mixture and its properties are not functions of the lithium concentration. This model incorporates the same property changes for the LiPb layer as that of the turbulent pool model above with one major difference. In this model the LiPb layer is assumed constant in concentration. Since lithium is being depleted by combustion, the excess lead is added to the pure lead layer which grows in thickness as the fire progresses. Eventually, the lead layer may retard the mass flow rate of lithium through the pool enough to be the limiting factor in the combustion rate. Therefore, the following two items represent the major difference to the LiPb turbulent pool model.

- Lithium diffusion rate through lead layer. The thickness of the lead layer is determined by the amount of excess lead in the pool due to removal of lithium by combustion. The mass of excess lead grows with time according to

$$M_{Pb} = \int_{t=0}^t \frac{(1-\chi)}{\chi} \times ASLI \times CMBR dt' \quad (4.7)$$

where $ASLI$ is the surface area of the pool, $CMBR$ is the lithium combustion rate in kg/sec, and χ is the weight fraction of lithium in the alloy. The thickness of the lead layer can then be calculated using

$$d_{Pb} = \frac{M_{Pb}}{\rho_{Pb} \times ASLI} \quad (4.8)$$

where the density of lead (ρ_{Pb}) is a known function of temperature.

The lithium that dissociates from the lead in the LiPb pool node is heated by conduction as it passes through the lead layer. The free lithium is assumed to travel through the lead layer according to a Fick's law diffusion of the form

$$\left(\frac{dM}{dt}\right)_{Li} = -D_{Li} \left(\frac{\rho_0 - \rho_{LiPb}}{d_{Pb}}\right) \quad (4.9)$$

where d is the thickness of the lead layer, ρ_0 is the lithium density at the pool surface (assumed to be zero for this calculation only), ρ_{LiPb} is the lithium atom density in the LiPb layer and D is the diffusion coefficient of lithium in lead. The assumption of zero lithium density at the pool surface is reasonable since this value will yield the highest diffusion rate of lithium for a given alloy. The diffusion coefficient, D is evaluated according to the estimate presented by Castleman and Conti [17] for liquid metal diffusion through liquid metals:

$$D = \frac{0.655T^{\frac{1}{2}}\sigma_{ij}}{M^{\frac{1}{2}}\left(\frac{\epsilon_{ij}}{k} \times 10^{-3}\right)\Sigma} \quad (4.10)$$

where M is the molecular weight of the solvent, T is the absolute diffusion temperature, Σ is a dimensionless force constant, σ_{ij} is the intermolecular separation where the Lennard-Jones potential is zero between unlike molecules, k is the boltzman constant and ϵ_{ij} is the well depth for the Lennard-Jones potential. Hovingh [18] gives an evaluation of these parameters for lead diffusion in lithium. Since all the factors in Eq. (4.10) are symmetric with respect to solute and solvent (except for the molecular weight) Hovingh's analysis can readily be transferred to lithium diffusion through lead. The resulting expression for the diffusion coefficient,

$$D = 6.0 \times 10^9 \exp\left(\frac{-680}{T}\right) \frac{\text{meter}^2}{\text{sec}} \quad (4.11)$$

for T in kelvin, is accurate to within 10% of the Eq. (4.10) value for temperatures between 500 and 1800 kelvin.

- **Limitations on combustion rate.** The thickness of the lead layer increases with the amount of lithium consumed, thereby decreasing the mass flow of the lithium through the pool to the combustion zone. Eventually the the mass diffusion rate may be sufficiently low enough to limit the combustion rate of lithium. LITFIRE models the combustion zone using a quasi-steady state analysis, especially for the mass balance. The mass of the combustion zone is based on the instantaneous combustion rate and does not include any mass buildup of unreacted gases or lithium vapor. This assumption may not be accurate when the combustion is lithium diffusion limited, but no change to the mass balance has been made at this time because of lack of experimental data on which to base a new model.

4.4. Major Changes to Litfire Encompassing Lithium-Lead Combustion in Air

The inclusion of lithium-lead combustion in LITFIRE was simplified by using the existing structure as much as possible. Two subroutines were added to the code that modified the pool

properties and heat transfer parameters in such a way as to make the pool "appear" to be a LiPb alloy. Many variable names were not changed, however, so that the same name may represent a single parameter for either pure lithium or lithium-lead depending on what stage of the calculation is being used.

The addition of one pool node required the addition of two more integrals into the main program. When all options are in effect, the number of integrals now approaches the stated limit (100 simultaneous integrations) of the integrator subroutines, however no decrease in accuracy because of this condition has yet been observed. The new integrals follow the mass and temperature of the top pool node which is a mass weighted average of all the excess lead and one third of the lithium-lead that remains in the pool. This average was necessary in order to increase the thickness of the top node of the pool so that computation time would stay within reasonable limits. Consistent with assumption, the thickness of the pure lead layer never exceeded a small fraction (less than 1/100th) of the total pool thickness. Yet this thickness was sufficient to retard the lithium mass flow rate enough to limit combustion. Therefore, the mass flow calculation is based on the "true" lead layer thickness while the heat transfer calculation is based on the lumped lead and lithium-lead thickness.

The surface pressure of lithium is assumed to be a function of the activity of the lithium-lead alloy according to

$$P_{Li} = a_{Li}P_o \quad (4.12)$$

where a_{Li} is the activity of lithium in the alloy (see section 4.2) and P_o is the vapor pressure of pure lithium which is a known function of temperature. The net effect of the reduced partial pressure is in a reduction of the film thickness between the combustion zone and pool but this effect tends to be very small due to the nitrogen pressure domination in this region.

4.5. LITFIRE Results

The comparison made in this section is again for the UWMAK-III reactor described earlier. However, the amount of alloy spilled was altered in each case so that the total volume of alloy spilled was the same. This was felt to be a more realistic comparison because of the lower lithium atom density in the lithium-lead alloys requiring a larger mass of breeder than pure lithium. However, lead acts as a neutron multiplier, enhancing the breeding ratio of the fewer lithium atoms, so that roughly equal volumes of the alternate breeders will most likely be required. It should be emphasized that the following analysis is not an indication of the consequences from a specific accident scenario but should be taken as an indication of the relative consequences of

pool fires for different alloys. Table 4.1 summarizes the important parameters governing the spills studied in this section.

4.5.1. Comparison of Turbulent Pool and Layered Pool Models

A comparison of the results from the layered pool model and the well mixed pool model are shown in Figures 4.9 and 4.10 where the cell gas and pool temperatures are plotted. In the case of the layered pool the top pool node is indicated by the dashed line. A more interesting comparison appears in Figure 4.11 where the effect of the lead layer on the combustion rate is shown. In both cases the alloy of interest was LiPb. The combustion rate is limited rather early in the fire due to the buildup of the lead layer on the surface. At the point where the combustion was lithium limited, the thickness of the lead layer was 0.15 mm., approximately one thousandth of the thickness of the entire pool. This indicates that LITFIRE's predictions will be very sensitive to the calculated diffusion rate and the lead layer thickness. As was expected, the diffusion model is less conservative than the turbulent pool model, but no evaluation of either model can be made at this time. Figure 4.12 shows the effect of a lithium-lead spill in the HEDL test facility used for LA-5. The models indicate that tests of this size will be much less severe than for the tests using pure lithium.

4.5.2. Comparison of LiPb Combustion to Pure Lithium Combustion

The comparison among the alternate coolants and breeders is shown in Figures 4.13 and 4.14 using the turbulent pool and layered pool models respectively. The temperature profiles are for the pool node since this is where the greatest variation occurred (except for the combustion zone). Comparison of the maximum temperatures predicted indicates that the turbulent pool model closely matches the predictions for a pure lithium fire. The layered pool model predictions show a substantial reduction in the peak temperatures but give higher temperatures after combustion has ceased. The major reason for this is due to the nodal structure of the layered pool model. The top node is made up of the lead layer in addition to one third of the LiPb pool layer, so that its conductivity is substantially reduced over that of pure lithium or LiPb. Since conduction from the pool is the principal heat transfer mechanism after combustion has stopped, the net effect is to reduce the rate of heat loss from the top pool node. This in turn reduces the heat loss of the lower pool node so that the average pool temperatures are higher than those predicted by the turbulent pool model. A trend that was consistent among the two models was that the lower the lithium atom concentration in the alloy, the lower the consequences of fires using that alloy. The variation in maximum cell gas temperature was $\sim 400^{\circ}\text{C}$ among the various alloys and models used in the calculation. The cell gas temperature time history is plotted in Figure 4.15.

TABLE 4.1

Summary of Lithium-Lead Calculations

<u>Alloy</u>	<u>Atom % Li</u>	<u>Volume Spilled (m³)</u>	<u>Mass Spilled (kg)</u>	<u>Initial Temp. (°C)</u>	<u>Maximum Temp. (°C)</u>
Li	1.00	475	22,000	980	1103 *
Li ₇ Pb ₂	0.78	475	202,900	980	1103
LiPb	0.50	475	346,630	980	1105
LiPb ₄	0.20	475	459,900	980	1125
LiPb	0.50	7.6	1,575	360	890
LiPb	0.50	0.49	100	360	710

*

Maximum temperatures are from LiPb turbulent pool model.

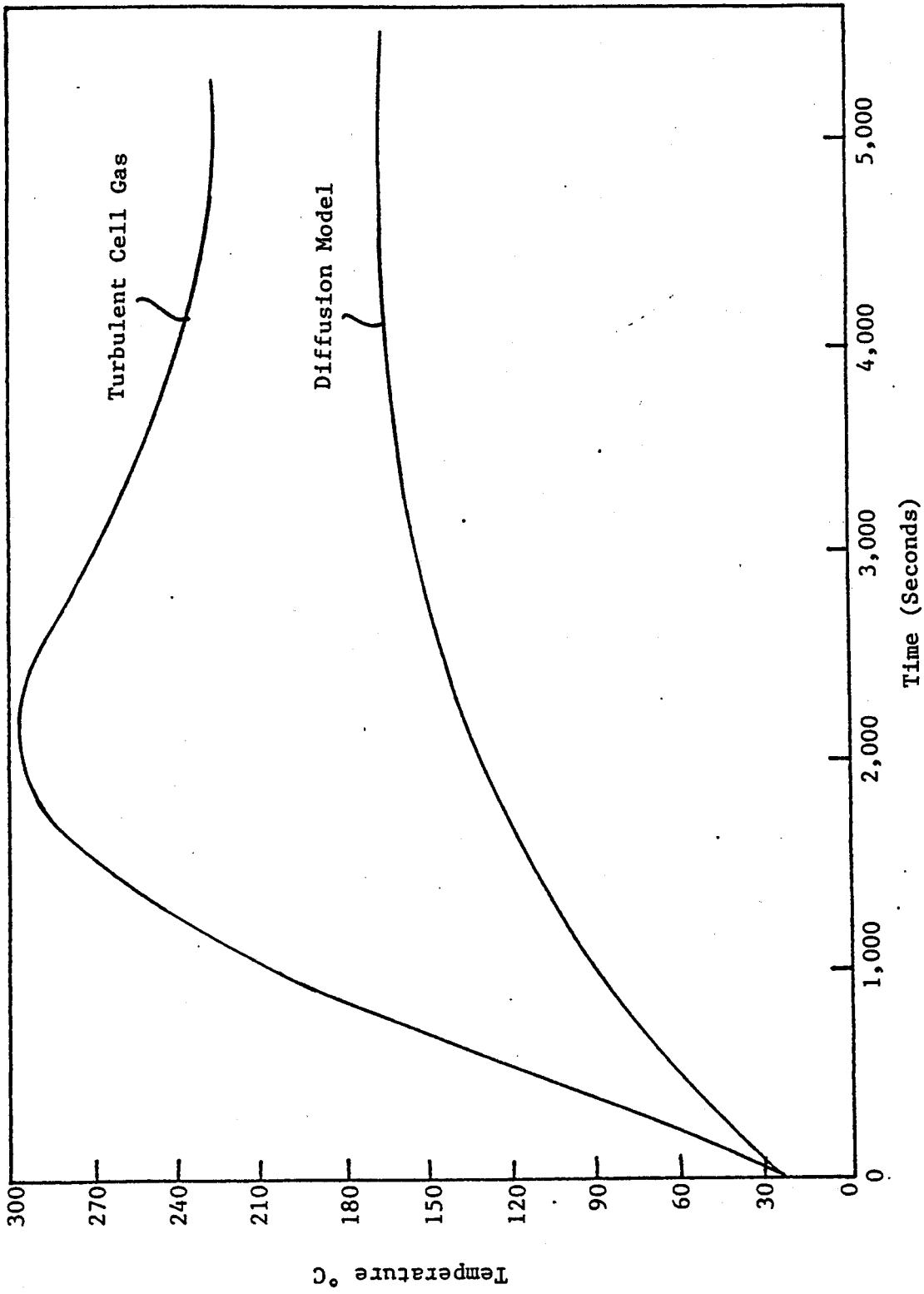


Figure 4.9: Cell Gas Temperatures for LiPb Alloy Using Layered and Turbulent Pool Models

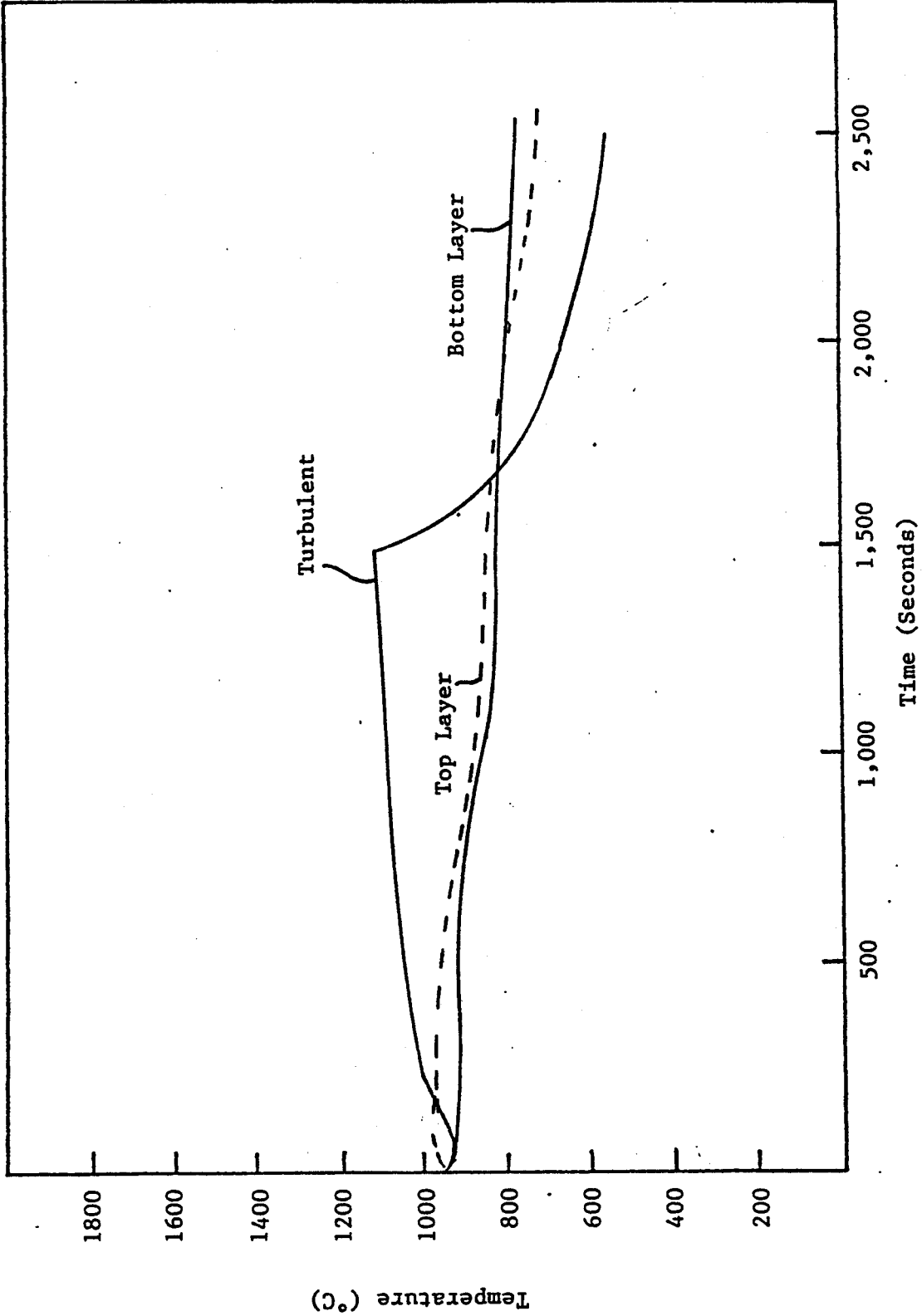


Figure 4.10: Pool Temperatures for LIPb using Layered and Turbulent Pool Models

Alloy = LiPb

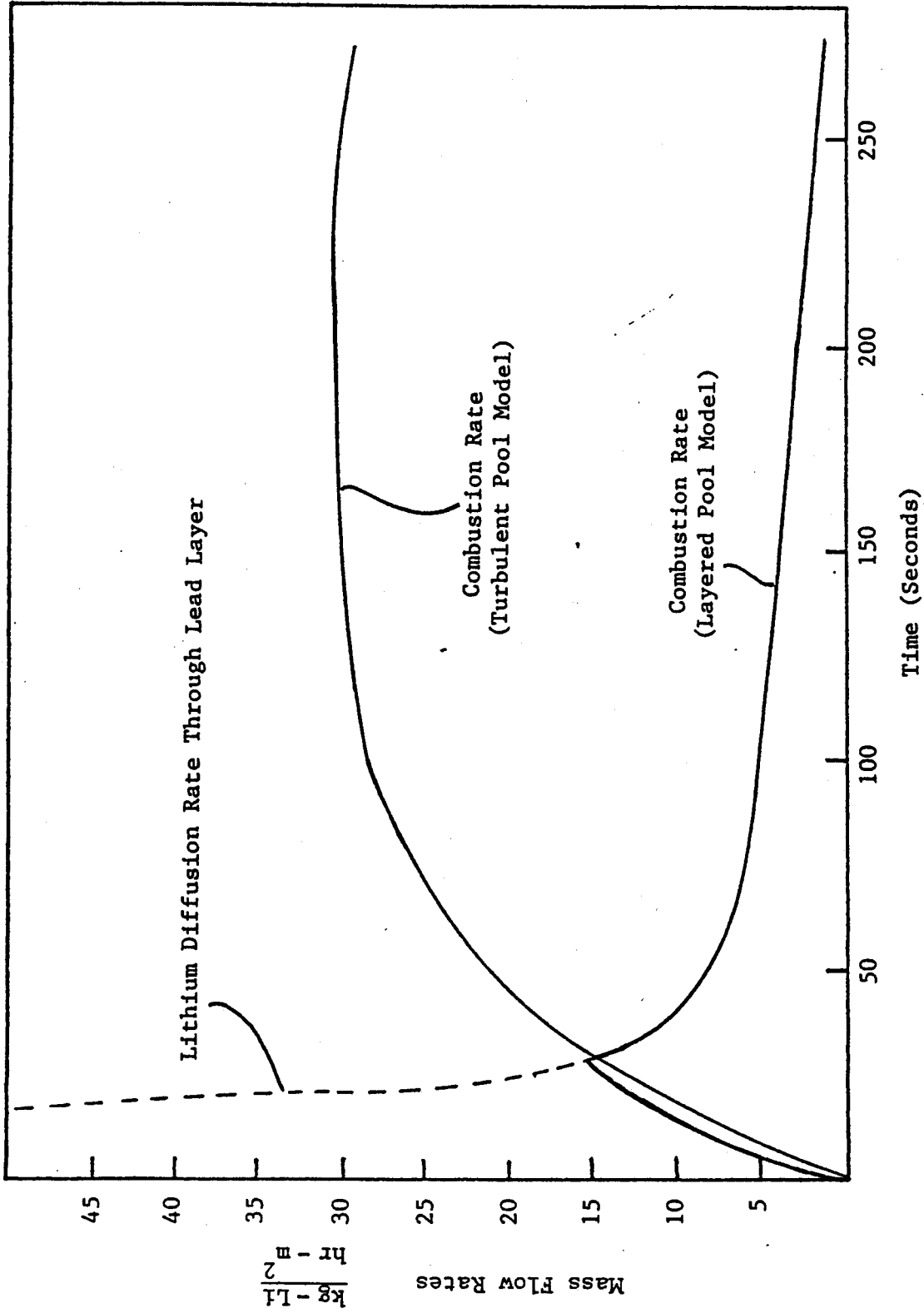


Figure 4.11: Effect of Lithium Diffusion Through Lithium-Lead on Combustion Rate

Alloy = LiPb

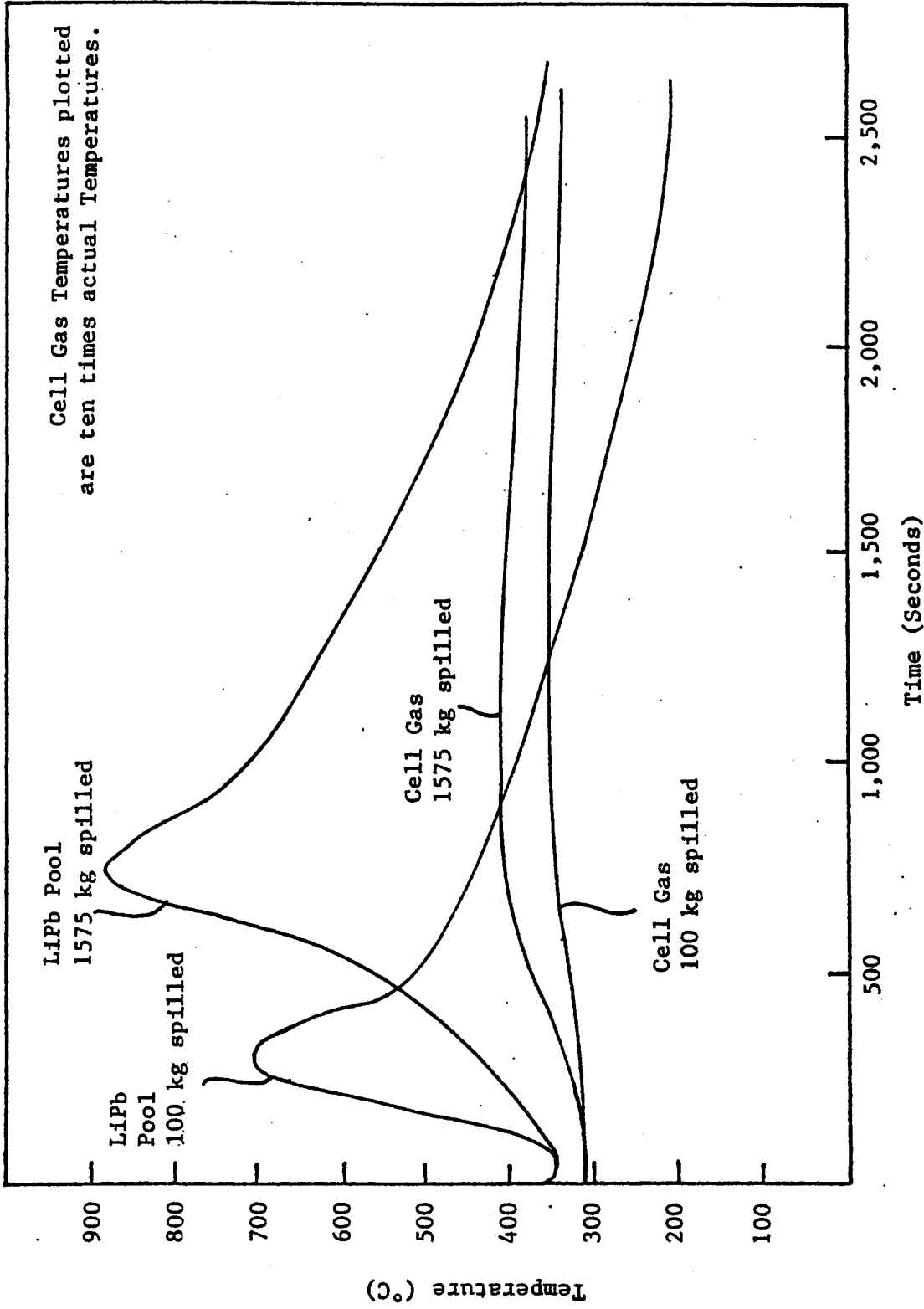


Figure 4.12: Predictions for Lithium-Lead Spill in HEDL Test Facility

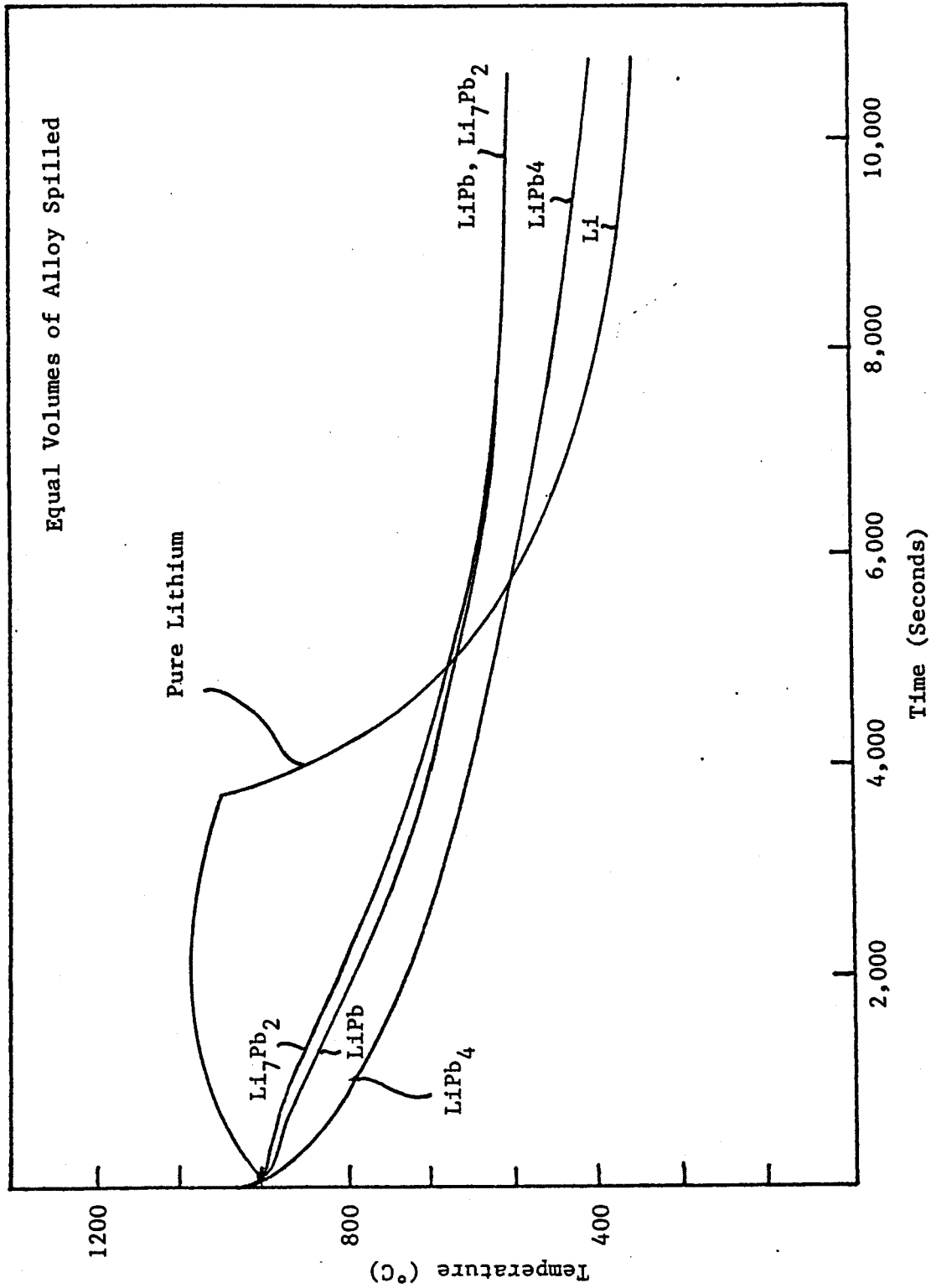


Figure 4.13: UWMK-III Average Pool Temperature History for Various LiPb Alloys Using Layered Pool Model.

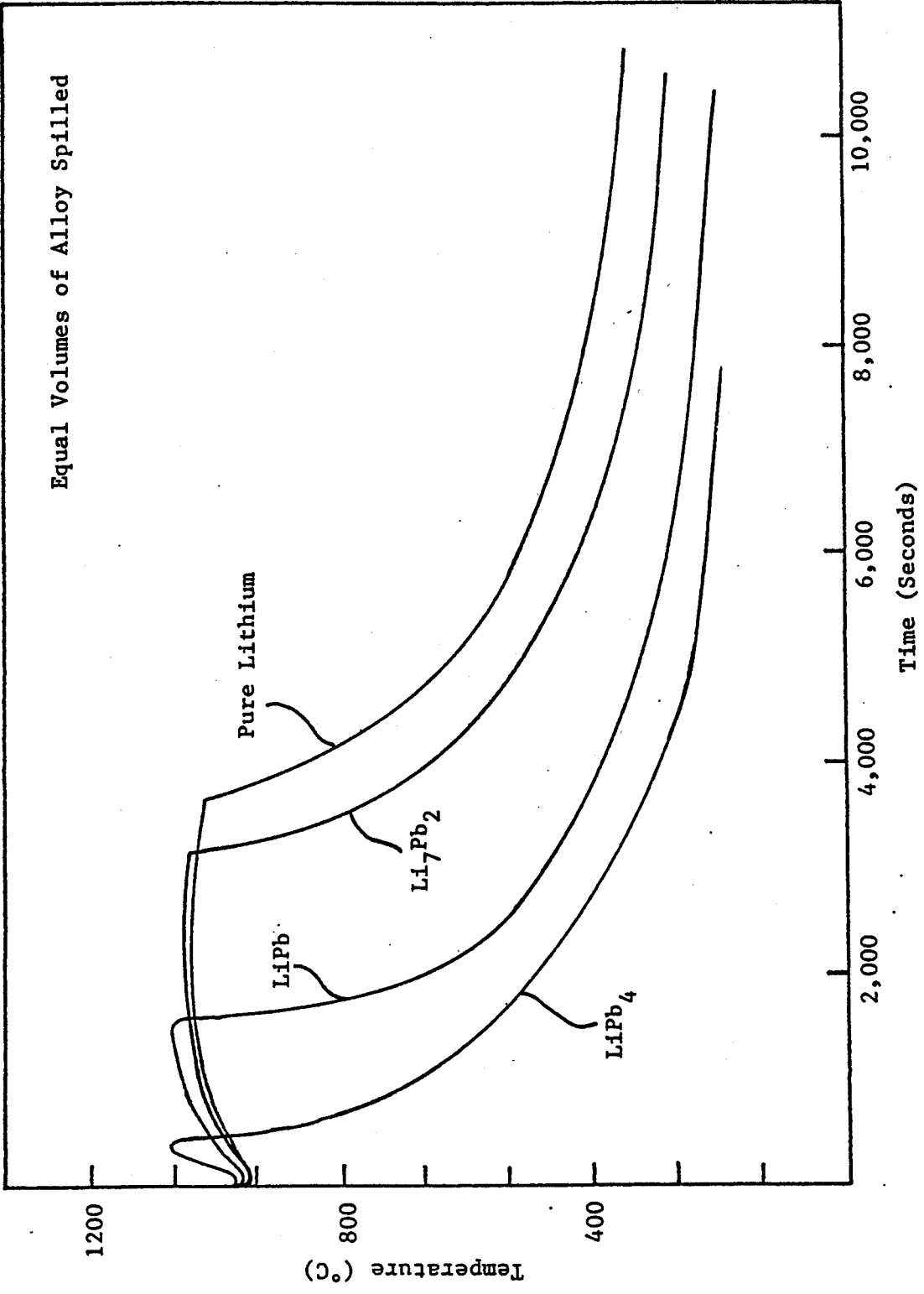


Figure 4.14: UWMAK-III Average Pool Temperature History for Various LiPb Alloys Using Turbulent Pool Model

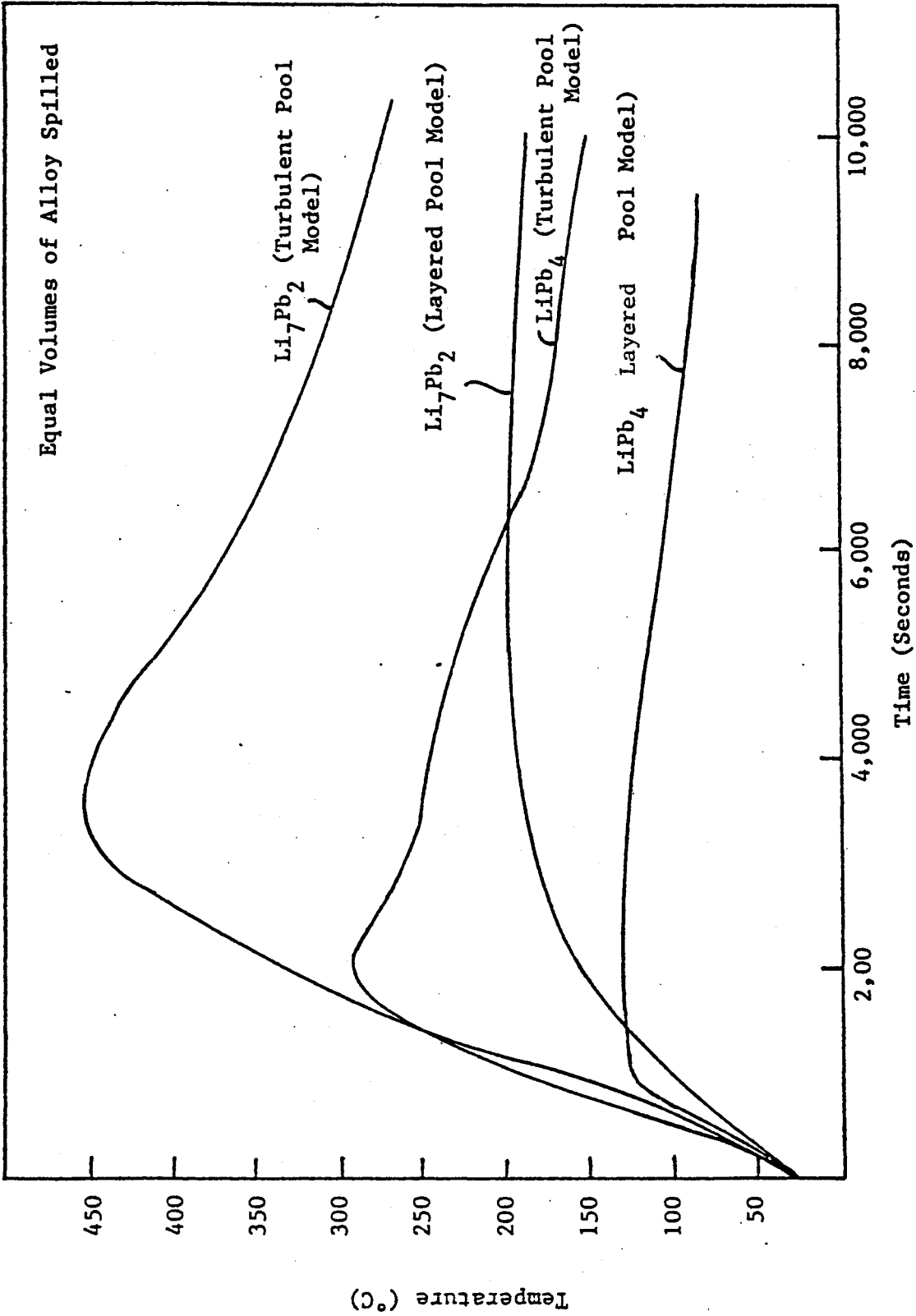


Figure 4.15: UWMK-III Cell Gas Temperature Profiles for Various Alloys

5. SUMMARY AND CONCLUSIONS

5.1. Code Development and Verification

The underlying purpose of this work was to continue the development of the LITFIRE computer code in order to more accurately assess the consequences of lithium spills and fires in fusion related systems. In order to evaluate the accuracy of the code, many comparisons with experiments have been performed. The most recent comparisons have been discussed in Chapter 2 and indicate that there is fairly close agreement for these particular test cases. However, this agreement was achieved at the expense of some discrepancy with earlier calculations, especially with respect to the combustion zone emissivity values. The present comparison indicates that high emissivities should be used (~ 0.9 or greater) while the work of Tillack indicated that very low emissivities (0.1 or less) would generate the closest agreement with experiment.

Results of the comparison for multiple species combustion indicate that LITFIRE tends to overpredict the combustion rate by more than a factor of three (on average) for both oxygen and nitrogen combustion. While this may be too conservative an estimate, no firm conclusions can be drawn from the present analysis because of the large inaccuracy in determining the actual experimental combustion rates. However, the temperatures and pressure predicted by LITFIRE for the HEDL test case LA-5 are in close agreement with the experimental results. This agreement would tend to validate the overall combustion rate prediction since the cell gas pressure and temperature are primarily dependent on the gas consumption rate and energy generation rate. The comparison of combustion zone and pool temperature coupling is presently limited in accuracy, since the relevant temperature profiles were not measured directly during the latest experiments.

The temperature and pressure profiles in the single containment scheme were found to be very sensitive to the combustion zone emissivity value chosen, less sensitive to the transmissivity of radiation through the combustion zone, and fairly insensitive to the removal of aerosols from the cell gas.

5.2. LITFIRE Applications

The applications of LITFIRE in the present work include use of both the single compartment and multi-compartment geometries. The single cell calculation was for a lithium spill in the containment building of UWMAK-III and updates predictions made by Tillack [10] and Dube [1] using earlier versions of the code. The most recent predictions indicate that the combustion zone and pool node's peak temperatures are lower by more than 100°C but the remaining nodes have temperature profiles quite similar in slope and magnitude to the earlier predictions.

The incorporation of an outer cell in the LITFIRE geometry, described in detail in Chapter 3, allowed much greater flexibility in modeling fusion related systems. The structural components associated with the vacuum torus within a reactor containment were modeled and the effect of cell gas communication on lithium fires was studied. The calculation presented is not indicative of any particular accident scenario but was chosen to compare the effects of a lithium fire within the torus to lithium fires within the larger reactor containment building. The results of this comparison indicate that the reduced amount of gas available inside the torus can significantly reduce the consequences of a large lithium spill. The effect is less pronounced when the lithium spill is smaller or when the orifice between the inner and outer cells is large enough to allow significant transport of gas to the reaction cell. In addition, the ignition time (time when fire begins after lithium is spilled) for a lithium fire in an initially evacuated cell (such as a torus) can be twenty minutes or longer, and is linearly dependent on the size of the orifice through which pressurization occurs.

5.3. Lithium-Lead Combustion

Experimental data on lithium-lead combustion is practically non-existent so two models were developed to sufficiently bound the problem from conservative and non-conservative viewpoints.

The inclusion of lithium-lead combustion in air greatly enhances the utility of LITFIRE in comparing safety aspects of alternate coolants and breeders in fusion reactors. In both of the models presented and discussed in Chapter 4 the geometry of LITFIRE is unchanged but the pool node properties and kinetics are significantly altered to include the effect of lead. The assessment of alternate coolants and breeders is by no means conclusive but should be taken as a preliminary indication as to which alloy may be less hazardous relative to the others considered.

Results of the comparison indicate that in both the conservative and non-conservative models the higher the concentration of lead in the alloy the lower the resulting temperatures will be. This effect is more pronounced in the layered pool model, due to the more rapid buildup of the lead layer with increasing lead concentration.

5.4. Recommendations for Further Development

LITFIRE now has the basic framework to perform many analyses of interest in lithium fire modeling. Among these are pure lithium reactions with air, water vapor, and concrete; lithium-lead reactions with air and water; in various containment schemes. However, all but the lithium-air reactions have not been compared with experimental data. It is expected in the near future that small scale experimental data will be available for all the remaining reactions modeled by LITFIRE.

Data is greatly needed to clarify the following parameters:

- **Combustion rate.** LITFIRE overpredicts the reaction rate for multiple species combustion. This may be due to incorrect modeling any combination of the following: mass diffusion rate of gases to the combustion zone by convection; the transport rate of lithium to the combustion zone by vapor diffusion; effect of product accumulation on either of the above; and the nitrogen hindrance factors for a given temperature and O₂ concentration. Accurate measurement of the gas consumption rates, temperatures, and O₂ concentration near the flames of the lithium fire would indicate which of the above effects are causing the discrepancy.
- **Pool and combustion zone coupling.** Values for the emissivity and transmissivity of the combustion zone have been inferred from various experiments. Recommended values for the emissivity vary widely depending on the size of the spill modeled, which may indicate that the emissivity is a strong function of combustion rate. Direct measurement of the radiative properties of flames in lithium fires is required to pinpoint the correct emissivity. In addition, the conductivity of the film region between the combustion zone and the pool may have a significant effect on the coupling of the two nodes but no measurements have yet been made to check the composition of this region. The effect of film conductivity would be greatly enhanced in LITFIRE if the pool region was divided into more than one node. The validity of using a single node for the pool is based on the high conductivity of lithium, but this assumption may be incorrect when lithium-lead is used due to the lower conductivity of lead.
- **Lithium-lead combustion.** Accurate measurement of the combustion rate of the lithium in lithium-lead alloys is needed before any evaluation of the two models presented in chapter 4 can be made. If possible, experiments should be designed to observe the pool kinetics as much as possible since this is the region that will be most affected by the presence of lead. If the experimental data that becomes available indicates that the present modeling in LITFIRE correctly bounds the reaction rate, then the next improvement in modeling might incorporate a diffusion model based on some degree of turbulence. This can be done using a lead layer whose thickness depends on the degree of turbulence and the magnitude of the combustion rate. In addition, direct measurement of the diffusion rate of lithium in lead would significantly improve the accuracy of the layered pool model.

The program itself has been extensively modified, modularized, and tested and now includes many options suggested by earlier developers. The following two suggestions are for improvements that would greatly increase the utility of LITFIRE use by the general fusion community, but at the expense of a fair amount of developmental effort. First, the addition of several nodes surrounding the inner steel wall and floor, with each node having unique physical properties. This would increase the flexibility of modeling a real tokamak, coolant piping system, or blanket module for example.

This change would be especially important for modeling the first wall and surrounding blanket and structural material. Second, to make LITFIRE compatible with other fusion related codes so that a comprehensive fusion safety code could be designed. This last suggestion is necessarily vague at this time but should be kept in mind whenever new developmental work is done on LITFIRE. A final suggestion is related to quality assurance but should not be underestimated in future efforts: each and every correlation in LITFIRE should be checked for coding accuracy and the source of the correlation well documented. The documentation is important since property data for lithium and other materials is continuously being updated and would indicate how contemporary the existing coding is.

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APPENDIX A

LITFIRE Data: HEDL Experiments LA-4 and LA-5

LA-4 HEDL TEST
USING VERSION OF LITFIRE: "LITFIR"
DATE: 17 AUGUST, 1982

OPTIONS IN EFFECT

IBLOW = 1 IESC = 0 ISFLC = 0 ISWICH = 0
IAROSL = 0 FLAGPN = T FLAG2 = F FLAGSI = T
FLAGAS = F FLAGC = F FLAGW = F FLAGF = F

PHYSICAL PROPERTIES

ENCONC = 0.9000 CPCON = 0.1560 KCON = 1.0000
RHCON = 144.0000 EMLI = 0.2000 CPLI = 0.9960
AKLI = 33.8000 RMLI = 30.0000 RHOLIO = 124.0000
RHOLIN = 66.9400 RHOLIN = 160.0000 EMGPF = 0.0400
EMCZ = 0.9000 TAUCZ = 0.1000

INNER CONTAINMENT DIMENSIONS

VP = 30086.0000 CMP = 66.7000 CPAP = 0.1247
XMOLA = 39.9000 FRA = 0.0250 RA = 3.0000

EXTRANEEOUS HEAT CAPACITY NODE DATA

TEHCZP = 643.0000 XMEHCP = 12300.0000 AEHCP = 5100.0000
CPEHCP = 0.1200 HINECP = 0.0900

SPIII PARAMETERS

ASLI = 1.3300 SPILL = 59.0000 SPRAY = 0.0000
ZLI = 1.4787

WALL AND FLOOR NODE DATA

NL = 6 NL1 = 6

THICKNESS OF CONCRETE WALL NODES

.200 .200 .200 .200 .200

THICKNESS OF CONCRETE FLOOR NODES

.200 .200 .200 .200 .200

PARAMETERS ASSOCIATED WITH OUTERMOST CONTAINMENT

THWC = 0.0000 THFC = 0.0000 GAP = 0.0000
 KGAP = 0.0150 KLEAK = 0.0000

PRIMARY STEEL WALL DATA

ESTLWP = 0.8500 CPSWP = 0.1200 KSTLWP = 30.0000
 RHSWP = 497.6498 AWP = 5600.0000 THWP = 0.0580

PRIAMRY STEEL FLOOR DATA

ESTLFP = 0.8500 CPSFP = 0.1200 KSTLFP = 30.0000
 RHSFP = 497.6498 AFP = 4000.0000 THFP = 0.0680

HEAT TRANSFER CORRELATION COEFFICIENTS

HIN = 0.1200 HINSAM = 0.0700 HINGSP = 0.1200
 HINGSS = 0.1200 HINPS = 0.0700 HINFAM = 0.0700
 HINFGS = 0.0700 HINFSG = 0.0700

COMBUSTION PARAMETERS

QCO = 18510.0000 RCMB0 = 0.8764 TVAP = 2456.0000
 RCMBH2 = 6.9300 PERCEN = 0.0000 QCO1 = 18510.0000
 QCO2 = 0.0000 RCMB01 = 0.8764 RCMB02 = 0.0000
 QCN = 4080.0000 RCMBN = 1.4870 TMELT = 353.0000
 QCW = 13784.0000 RCMBW = 0.3830 QVAP = 8431.0000

INITIAL CONDITIONS

PRIMARY

TGPZER = 548.0000 TSPZER = 543.0000 TCZI = 1560.0000
 TLII = 1660.0000 TSFPI = 541.0000 TA = 535.0000
 WOZP = 0.2316 WAP = 0.0094 WWAP = 0.0062
 PAPZER = 16.8700

INTEGRATION CONTROL PARAMETERS

IMETH = 3 DTMIN = 0.2000 TIMEF = 12000.0000
 RELERR = 0.0060 DELOUT = 2000.0000

MISCELLANEOUS INPUT ASSOCIATED WITH VARIOUS OPTIONS

INERT GAS FLOODING

W02B =	0.0000	BLOWV =	24.0000	CPAP =	0.1247
WWAB =	0.0000	TBLOUT =	325.0000	CPAB =	0.1247
WN2B =	0.0000	TBLIN =	310.0000	EXHSTV =	0.0000
TBLOW =	535.0000	XMOLAB =	4.0000		

STEEL FLOOR COOLING

SFLTIN =	0.0000	SFLCR =	0.0000	SFLEND =	0.0000
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EMERGENCY SPACE COOLING

ESCTIN =	0.0000	ESCR =	0.0000	ESCEND =	0.0000
----------	--------	--------	--------	----------	--------

DATA FOR SUSPENDED PAN OPTIONAL GEOMETRY:

TPANZO =	1560.0000	APAN =	9.7000	CPPAN =	0.1100
THKPAN =	0.0157	BREDTH =	4.1900		
KPAN =	13.0000	RHPAN =	488.0000		
THKIN1 =	0.2080	THKIN2 =	0.0416	AINS =	14.1500
RHINS =	8.0000	CPINS =	0.2550	EMINS =	0.9000
HINGPF =	0.0000				

SPRAY FIRE RESULTS

TGPZER =	548.0	PZEROP =	16.870
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LA-5 HEDL TEST THESIS RUN
USING VERSION OF LITFIRE: "LITFIR"
DATE: 17 AUGUST, 1982

OPTIONS IN EFFECT

IBLOW = 0 IESC = 0 ISFLC = 0 ISWICH = 0
IAROSL = 1 FLAGPN = T FLAG2 = F FLAGSI = T
FLAGAS = F FLAGC = F FLAGW = T FLAGF = T

PHYSICAL PROPERTIES

EMCONC = 0.9000 CPCON = 0.2650 KCON = 0.0227
RHCON = 144.0000 EMLI = 0.2000 CPLI = 0.9960
AKLI = 33.8000 RHLI = 30.0000 RHOLIO = 124.0000
RHOLIN = 86.9400 RHOLIH = 160.0000 EMGPF = 0.0400
EMCZ = 0.9000 TAUCZ = 0.1000

INNER CONTAINMENT DIMENSIONS

VP = 30086.0000 CHP = 66.7000 CPAP = 0.1247
XMOLA = 39.9000 FRA = 0.0500 RA = 5.0000

EXTRANEOUS HEAT CAPACITY NODE DATA

TEHCZP = 543.0000 XMEHCP = 12300.0000 AEHCP = 5100.0000
CPENCZP = 0.1200 HINECP = 0.0900

SPILL PARAMETERS

ASLI = 21.6500 SPILL = 220.0000 SPRAY = 0.0000
ZLI = 0.3387

WALL AND FLOOR NODE DATA

NL = 6 NL1 = 6

THICKNESS OF CONCRETE WALL NODES

.200 .200 .200 .200 .200

THICKNESS OF CONCRETE FLOOR NODES

.200 .200 .200 .200 .200

PARAMETERS ASSOCIATED WITH OUTERMOST CONTAINMENT

THWC = 0.0840 THFC = 0.0840 GAP = 0.0000
 KGAP = 0.0160 KLEAK = 0.0000

PRIMARY STEEL WALL DATA

ESTLWP = 0.8500 CPSWP = 0.1200 KSTLWP = 30.0000
 RHSWP = 497.6498 AWP = 5600.0000 THWP = 0.0580

PRIMARY STEEL FLOOR DATA

ESTLFP = 0.8500 CPSFP = 0.1200 KSTLFP = 30.0000
 RHSFP = 497.6498 AFP = 4000.0000 THFP = 0.0580

HEAT TRANSFER CORRELATION COEFFICIENTS

HIN = 0.1200 HINSAM = 0.0700 HINGSP = 0.1200
 HINGSS = 0.1200 HINPS = 0.0700 HINFAM = 0.0700
 HINFGS = 0.0700 HINFSG = 0.0700

COMBUSTION PARAMETERS

QCO = 18510.0000 RCMBO = 0.8764 TVAP = 2916.0000
 RCMBH2 = 6.8300 PERCEN = 0.0000 QCO1 = 18510.0000
 QCO2 = 0.0000 RCMBO1 = 0.8764 RCMBO2 = 0.0000
 QCN = 4080.0000 RCMBN = 1.4870 TMELT = 353.0000
 QCW = 13784.0000 RCMBW = 0.3830 QVAP = 8431.0000

INITIAL CONDITIONS

PRIMARY

TGPZER = 549.1750 TSPZER = 546.9600 TCZI = 1140.0000
 TLII = 1140.0000 TSFPI = 546.0000 TA = 540.5300
 W02P = 0.2316 WAP = 0.0094 WWAP = 0.0062
 PAPZER = 16.4330

INTEGRATION CONTROL PARAMETERS

IMETH = 3 DTMIN = 0.2000 TIMEF = 12000.0000
 RELERR = 0.0060 DELOUT = 2000.0000

AEROSOL REMOVAL FROM PRIMARY CONTAINMENT

BETA = 100.0000

DATA FOR SUSPENDED PAN OPTIONAL GEOMETRY:

TPANZO = 535.0000 APAN = 35.2900 CPPAN = 0.1200
THKPAN = 0.0157 BREDTH = 18.5000
KPAN = 13.0000 RHPAN = 490.0000

THKIN1 = 0.1867 THKIN2 = 0.0833 AINS = 14.1500
RHINS = 10.0000 CPINS = 0.2000 EMINS = 0.9000
HINGPF = 0.0000

SPRAY FIRE RESULTS

TGPZER = 549.2 PZEROP = 16.433

APPENDIX B

LITFIRE Data: Two-Cell Calculation

UWMAK-III TWO CELL TEST CASES WITH CRACK=0.0 CM**2
USING VERSION OF LITFIRE: "LITFIR" IN SI UNITS
DATE: 23 august, 1982

OPTIONS IN EFFECT

IBLOW = 0 IESC = 0 ISFLC = 0 ISWICH = 0
IAROSL = 0 FLAGPN = F FLAG2 = T FLAGSI = T
FLAGAS = F FLAGC = F FLAGW = T FLAGF = T

PHYSICAL PROPERTIES

EMCONC = 0.9000 CPCON = 653.0000 KCON = 1.7300
RHCON = 2306.6600 ENLI = 0.2000 CPLI = 4170.0000
AKLI = 48.4400 RHLI = 480.6500 RHOLIO = 1986.2900
RIOLIN = 1392.6400 RHOLIH = 2562.9500 EMGPF = 0.0400
ENCZ = 0.1000 TAUCZ = 0.5000

INNER CONTAINMENT DIMENSIONS

VP = 950.0000 CHP = 6.2000 CPAP = 622.0000
XMOLA = 40.0000 FRA = 0.7500 RA = 300.0000

EXTRANEEOUS HEAT CAPACITY NODE DATA

TEHCZP = 543.0000 XMEHCP = 12300.0000 AEHCP = 0.0000
CPEHCP = 502.0000 HINECP = 0.0000

SPILL PARAMETERS

ASLI = 150.0000 SPILL = 22000.0000 SPRAY = 0.0000
ZLI = 0.3052

WALL AND FLOOR NODE DATA

NL = 8 NL1 = 8

THICKNESS OF CONCRETE WALL NODES

.100 .100 .100 .150 .150 .150 .150 .100

THICKNESS OF CONCRETE FLOOR NODES

.100 .100 .100 .150 .150 .150 .150 .100

PARAMETERS ASSOCIATED WITH OUTERMOST CONTAINMENT

THWC = 0.2540 THFC = 0.6350 GAP = 0.0076
 KGAP = 0.0260 KLEAK = 0.0000

PRIMARY STEEL WALL DATA

ESTLWP = 0.8500 CPSWP = 502.0000 KSTLWP = 51.9000
 RHSWP = 7970.0000 AMP = 650.0000 THWP = 0.0500

PRIMARY STEEL FLOOR DATA

ESTLFP = 0.8500 CPSFP = 502.0000 KSTLFP = 51.9000
 RHSFP = 7970.0000 AFP = 160.0000 THFP = 0.0500

HEAT TRANSFER CORRELATION COEFFICIENTS

HIN = 0.1200 HINSAM = 0.0700 HINGSP = 0.1200
 HINGSS = 0.1200 HINPS = 0.0700 HINFAN = 0.0700
 HINFGS = 0.0700 HINFSG = 0.0700

COMBUSTION PARAMETERS

QCO = 42936.7002 RCMB0 = 0.8764 TVAP = 1615.0000
 RCMBH2 = 6.9300 PERCEN = 0.0000 QC01 = 42936.7002
 QCO2 = 0.0000 RCMB01 = 0.8764 RCMB02 = 0.0000
 QCN = 9464.1600 RCMBN = 1.4870 TMELT = 453.7000
 QCW = 31974.0000 RCMBW = 0.3830 QVAP = 19370.0000

INITIAL CONDITIONS

PRIMARY

TGPZER = 523.0000 TSPZER = 523.0000 TCZI = 593.0000
 TLII = 593.0000 TSFPI = 523.0000 TA = 300.0000
 W02P = 0.2316 WAP = 0.0000 WWAP = 0.0000
 PAPZER = 1.0000

INTEGRATION CONTROL PARAMETERS

IMETH = 3 DTHIN = 0.0300 TIMEF = 50222.0000
 RELERR = 0.00E0 DEIOUT = 2000.0000

SECONDARY CONTAINMENT DIMENSIONS

CHS =	45.0000	VS =	255000.0000	W02S =	0.2320
WWAS =	0.0000	WAS =	0.0000	CPAS =	522.0000
CRACK =	10.0000				

EXTRANEOUS HEAT CAPACITY NODE DATA

TEHCZS =	300.0000	XMEHCS =	11500.0000	AEHCS =	50.0000
CPEHCS =	502.0000	HINECS =	0.0900		

SECONDARY INITIAL CONDITIONS

TGSZER =	300.0000	TSSZER =	300.0000	TFSZER =	300.0000
PASZER =	101.4000				

SECONDARY STEEL WALL DATA

ESTLWS =	0.8500	CPSWS =	502.0000	KSTLWS =	51.9000
RHSWS =	7870.0000	AWS =	17000.0000	THWS =	0.0060

SECONDARY STEEL FLOOR DATA

ESTLFS =	0.8500	CPSFS =	502.0000	KSTLFS =	51.9000
RHSFS =	7870.0000	AFS =	6000.0000	THFS =	0.0060

SPRAY FIRE RESULTS

TGPZER =	941.4	PZEROP =	0.145
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APPENDIX C

LITFIRE Data: LiPb Combustion

UWMAK-III GEOMETRY LARGE SPILL COMPARISON.
USING VERSION OF LITFIRE: DIFSI
DATE: 13 SEPTEMBER 1982 RUN NUMBER: ONE

OPTIONS IN EFFECT

IBLOW = 0 IESC = 0 ISFLC = 0 ISWICH = 0
IAROSL = 0 FLAGPN = F FLAG2 = F FLAGSI = T
FLAGAS = F FLAGC = F FLAGW = T FLAGF = T
 FLAGPB = T FLAGDF = T

PHYSICAL PROPERTIES

EMCONC = 0.8000 CPCON = 0.1560 KCON = 1.0000
RHCON = 144.0000 EMLI = 0.2000 CPLI = 0.9960
AKLI = 28.0000 RHLI = 30.0000 RHOLIO = 124.0000
RHOLIM = 86.9400 RHOLIM = 160.0000 EMGPF = 0.0400
EMCZ = 0.1000 TAUCZ = 0.9000

INNER CONTAINMENT DIMENSIONS

VP = 8855700.0000 CHP = 150.0000 CPAP = 0.1247
XMOLA = 39.9000 FRA = 0.7500 RA = 300.0000

EXTRANEOUS HEAT CAPACITY NODE DATA

TEHCZP = 538.0000 XMEHCF = 6.0000 AENCP = 10.0000
CPEHCP = 0.1200 HINECP = 0.0900

SPILL PARAMETERS

ASLI = 10386.0000 SPILL = 763418.0000 SPRAY = 0.0000
ZLI = 2.4502

WALL AND FLOOR NODE DATA

NL = 8 NL1 = 8

THICKNESS OF CONCRETE WALL NODES

.100 .100 .100 .150 .150 .150 .150 .100

THICKNESS OF CONCRETE FLOOR NODES

.100 .100 .100 .150 .150 .150 .150 .100

PARAMETERS ASSOCIATED WITH OUTERMOST CONTAINMENT

THWC = 0.8333 THFC = 2.0833 GAP = 0.0021
KGAP = 0.0160 KLEAK = 0.0000

PRIMARY STEEL WALL DATA

ESTLWP = 0.8500 CPSWP = 0.1200 KSTLWP = 30.0000
RHSWP = 497.6498 ANP = 183532.0000 THWP = 0.0210

PRIMARY STEEL FLOOR DATA

ESTLFP = 0.8500 CPSFP = 0.1200 KSTLFP = 30.0000
RHSFP = 497.6498 AFP = 10386.0000 THFP = 0.0210

HEAT TRANSFER CORRELATION COEFFICIENTS

HIN = 0.1200 HINSAM = 0.0700 HINGSP = 0.1200
HINGSS = 0.0700 HINPS = 0.0700 HINFAM = 0.0700
HINFGS = 0.0700 HINFGS = 0.0700

COMBUSTION PARAMETERS

QCO = 18510.0000 RCMB0 = 0.8764 TVAP = 2916.0000
RCMBH2 = 6.9300 PERCEN = 0.0000 QCO1 = 18510.0000
QCO2 = 0.0000 RCMB01 = 0.8764 RCMB02 = 0.0000
QCN = 4080.0000 RCMBN = 1.4870 TMELT = 813.0000
QCW = 13784.0000 RCMBW = 0.3830 QVAP = 8350.0000

INITIAL CONDITIONS

PRIMARY

TGPZER = 538.0000 TSPZER = 538.0000 TCZI = 2300.0000
TLII = 2286.0000 TSFPI = 538.0000 TA = 538.0000
WO2P = 0.2310 WAP = 0.0000 WMAP = 0.0000
PAPZER = 14.7000

INTEGRATION CONTROL PARAMETERS

IMETH = 3 DTMIN = 1.0000 TIMEF = 12121.1000
RELERR = 0.0060 DELOUT = 2000.0000

DATA FOR LITHIUM LEAD COMBUSTION OPTION:

CPLEAD = 0.0350 KLEAD = 9.3000 RHLEAD = 708.0000
ALLOYI = 0.6000 QDISS = 3318.0000

MODIFIED PARAMETERS FOR LITHIUM IN LITHIUM LEAD POOL

AMOUNT OF LITHIUM AVAILABLE FOR COMBUSTION = 24744.8379

THICKNESS OF LIPB POOL IS LESS THAN ZLI ABOVE AND
IS CALCULATED IN PROGRAM

SPRAY FIRE RESULTS

TGPZER = 538.0 PZEROP = 14.700

APPENDIX D

Listing of the LITFIRE Computer Code

C -- forttran --

LIBP COMBUSTION MODELING INCLUDED

AKEXX SUBROUTINE INCLUDED

MODELED WITH: TAUCZ,EMGP=1.0ETC.,EMGF IS INCLUDED,KMIT/KLIT.
BETA AND STICK
SEPERATE EMISSIVIITES AND STEEL PROPERTIES.
NEW FLOOR NODE IN SECODARY.

IMPLICIT REAL (K,L,N)
LOGICAL FLAGW,FLAGF,FLAGL,FLAGPN,FLAGAS,FLAGH,FLAG2,FLAGSI,FLAGN,
FLAGC,FLAGPB
REAL INTGRL
COMMON // NAME(320),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGDF,ICZ
COMMON /LITH/ AKLI,ASLI,CPLI,CSBLI,HB,LIBP,LIL,LILP,LIT,
RHLI,SPILL,TLI,TLII,ZLI
COMMON /LEAD/ CPLEAD,KLEAD,RHLEAD,MLIPB,XALLDY,ATML,ATMPB,CMBR
COMMON /PBPOOL/ DMPBOT,ZZPB,MLEAD,TLEADI,XWLI,DFLIPB,XLIDOT,
THPB,TLEADF
COMMON /STEEL/ CPSFP,CPSFS,CPSWP,CPSWS,ESTLFP,ESTLWP,KSTLFP,
KSTLFS,KSTLWP,KSTLWS,RHSFP,RHSFS,RHSWP,RHSWS
COMMON /MISC/ AFP,AFS,AMP,AWS,C7,C21,GIN,
HA,HINFAM,HINSAM,HTCPGP,QRADC,RADC,RCZW,
RHOAP,RLIW,RWPWS,SIGMA,TA,TC(20),TFS,
TFSZER,TGP,TGS,TGPZER,TSFP,TSP,TSS,
TSSZER,THFP,THFS,THWP,THWS,ZZES,ZZS,ZZI,ZZ7
COMMON /INTGL/ IMETH,ICOUNT,ISTORE,INOIN,IPASS,DELT,
XIC(101),ZZZ(601)
COMMON /INJOP/ DP1,DP2,DP3,MNIINJ,MOXINJ,TIME,VP
COMMON /PANOP/ AINS,APAN,BREDTH,CLIST,CPINS,CPPAN,EMGP,FPG,FPW,
KPAN,RHINS,RHPAN,THKIN1,THKIN2,THKPAN,
TINS1,TINS1F,TINS1I,TINS2,TINS2F,TINS2I,
TPAN,TPANF,TPANZO,ZZ2,ZZ4,ZZ8,ZZ9
COMMON /CONOP/ CB,CPCON,DTBDT(20),DTCDT(20),GAP,KCON,KGAP,
L(20),L1(20),NL,NL1,QRADB,RADB,RHCON,
SFLCR,TB(20),TBF(20),TBIC(20),TCF(20),
TCIC(20),THFC,THWC,TSFPI,TSPZER,XSFL
COMMON /CCOP/ CMBRO,CRACON,DCOCZ,H2LEFT,QCCONC,RCMBO,RCMBW,
RELESE,TCIGNI,TCON,TCONF,XMHZOI,ZZC,ZZD,ZZDIN
COMMON /SECOF/ AEHCS,C11,C20,CHS,CPEHCS,CPH2,CPLIN,CPWA,CRACK,
FOUTP,FOUTS,FOUTT,HINF6S,HINF6G,HINF6SS,HINPS,KLEAK,
LEAK,MAIRP,MAIRS,MAIS,MAS,MH2S,MLIHS,MLINIS,MLINS,
MLI0IS,MLI0S,MNIIS,MNIS,MOXIS,MOXS,MWAIS,
MWAS,PAP,PAS,PASZER,RA,RBREAK,RHOLIN,
RHOLIN,RHOLIO,RWPGAS,TEHCS,TEHCSF,TEHCZS,TGSF,
TFSF,TGSZER,TSSF,VS,XMDOT,XMENC,XMOLA,ZZ3,ZZFS
COMMON /UNITS/ AENCP,BETA,CHP,CMBRH,CPAP,CPEHCP,MAP,MNIP,
MOXP,MWAP,PAPZER,QCN,QCO,QCO1,QCO2,QCW,QVAP,
TCZ,TCZF,TCZI,TEHCP,TEHCPF,TEHCZP,TGPF,
TLIF,TMELT,TSFPF,TSPF,TVAP,XMENC
COMMON /PBDIF/ CCZP,CGLI,CLIG,CPCZ,CPMCZ,DFILM,KFILM,PYUP,
QRADP,RCZP,RGLI,RIFCZP,RIFPG,RIFPW,RLIG,RWLI,
TLEAD,YAPCZ,ZZ6

open(unit=1,device='dsk',access='seqin',
file='indat1',mode='ascii')
open(unit=2,device='dsk',access='seqin',
file='indat2',mode='ascii')
open(unit=3,device='dsk',access='seqin',
file='indat3',mode='ascii')
open(unit=4,device='dsk',access='seqin',
file='indat4',mode='ascii')
open(unit=10,device='dsk',access='seqout',
file='outd1',mode='ascii')
open(unit=11,device='dsk',access='seqout',
file='outd2',mode='ascii')
open(unit=12,device='dsk',access='seqout',
file='outd3',mode='ascii')

```

      open(unit=13,device='dsk',access='seqout',
           file='outd4',mode='ascii')
      open(unit=14,device='dsk',access='seqout',
           file='outd5',mode='ascii')
C
C.....
C                               INPUT SECTION
C.....
C  SEE LITFIRE USERS GUIDE FOR DEFINITIONS AND DIMENSIONS OF INPUT VARIABLES
C
C.....      READ IN TITLE AND HEADINGS      .....
C
      READ (1,700) (NAME(I),I=1,80)
      READ (2,700) (NAME(I),I=81,160)
      READ (3,700) (NAME(I),I=161,240)
      READ (4,700) (NAME(I),I=241,320)
      700 FORMAT(20A4)
C
C.....      READ IN FLAGS AND OPTIONS      .....
C
C THE NEXT BUNCH OF STATEMENTS ARE HERE BECAUSE OF COMPILE TROUBLE AT
C LIVERMORE. HOPEFULLY THIS WILL BE CORRECTED SOON. (1/26/82).
C
      READ (1,701) IFLAGW,IFLAGF,IFLAGP,IFLAG2,IFLAGS,IFLAGC,
                  IFLAGU,IFLAGB,IBLOW,IESC,ISFLC,ISWICH,IAROSL,IFLAGD
      701 FORMAT(1X,14(I1,1X))
      FLAGW=.FALSE.
      FLAGF=.FALSE.
      FLAGP=.FALSE.
      FLAG2=.FALSE.
      FLAGAS=.FALSE.
      FLAGC=.FALSE.
      FLAGSI=.FALSE.
      FLAGPB=.FALSE.
      FLAGDF=.FALSE.
      IF (IFLAGW .EQ. 1) FLAGW=.TRUE.
      IF (IFLAGF .EQ. 1) FLAGF=.TRUE.
      IF (IFLAGP .EQ. 1) FLAGP=.TRUE.
      IF (IFLAG2 .EQ. 1) FLAG2=.TRUE.
      IF (IFLAGS .EQ. 1) FLAGAS=.TRUE.
      IF (IFLAGC .EQ. 1) FLAGC=.TRUE.
      IF (IFLAGU .EQ. 1) FLAGSI=.TRUE.
      IF (IFLAGB .EQ. 1) FLAGPB=.TRUE.
      IF (IFLAGD .EQ. 1) FLAGDF=.TRUE.
C
C.....      READ IN PRIMARY CONTAINMENT SPECIFICATIONS      .....
C
      READ (1,703) NL,NL1
      READ (1,704) (L(I),I=1,NL)
      READ (1,704) (L1(I),I=1,NL1)
      READ (1,702) VP,CNP,CPAP,XMOLA
      READ (1,702) TEHCZP,XMEHCP,AEHCP,CPEHCP,HINECP
      702 FORMAT (8F12.4)
      703 FORMAT (I4,I4)
      704 FORMAT (10F5.3/10F5.3)
C
C.....      READ IN PARAMETERS ASSOCIATED WITH      .....
C                               OUTERMOST CONTAINMENT SHELL AND CONCRETE
C
      READ (1,702) THWC,THFC,GAP,KGAP,KLEAK
      IF (THWC .LT. 0.001) FLAGW=.FALSE.
      IF (THFC .LT. 0.001) FLAGF=.FALSE.
C
C.....      READ IN PHYSICAL CONSTANTS      .....
C                               AND EMISSIVITIES
C
      READ (1,702) ESTLWP,CPSWP,KSTLWP,RHSWP,AWP,THWP
      READ (1,702) ESTLFP,CPSFP,KSTLFP,RHSFP,AFP,THFP
      READ (1,702) EMLI,CPLI,AKLI,RHLI
      READ (1,702) EMCONC,CPCON,KCON,RHCON
      READ (1,702) RHOLIO,RHOLIN,RHOLIH,EMGPF,EMCZ,TAUCZ
C

```

```

C..... READ IN REACTION CONSTANTS .....
C
  READ (1,702) QCO1,QCO2,QCN,QCW
  READ (1,702) RCMB01,RCNBO2,RCMBN,RCMBW,RCMBH2
  READ (1,702) TMELT,TVAP,QVAP,PERCEN
  RCMB0=((100.-PERCEN)*RCMB01+PERCEN*RCMB02)/100.
  QCO=((100.-PERCEN)*RCMB01*QCO1+PERCEN*RCMB02*QCO2)/(RCMB0*100.)
C
C..... READ IN HEAT TRANSFER CORRELATION COEFFICIENTS .....
C
  READ (1,702) HIN,HINGSP,HINGSS,HINPS,HINSAM,HINFAN
  READ (1,702) HINFGS,HINFSG
C
C..... READ IN SPILL PARAMETERS .....
C
  READ (1,702) ASLI,SPILL,SPRAY,FRA,RA
  ZLI=SPILL/RHLI/ASLI
C
C..... READ IN INITIAL CONDITIONS .....
C
  READ (1,702) TCZI,TGPZER,TSPZER,TSFPI,TA,TLII
  READ (1,702) PAPZER,W02P,WVAP,WAP
C
C..... READ IN INTEGRATION CONTROL PARAMETERS .....
C
  READ (1,705) IMETH,DTMIN,TIMEF,RELERR,DELOUT
  705 FORMAT(I4,5F12.4)
C
C..... OPTIONS .....
C
C..... CONTAINMENT FLOODING WITH INERT GAS OPTION .....
C
  DATA TBLIN,TBLOUT,BLOWV,EXHSTV,XBLOW,W02B,WN2B,WWAB,XMOLAB,CPAB,
  TBLOW/8*0.0,3*1.0/
C
C** READ IN GAS FLOODING PARAMETERS IF USING OPTION **
C
  IF (IBLOW.NE.1) GO TO 900
  READ (4,702) W02B,WWAB,WN2B,XMOLAB,CPAB,TBLOW
  READ (4,702) BLOWV,EXHSTV,TBLIN,TBLOUT
C
  900 CONTINUE
  WAB=1.-W02B-WN2B-WVAB
C
C..... EMERGENCY SPACE COOLING OF CONTAINMENT OPTION .....
C
  DATA XESC,ESCR,ESCTIN,ESCEND/4*0.0/
  IF (IESC.EQ.1) READ (4,702) ESCR,ESCTIN,ESCEND
C
C..... EMERGENCY STEEL FLOOR LINER COOLING OPTION .....
C
  DATA XSFL,SFLCR,SFLTIN,SFLEND/4*0.0/
  IF (ISFLC.EQ.1) READ (4,702) SFLCR,SFLTIN,SFLEND
C
C..... AEROSOL REMOVAL FROM PRIMARY CONTAINMENT .....
C
  IF (IAROSL .EQ. 1) READ (4,702) BETA
C
C..... CLOSURE OF CRACK BETWEEN PRIMARY AND SECONDARY .....
C
C.....
C
C..... PRINT OUT THE INPUT .....
C
C.....
C
  WRITE (10,800) (NAME(I),I=1,60)
  WRITE (10,801) IBLOW,IESC,ISFLC,ISWICH,IAROSL,FLAGPN,FLAG2,
  FLAGSI,FLAGAS,FLAGC,FLAGW,FLAGF,FLAGPB,FLAGDF

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WRITE (10,802) EMCONC,CPCON,KCON,RHCON,EMLI,CPLI,AKLI,RHLI,
      RHOLIO,RHOLIN,RHOLIH,EMGPF,EMCZ,TAUCZ
WRITE (10,803) VP,CHP,CPAP,XMOLA,FRA,RA
WRITE (10,804) TEHCZP,XMEHCP,AEHCP,CPEHCP,HINECP
WRITE (10,805) ASLI,SPILL,SPRAY,ZLI
WRITE (10,806) NL,NL1
WRITE (10,807) (L(I),I=1,NL)
WRITE (10,808) (L1(I),I=1,NL1)
WRITE (10,809) THWC,THFC,GAP,KGAP,KLEAK
WRITE (10,810) ESTLWP,CPSWP,KSTLWP,RHSWP,AWP,THWP
WRITE (10,811) ESTLFP,CPSFP,KSTLFP,RHSFP,AFP,THFP
WRITE (10,812) HIN,HINSAM,HINGSP,HINGSS,HINPS,HINFAM,HINFGS,HINFSG
WRITE (10,813) QCO,RCMBO,TVAP,RCMBH2,PERCEN,QCO1,QCO2,RCMBO1,
      RCMBO2,QCN,RCMBN,TMELT,QCW,RCMBW,QVAP
WRITE (10,814) TGPZER,TSPZER,TCZI,TLII,TSFPI,
      TA,WOPZ,WAP,WVAP,PAPZER
WRITE (10,815) IMETH,DTMIN,TIMEF,RELERR,DELOUT
C
C***** THE FOLLOWING PARAMETERS ARE ASSOCIATED WITH THE *****
C          DIFFERENT OPTIONS AND ARE WRITTEN ONLY WHEN USED
C
      IF (IBLOW.EQ.1.OR.ISFLC.EQ.1.OR.IESC.EQ.1) WRITE (10,819) W02B,
      BLOW,CPAP,WVAB,TBLOUT,CPAB,WN2B,TBLIN,EXHSTV,TBLOW,
      XMOLAB,SFLTIN,SFLCR,SFLEND,ESCTIN,ESCR,ESCEVO
C
      IF (IAROSL.EQ.1) WRITE (10,820) BETA
C
800 FORMAT (' ',3(20A4.)/,/)
801 FORMAT(' OPTIONS IN EFFECT'/1X,17(1H-)//T10,'IBLOW = ',I4,T25,
      'IESC = ',I4,T40,'ISFLC = ',I4,T55,'ISWICH = ',I4//T10,'IAROSL = ',
      I4,T25,'FLAGPN = ',L4,T40,'FLAG2 = ',L4,T55,'FLAGSI = ',L4//T10,
      'FLAGAS = ',L4,T25,'FLAGC = ',L4,T40,'FLAGW = ',L4,T55,'FLAGF = ',
      L4//T25,'FLAGPB = ',L4,T40,'FLAGDF = ',L4//)
802 FORMAT(' PHYSICAL PROPERTIES'/1X,19(1H-)//T10,'EMCONC = ',F12.4,
      T35,'CPCON = ',F12.4,T60,'KCON = ',F12.4//T10,'RHCON = ',F12.4,
      T35,'EMLI = ',F12.4,T60,'CPLI = ',F12.4//T10,'AKLI = ',F12.4,
      T35,'RHLI = ',F12.4,T60,'RHOLIO = ',F12.4//T10,'RHOLIN = ',F12.4,
      T35,'RHOLIH = ',F12.4,T60,'EMGPF = ',F12.4//T10,'EMCZ = ',F12.4,
      T35,'TAUCZ = ',F12.4//)
803 FORMAT(' INNER CONTAINMENT DIMENSIONS'/1X,28(1H-)//T10,'VP = ',
      F12.4,T35,'CHP = ',F12.4,T60,'CPAP = ',F12.4//T10,'XMOLA = ',
      F12.4,T35,'FRA = ',F12.4,T60,'RA = ',F12.4//)
804 FORMAT(' EXTRANEIOUS HEAT CAPACITY NODE DATA'/1X,33(1H-)//T10,
      'TEHCZP = ',F12.4,T35,'XMEHCP = ',F12.4,T60,'AEHCP = ',F12.4//
      T10,'CPEHCP = ',F12.4,T35,'HINECP = ',F12.4//)
805 FORMAT(' SPILL PARAMETERS'/1X,16(1H-)//T10,'ASLI = ',F12.4,T35,
      'SPILL = ',F12.4,T60,'SPRAY = ',F12.4//T10,'ZLI = ',F12.4//)
806 FORMAT(' WALL AND FLOOR NODE DATA'/1X,24(1H-)//T10,'NL = ',
      I2,T35,'NL1 = ',I2//)
807 FORMAT(' THICKNESS OF CONCRETE WALL NODES'/1X,31(1H-)//T10,
      '10(F5.3)//T10,10(F5.3)//)
808 FORMAT(' THICKNESS OF CONCRETE FLOOR NODES'/1X,32(1H-)//T10,
      '10(F5.3)//T10,10(F5.3)//)
809 FORMAT(' PARAMETERS ASSOCIATED WITH OUTERMOST CONTAINMENT'/1X,
      48(1H-)//T10,'THWC = ',F12.4,T35,'THFC = ',F12.4,T60,
      'GAP = ',F12.4//T10,'KGAP = ',F12.4,T35,'KLEAK = ',F12.4//)
810 FORMAT(' PRIMARY STEEL WALL DATA'/1X,23(1H-)//T10,
      'ESTLWP = ',F12.4,T35,'CPSWP = ',F12.4,T60,'KSTLWP = ',F12.4//T10,
      'RHSWP = ',F12.4,T35,'AWP = ',F12.4,T60,'THWP = ',F12.4//)
811 FORMAT(' PRIAMRY STEEL FLOOR DATA'/1X,24(1H-)//T10,
      'ESTLFP = ',F12.4,T35,'CPSFP = ',F12.4,T60,'KSTLFP = ',F12.4//T10,
      'RHSFP = ',F12.4,T35,'AFP = ',F12.4,T60,'THFP = ',F12.4//)
812 FORMAT(' HEAT TRANSFER CORRELATION COEFFICIENTS'/1X,38(1H-)//
      T10,'HIN = ',F12.4,T35,'HINSAM = ',F12.4,T60,'HINGSP = ',F12.4//
      T10,'HINGSS = ',F12.4,T35,'HINPS = ',F12.4,T60,'HINFAM = ',F12.4//
      T10,'HINFGS = ',F12.4,T35,'HINFSG = ',F12.4//)
813 FORMAT(' COMBUSTION PARAMETERS'/1X,21(1H-)//T10,'QCO = ',F12.4,
      T35,'RCMBO = ',F12.4,T60,'TVAP = ',F12.4//T10,'RCMBH2 = ',F12.4,
      T35,'PERCEN = ',F12.4,T60,'QCO1 = ',F12.4//T10,'QCO2 = ',F12.4,
      T35,'RCMBO1 = ',F12.4,T60,'RCMBO2 = ',F12.4//T10,'QCN = ',F12.4,
      T35,'RCMBN = ',F12.4,T60,'TMELT = ',F12.4//T10,'QCW = ',F12.4,
      T35,'RCMBW = ',F12.4,T60,'QVAP = ',F12.4//)

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WN2P=1.-WO2P-WWAP-WAP
XMOLP=1./(WO2P/32.+WN2P/28.+WWAP/18.+WAP/XMOLA)
RINP=1645./XMOLP
TEHCP=TEHCZP
TLI=TLII
TCZ=TCZI
TSP=TSPZER
TSFP=TSFPI
RHOAIP=PAPZER*144./RINP/TGPZER
RHOAP=RHOAIP
MNIIP=WN2P*RHOAIP*VP
MOXIP=WO2P*RHOAIP*VP
MNIP=MNIIP
MLIOIP=LIS*(1.+RCMBO)/RCMBO
MWAIP=WWAP*RHOAIP*VP
MWAIP=MWAIP
MAIP=WAP*RHOAIP*VP
MAP=MAIP
C
C***** INITIALIZE OPTION VARIABLES *****
C
IF (FLAG2) CALL CELL2
IF (.NOT. FLAG2) RBREAK=0.0
IF (FLAGN) CALL PAN
IF (FLAGC) CALL CONCC
FLAGN=.TRUE.
IF (FLAGW) CALL CONCW
IF (FLAGF) CALL CONCF
FLAGN=.FALSE.
BLOWR=1.35E-03*BLOWV
EXHSTR=1.35E-03*EXHSTV
STICK=0.0
IF (IAROSL .EQ. 1) STICK=AWP/(VP*BETA)/12.
IF (STICK .GE. 1.0) GO TO 986
IF (STICK .GT. .25) WRITE (11,823)
823 FORMAT (' AEROSOL REMOVAL FRACTION IS GREATER THAN ONE QUARTER
. OF AEROSOL INVENTORY. TIME STEP HAS BEEN DECREASED TO INSURE
. STABILITY.')
IF (STICK .GT. .25) IPAGE=IPAGE+2
C
C***** CONVERSION TO FT. - LB. - SEC. *****
C
AKLI=AKLI/3600.
KSTLWP=KSTLWP/3600.
KSTLFP=KSTLFP/3600.
KCON=KCON/3600.
KGAP=KGAP/3600.
C
C
C*****
C* SPRAY FIRE COMPUTATION STARTED *
C*****
C
C***** CHECK THAT ENOUGH OXYGEN IS LEFT FOR POOL FIRE AFTER SPRAY FIRE ***
C
OXLFS=WO2P*RHOAP*VP-LIS/RCMBO
IF (OXLFS .LT. 0.0) LIS=RCMBO*WO2P*RHOAIP*VP
IF (OXLFS .LT. 0.0) OXLFS=0.0
C
IF (LIS.LE.0.0) GO TO 902
TO=TGPZER
QIN= LIS*(QCO+CPLI*(TLI-TO))
FF2=QIN
TE=TGPZER+1.
901 CONTINUE
C***** SPECIFIC HEAT FOR DILITHIUM OXIDE *****
C CP = .0602*T**.326 T = DEG. R
C IF A DIFFERENT REACTION PRODUCT IS DESIRED, THE INTEGRAL OF THE
C DESIRED PRODUCT MUST BE SUBSTITUTED IN QOUT1.
C*****
QOUT1=(1.+RCMBO)/RCMBO*LIS*(0.0602/1.326)*(TE**1.326-TO**1.326)

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QOUT2=WN2P*RHOAP*VP*(.172*(TE-TO)+8.57E-06/2.*(TE*TE-TO*TO)+
1.02E-09/3.*(TE**3.-TO**3.))
QOUT3=OXLFS*(.184*(TE-TO)+3.2E-6/2.*(TE**2.-TO**2.))+1.36E04*
(1./TE-1./TO)
QOUT4=WWAP*RHOAP*VP*(0.44*(TE-TO))+WAP*RHOAP*VP*CPAP*(TE-TO)
FF1=QIN-QOUT1-QOUT2-QOUT3-QOUT4
IF (FF1*FF2.LT.0.) GO TO 903
TE=TE+1.
IF (TE.GT.1.0E06) GO TO 979
FF2=FF1
GO TO 901
C***** PORTION OF PROGRAM FOR GETTING INITIAL GAS TEMP. AND PRESS. ****
902 CONTINUE
TE=TGPZER
903 CONTINUE
TGP=TE
MOXP=MOXIP-LIS/RCMBO
MOXIP=MOXP
MLIOP=MLIOP
XMAIRP=MNIP/28.+MOXP/32.+MAP/XMOLA+MWAP/18.
PZEROP=1545.*XMAIRP*TGP/144./VP
PAP=PZEROP
TGPZER=TGP
WRITE (10,825) TGP,PZEROP
825 FORMAT (// ' SPRAY FIRE RESULTS'//1X,18(1H-)//6X,'TGPZER = ',F6.1,
' PZEROP = ',F8.3//)
C***** SPRAY FIRE COMPUTATION CONCLUDED *****
C
CALL INIT
C
C*****
C* START OF DYNAMIC CYCLE *
C* ----- *
C* START OF INTEGRATION CYCLE *
C*****
C
200 CONTINUE
C***** INJECTION OF GASES TO MODEL HEDL EXPERIMENT *****
MOXINJ=0.0
MNIINJ=0.0
IF (FLAGAS) CALL INJEC
C
C***** COMPUTE PHYSICAL PROPERTIES DEPENDENT ON TEMPERATURE *****
C***** CALCULATE AIR COMPOSITION AND SPECIFIC HEAT AT CONST. VOLUME *****
C
MAIRP=MOXP+MNIP+MWAP+MH2P+MAP
RHOAP=MAIRP/VP
FOXP=MOXP/MAIRP
FWAP=MWAP/MAIRP
FNIP=MNIP/MAIRP
CPO2P=(0.184+3.2E-06*TGP-1.36E04/(TGP*TGP))
CPMOXP=CPO2P*MOXP
CPN2P=(0.172+8.57E-06*TGP+1.02E-09*TGP*TGP)
CPMNIP=CPN2P*MNIP
CPWA=0.44
CPH2=3.76
CPLIN=0.67
CPLIOP=0.0602*TGP**.326
CPLINP=0.3368+3.67E-04*TGP
CPMLOP=CPLIOP*MLIOP
C
C
RHLI=33.49-.0035*(TLI-460.)
AKLI=(10.48+2.767E-03*(TLI-817.))-0.322E-06*(TLI-817.)**2/1488.
CPFAC=0.004938*TLI-6.20741
CPLI=1.0037-.01063*CPFAC-.00564*CPFAC**2-.001279*CPFAC**3
CPLI=((LIT-LIBP)*CPLI+LILOX*CPLIOP+LILNI*CPLINP)/LILP
C
IF (FLAGPB) CALL LIPB
C
C***** TWO MILLIMETERS ARE ASSUMED TO COVER THE POOL OPTICALLY *****
ZP=(LILOX/RHOLIO-LILNI/RHOLIN)/ASLI

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EMF=0.0
IF (EMLI.LT.EMF)EMLI=0.2+(EMF-0.2)*ZP/0.00666
C
HTCPGP=CPMOXP+CPMNIP+CPMLOP+CPAP*NAP+CPLINP*MLINP+CPLIH*MLIHP+
CPH2*MHZP+CPWA*WAP
C
EMGP=1.-EXP(-(MLIOP/RHOLIO+MLINP/RHOLIN+MLIHP/RHOLIN)*
2.27E06*CHP/VP/RA)
EMGP=EMGP*EMGPF
IF (EMGP .LE. 0.005) EMGP=0.005
C
C***** CALCULATING RADIATIVE INTERCHANGE FACTORS *****
C FPG AND FPW REPRESENT VIEW FACTORS FROM THE POOL. THEY ARE
C INITIALIZED AS UNITY IF PAN IS NOT PRESEN. INITIALIZED IN
C PAN OPTION IF IT IS USED. TAUCZ IS USED INSTEAD OF (1.-EMCZ)
C TO MORE FLEXIBLY MODEL COMBUSTION ZONE-POOL COUPLING.
C
RIFPW=1./(((1.-EMLI)/EMLI+(1.-ESTLWP)*ASLI/ESTLWP/AWP+1./
((1.-EMGP)*(ICZ*(TAUCZ-1.)+1.)*FPW+EMGP/(ASLI/AWP+1./
FPG/(ICZ*(TAUCZ-1.)+1.))))
RIFCZW=1./(((1.-EMCZ)/EMCZ+(1.-ESTLWP)*ASLI/ESTLWP/AWP+1./
((1.-EMGP)+EMGP/(1.+ASLI/AWP))))
RIFPG=(EMLI*EMGP)/((1.-EMLI)*EMGP+EMLI/FPG/(ICZ*(TAUCZ-1.)+1.))
RIFCZG=(EMCZ*EMGP)/((1.-EMCZ)*EMGP+EMCZ)
RIFSCW=(ESTLWP*EMCONC)/(ESTLWP+EMCONC-ESTLWP*EMCONC)
RIFSCF=(ESTLFP*EMCONC)/(ESTLFP+EMCONC-ESTLFP*EMCONC)
RIFCZP=(EMLI*EMCZ)/(EMCZ+EMLI-EMCZ*EMLI)
C
C***** CALCULATING GAS CONVECTION COEFFICIENT *****
C
C the following calculation invokes Reynold's analogy between
C heat and mass transfer by assuming that
C
C 
$$Sh=c(GrSc)^{1/3}$$

C
C The Sherwood number,  $(h L / D)$ , is defined by the relation:
C
C 
$$j = \frac{h}{m} \frac{\rho_1 (w_1 - w_2)}{\rho_2}$$

C
C Reynold's analogy, together with the Lewis relation, gives us:
C
C 
$$\frac{h}{m} = \frac{h}{c} \frac{\rho_1}{\rho_2} \frac{C}{p}$$

C
C In LITFIRE,  $w_2$  is assumed to be zero.
C
C
C POOL OR COMBUSTION ZONE TO PRIMARY GAS
IF (ICZ .EQ. 1) T1=0.5*(TGP+TCZ)
IF (ICZ .EQ. 0) T1=0.5*(TGP+TLI)
B1= 1.0/T1
D1=((4.94E-05*T1+0.0188)/(RHOAP*3600.))**2
AK1=(0.014+1.92E-05*(T1-480.))/3600.
IF (ICZ .EQ. 1) EXX=(GIN*B1*ABS(TCZ-TGP)/D1)
IF (ICZ .EQ. 0) EXX=(GIN*B1*ABS(TLI-TGP)/D1)
IF (EXX .LE. 0.0) GO TO 985
EX1 = (EXX)**0.3333
DIFF=241.57/(132.0+T1/1.8)*(T1/493.2)**2.5/3600.
HFINF=HIN*DIFF*EX1
HBINF=HIN*AK1*EX1
IF (TAU .LT. DELT) TAU=DELT
HF=HF+(HFINF-HF)*DELT/TAU
HB=HB+(HBINF-HB)*DELT/TAU
C
C***** CALCULATING GAS HEAT TRANSFER COEFFICIENTS *****
C PRIMARY GAS TO PRIMARY STEEL LINER
HGWP=HINGSP*AKEXX(TGP,ISP,RHOAP)
C PRIMARY GAS TO PRIMARY EXTRANCOUS HEAT CAPACITY
HEHCP=HINECP*AKEXX(TGP,TEHCP,RHOAP)

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C PRIMARY STEEL LINER TO AMBIENT IF NOT TWO CELL OR CONCRETE OPTION
  IF (.NOT. (FLAG2 .OR. FLAGW)) HA=MINSAM*AKEXX(TSP,TA,.074)
C PRIMARY STEEL FLOOR TO AMBIENT (IF NOT TWO CELL OR CONCRETE)
  IF (.NOT. (FLAG2 .OR. FLAGF)) HAMF=HINFAM*AKEXX(TSFP,TA,.074)
C ***** CALCULATING THERMAL DIFFUSIVITIES BETWEEN NODES *****
  IF (FLAGW) CALL CONCW
  IF (FLAGF) CALL CONCF
  CEHCGP=HEHCP*AEHCP/HTCPGP
  CGPEHC=HEHCP*AEHCP/XMEHCP/CPEHCP
  C1=KSTLWP*HGWP*AWP/HTCPGP/(THWP*HGWP/2.+KSTLWP)
  C6=KSTLWP*HGWP/(RHSWP*CPSWP*THWP*(THWP*HGWP/2.+KSTLWP))
C THE NEXT THERMAL DIFFUSIVITY IS VALID ONLY IF NO WALL CONCRETE AND
C NO SECONDARY CONTAINMENT CELL, AND IS BETWEEN STEEL LINER AND AMBIENT
  IF (.NOT. (FLAGW.OR.FLAG2)) C11=KSTLWP*HA/(RHSWP*CPSWP*THWP*
    (KSTLWP*THWP*HA/2.))
  IF (.NOT. (FLAGW.OR.FLAG2)) C12=KSTLFP*HAMF/(RHSFP*CPSFP*THFP*
    (KSTLFP*THFP*HAMF/2.))
C
C
C.....
C REPEAT ABOVE CALCULATIONS DEPENDENT ON TEMPERATURE FOR SECONDARY
C CONTAINMENT
C
C IF (FLAG2) CALL CELL2
C.....
C
C***** TESTING TO SEE IF EMERGENCY SPACE COOLING OR STEEL COOLING IN EFFECT
  IF (TIME .GT. ESCFIN) XESC=1.
  IF (TIME .GT. ESCEND) XESC=0.
  IF (TIME .GT. SFLFIN) XSFL=1.
  IF (TIME .GT. SFLEND) XSFL=0.
C
C***** LITHIUM LEAD DIFFUSION CALCULATION IN PREPERATION *****
C FOR COMBUSTION RATE CALCULATION
C IF (FLAGDF) CALL LIDIFF
C***** TESTING FOR COMBUSTION *****
  ICNI=0
  TEZ=(TCZ+TLI)/2.
  IF (TEZ .LE. 2340. .AND. FOXP.LE.0.28 .AND. MNIP.GT.0.0) ICNI=1
  IF (.NOT.(ILIT.EQ.0 .OR.(ICMB.EQ.0 .AND. ICNI.EQ.0) .OR. TLI.LT.
    TMELT)) GO TO 909
  IF (ICZ.EQ.1)WRITE (11,827)ICZ,ICNI,ILIT,ICMB,TCZ,FOXP,TLI,TIME
827 FORMAT(' COMBUSTION HAS JUST STOPPED. PARAMETERS ARE ICZ=',I1,
  ' ICNI=',I1,' ILIT=',I1,' ICMB=',I1,' TCZ=',F8.2,' FOXP=',
  F7.3,' TLI=',F8.2,' AT TIME=',F9.2)
  IF (ICZ.EQ.1) IPAGE=IPAGE+2
  GO TO 910
C
C
C.....
C COMPUTATIONS USING COMBUSTION ZONE MODEL *****
C
C***** COMPUTING RATE OF LITHIUM COMBUSTION *****
909 RN2=0.
  ICZ=1
  IF (TEZ.LT.1900. .AND. FOXP .LE. 0.28) RN2=
    (1.0-FOXP/0.28)/EXP(((1900.-TEZ)/666.)**2.76)
  IF (TEZ.GE.1900. .AND. TEZ.LE. 2340. .AND. FOXP.LE.0.28) RN2=
    (1.0-FOXP/0.28)*(1.-((TEZ-1900.)/440.)**2)
  CMBRO=HF*FOXP*RHOAP*RCMBO
  CMBRN=HF*FNIP*RHOAP*RCMBN*RN2
  CMBRW=HF*FWAP*RHOAP*RCMBW
  CMBR = CMBRO + CMBRN + CMBRW
  IF (.NOT. FLAGDF) GO TO 1909
  IF (CMBR .LT. XLIDOT) GO TO 1909
  CMBRO=CMBRO*XLIDOT/CMBR
  CMBRN=CMBRN*XLIDOT/CMBR
  CMBRW=CMBRW*XLIDOT/CMBR
  CMBR=CMBRO+CMBRN+CMBRW
1909 CONTINUE
  IF (CMBR*3600. .LT. 0.2) GO TO 910
  RNILB=CMBRN*ASLI/RCMBN

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ROXLB=CMBRO*ASLI/RCMBO
RWALB=CMBRW*ASLI/RCMBW
C
C***** COMPUTATION OF LITHIUM VAPOR DIFFUSION *****
TFEFF=0.002*(TCZ+TLI)/2.-3.92
PLIV=(10.***(4.8831-14180.2/TLI))**14.
IF (FLAGPB) PLIV=ACTVTV(XALLOY)*PLIV
RHOLIV=PLIV**144./RINP/TLI
DIFFLI=3.56E-03*((TLI/460.))**1.81)/PAP
DFILM=DIFFLI*RHOLIV/CMBR
EFILM=DFILM**12.
C
KNIT=.0432+TFEFF*(.0078-TFEFF*(8.2E-04+TFEFF*2.08E-04))
KLIT=0.65+TFEFF*(-4.99E-04+TFEFF*1.208E-07)
KFILM=(PLIV*(KLIT-KNIT)+PAP*KNIT)/14.7
C***** COMPUTATION OF HEAT TRANSFER COEFFICIENTS *****
YAPCZ=KFILM*AKLI*ASLI/(DFILM*AKLI+KFILM*ZLI/2.)
C***** THIS HEAT CAPACITY IS SHEER GUESS WORK THE 0.1 IS FOR LOW COMB. RATES
CPMCZ=ASLI*((1.+RCMBO)/RCMBO*CMBRO*CPLIOP+(1.+RCMBN)/RCMBN*CMBRN*
CPLIN+((1.+RCMBW)/RCMBW-(1./RCMBH2))*CMBRW*CPWA+(1.+RCMBH2)/
RCMBH2*CMBRW*CPH2+RN2*HF*FNIP*RHOAP*CPN2P)*300.+1.
IF (CPMCZ/ASLI .LE. 0.001) CPMCZ=0.001*ASLI
CGCZ=HB*ASLI/CPMCZ
CCZG=HB*ASLI/HTCPGP
CPCZ=YAPCZ/CPMCZ
CCZP=YAPCZ/(CPLI*LIL)
CCZ=(CMBRO*QCO+CMBRN*QCN+CMBRW*QCW)*ASLI
CLIST=2.*AKLI*AKLI*KSTLFP/(LIL*CPLI*(ZLI*KSTLFP+THFP*AKLI))
CSBLI=2.*AKLI*KSTLFP/(RHSFP*THFP*CPSFP*(ZLI*KSTLFP+THFP*AKLI))
QRADP=SIGMA*ASLI*(TCZ**4-TLI**4)*RIFCZP
QRADW=SIGMA*ASLI*(TCZ**4-TSP**4)*RIFCZW
QRADG=SIGMA*ASLI*(TCZ**4-TGP**4)*RIFCZG
RCZW=QRADW/(THWP*AMP*RHSWP*CPSWP)
RCZP=QRADP/(LIL*CPLI)
RCZG=QRADG/HTCPGP
QRADY=SIGMA*ASLI*(TLI**4-TSP**4)*RIFPW
QRADZ=SIGMA*ASLI*(TLI**4-TGP**4)*RIFPG
RLIW=QRADY/(THWP*AMP*RHSWP*CPSWP)
RWLI=QRADY/CPLI/LIL
RGLI=QRADZ/CPLI/LIL
RLIG=QRADZ/HTCPGP
C
C
C*****
C* CALCULATING TEMPERATURE RATES OF CHANGE WITH COMBUSTION *
C*****
C
C***** CALCULATE COMB. ZONE TEMP. RATE OF CHANGE DEG. R/SEC. *****
ZZ6=(CCZ-(QRADP+QRADW+QRADG))/CPMCZ+QVAP*CMBR*ASLI/CPMCZ
-CPCZ*(TCZ-TLI)-CGCZ*(TCZ-TGP)
C
C***** CALC. LITHIUM TEMP. RATE OF CHANGE DEG. R/SEC. *****
ZZ1=CCZP*(TCZ-TLI)+RCZP-CLIST*(TLI-TSFP)-QVAP*CMBR*ASLI*CCZP/YAPCZ
-RWLI-RGLI
C
C***** CALC. CELL GAS TEMP. RATE OF CHANGE DEG. R/SEC. *****
ZZ4=C1*(TSP-TGP)+CCZG*(TCZ-TGP)+RCZG+RBREAK+XBLOW*BLOWR*CPAB*
(TBLOW-TGP)/HTCPGP-ESCR*XESC/HTCPGP+CEHCGP*(TEHCP-TGP)+RLIG
C
C***** CALC. WALL STEEL TEMP. RATE OF CHANGE DEG. R/SEC. *****
ZZ5=C6*(TGP-TSP)+RCZW+RLIW
GO TO 911
C
C
C*****
C* COMPUTATIONS WITHOUT COMBUSTION ZONE MODEL *
C*****
C
910 CONTINUE
ICZ=0
CMBR=0.0
RNZ=0.0

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YALIG=AKLI*HB*ASLI/(AKLI*HB*ZLI/2.)
CLIG=YALIG/HTCPGP
QRADW=SIGMA*ASLI*(TLI**4-TSP**4)*RIFPW
QRADG=SIGMA*ASLI*(TLI**4-TGP**4)*RIFPG
RLIW=QRADW/(THWP*AWP*RHSWP*CPSWP)
RWLI=QRADW/CPLI/LIL
RGLI=QRADG/CPLI/LIL
RLIG=QRADG/HTCPGP
CGLI=YALIG/(LIL*CPLI)
CLIST=2.*ASLI*AKLI*KSTLFP/(LIL*CPLI*(ZLI*KSTLFP+THFP*AKLI))
CSBLI=2.*AKLI*KSTLFP/(RHSFP*THFP*CPSFP*(ZLI*KSTLFP+THFP*AKLI))
C
C*****
C* CALCULATING TEMPERATURE RATES OF CHANGE *
C*****
C
C***** CALC. LITHIUM TEMP. RATE OF CHANGE DEG. R/SEC. *****
Z21=CGLI*(TGP-TLI)-CLIST*(TLI-TSFP)-RWLI-RGLI
C LET COMBUSTION FOLLOW POOL TEMPERATURE FOR POSSIBLE REIGNITION
Z26=(TLI-TCZ)/DELT
C
C***** CALC. CELL GAS TEMP. RATE OF CHANGE DEG. R/SEC. *****
Z24=C1*(TSP-TGP)+CLIG*(TLI-TGP)+RLIG+RBREAK+XBLOW*BLOWR*CPAB*
(TBLOW-TGP)/HTCPGP-ESCR*XESC/HTCPGP+CEHCGP*(TEHCP-TGP)
C
C***** CALC. WALL STEEL TEMP. RATE OF CHANGE DEG. R/SEC. *****
Z25=C6*(TGP-TSP)+RLIW
011 CONTINUE
C
C*****
C* COMPUTATIONS VALID WITH EITHER MODEL *
C*****
C
Z2EP=CGPEHC*(TGP-TEHCP)
C***** CALC. FLOOR STEEL TEMP. RATE OF CHANGE DEG. R/SEC. *****
Z27=-XSFL*SFLCR*12./(THFP*AFP*RHSFP*CPSFP)
C
IF (FLAG2) GO TO 015
IF (.NOT. FLAGW) QRADC=SIGMA*AWP*(TSP**4-TA**4)*ESTLWP
IF (FLAGW) QRADC=SIGMA*AWP*(TSP**4-TC(1)**4)*RIFSCW
RADC=QRADC/(THWP*AWP*RHSWP*CPSWP)
IF (.NOT. FLAGW) Z25=Z25-C11*(TSP-TA)-RADC
IF (FLAGW) Z25=Z25-C7*(TSP-TC(1))-RADC
IF (.NOT. FLAGF) QRADB=SIGMA*AFP*(TSFP**4-TA**4)*ESTLFP
IF (FLAGF) QRADB=SIGMA*AFP*(TSFP**4-TB(1)**4)*RIFSCF
RADB=QRADB/(THFP*AFP*RHSFP*CPSFP)
IF (.NOT. FLAGF) Z27=Z27+CSBLI*(TLI-TSFP)-C12*(TSFP-TA)-RADB
IF (FLAGF) Z27=Z27+CSBLI*(TLI-TSFP)-C8*(TSFP-TB(1))-RADB
015 CONTINUE
IF (FLAG2) CALL CELL2
IF (FLAGF) CALL CONC2
IF (FLAGW) CALL CONC2
IF (FLAGFB) CALL LIPB
IF (FLAGDF) CALL LIDIFF
C
C
C*****CALCULATIONS WITH SUSPENDED PAN GEOMETRY*****
C
IF (FLAGPN) CALL PAN
C
C***** CALCULATIONS USING COMBUSTION OF CONCRETE (BREACH OF STEEL LINER)****
C
IF (FLAGC) CALL CONCC
C
C*****
C* CALCULATING OVERPRESSURE *
C*****
XMAIRP=MOXP/32.+MNIP/28.+MWAP/18.+MAP/XMOLA
PAP=1546.*XMAIRP*TGP/144./VP
OVRPP=PAP-PAPZER
IF (TIME.GT.TBLIN) XBLOW=1.
IF (TIME.GT.TBLOUT) XBLOW=0.

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C
C.....
C**  CALCU. TOTAL LEAKAGE  ***
C.....
C
    LEAK=0.0
    IF (FLAG2) CALL CELL2
    IF (FLAG2) GO TO 932
    IF (PAP .GT. 14.7) LEAK=KLEAK*(PAP-14.7)**0.6
    XMDOT=0.0
    FOUTS=0.0
    FOUTP=EXHSTR/MAIRP*XBLOW+LEAK
932 CONTINUE
    FMLEFT= EXP(-OUTINT)
    FMLEAK=1.-FMLEFT
C
C.....
C*  DO INTEGRATIONS  *
C.....
C
    LIBP=INTGRL(0.,CMBR*ASLI)
    LILOX=INTGRL(0.,(1.+RCMBO)/RCMBO*CMBRO*ASLI*(1.-FRA))
    LILNI=INTGRL(0.,(1.+RCMBN)/RCMBN*CMBRN*ASLI*(1.-FRA))
    OXLB=INTGRL(OXLBI,ROXLB)
    TC2=INTGRL(TC2I,ZZ6)
    TLI=INTGRL(TLII,ZZ1)
    TGP=INTGRL(TGPZER,ZZ4)
    TSP=INTGRL(TSPZER,ZZ6)
    TEHCP=INTGRL(TEHCZP,ZZEP)
    TSFP=INTGRL(TSFPI,ZZ7)
    MOXP=INTGRL(MOXIP,W02B*BLOWR*XBLOW+MOXS*FOUTS-MOXP*FOUTP-
    ROXLB+MOXINJ)
    MNIP=INTGRL(MNIP,WN2B*BLOWR*XBLOW+MNIS*FOUTS-MNIP*FOUTP
    -RNILB*MNIINJ)
    MAP=INTGRL(MAIP,WAB*BLOWR*XBLOW+MAS*FOUTS-MAP*FOUTP)
    MWAP=INTGRL(MWAIP,WAB*BLOWR*XBLOW+MWAS*FOUTS-MWAP*FOUTP-RWALB)
    MLIOP=INTGRL(MLIOIP,-MLIOP*FOUTP+(1.+RCMBO)/RCMBO*CMBRO*ASLI*FRA+
    MLIOS*FOUTS-MLIOP*STICK)
    MLINP=INTGRL(MLINIP,-MLINP*FOUTP+(1.+RCMBN)/RCMBN*CMBRN*ASLI*FRA+
    MLINS*FOUTS-MLINP*STICK)
    MLIHP=INTGRL(0.,-MLIHP*FOUTP+CMBRW*ASLI*((1.+RCMBW)/RCMBW-
    1./RCMBH2)+MLIHS*FOUTS-MLIHP*STICK)
    MH2P=INTGRL(0.,MH2S*FOUTS-MH2P*FOUTP+(1.+RCMBH2)/RCMBH2*
    CMBRW*ASLI)
    OUTINT=INTGRL(LEAKO,LEAK)
    IF (.NOT. FLAGPW) GO TO 935
    TPAN=INTGRL(TPANZO,ZZ2)
    TINS1=INTGRL(TINS1I,ZZ8)
    TINS2=INTGRL(TINS2I,ZZ9)
935 CONTINUE
    IF (.NOT. FLAG2) GO TO 938
    MOXS=INTGRL(MOXIS,MOXP*FOUTP-MOXS*FOUTT)
    MNIS=INTGRL(MHIIS,MNIP*FOUTP-MNIS*FOUTT)
    MAS=INTGRL(MAIS,MAP*FOUTP-MAS*FOUTT)
    MWAS=INTGRL(MWAIS,MWAP*FOUTP-MWAS*FOUTT)
    MLIOS=INTGRL(MLIOIS,MLIOP*FOUTP-MLIOS*FOUTT)
    MLINS=INTGRL(MLINIS,MLINP*FOUTP-MLINS*FOUTT)
    MLIHS=INTGRL(0.,MLIHP*FOUTP-MLIHS*FOUTT)
    MH2S=INTGRL(0.,MH2P*FOUTP-MH2S*FOUTT)
    TGS=INTGRL(TGSZER,ZZ3)
    TSS=INTGRL(TSSZER,ZZ5)
    TFS=INTGRL(TFSZER,ZZFS)
    TEHCS=INTGRL(TEHCZS,ZZES)
938 CONTINUE
    IF (.NOT. FLAGW) GO TO 1008
    DO 1008 I=1,NL
    TC(I)=INTGRL(TCIC(I),DTCDT(I))
1008 CONTINUE
    IF (.NOT. FLAGV) GO TO 1009
    DO 1009 I=1,NL1
    TB(I)=INTGRL(TBIC(I),DTBOT(I))
1009 CONTINUE

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IF (.NOT. FLAGC) GO TO 941
TCON=INTGRL(TSFPI,ZZC)
DCOC2=INTGRL(0.01,ZZD)
HZLEIT=INTGRL(XMH2OI,-RELEASE)
941 CONTINUE
IF (FLAGDF) MLEAD=INTGRL(0.,DMPBOT)
IF (FLAGDF) TLEAD=INTGRL(TLEADI,ZZPB)
C
CALL DYNAMI(TIME,&Z00)
C
C.....
C* POST INTEGRATION SECTION
C CHECK OVERP AND TLI FOR STOP CONDITON
C CHECK AND CORRECT FOR LITHIUM AND OXYGEN SUPPLY
C.....
C
950 CONTINUE
IF (TMPB .GT. .333*ZLI) GO TO 987
IF (TLI .GE. TVAP) GO TO 978
LILP=LIT-LIBP+LILOX+LILNI
IF (LILP .LE. 0.) LILP=0.0
IF (.NOT. FLAGPB) ZLI=LILP/RHLI/ASLI
ALPHA=AKLI/(RHLI*CPLI)
IF ((LILP .LT. 0.1*LIT) .AND. (ALPHA*DELT .GT. ZLI*ZLI .OR. LILP
.LT. 1.0) .AND. (.NOT. FLAGPB)) FLAGL=.TRUE.
IF (FLAGL) LIL=LIT/10.
IF (.NOT. FLAGL .AND. .NOT. FLAGPB) LIL=LILP
IF (TGP .LT. 500. .AND. OVERPP .LT. 1. .AND. ABS(XMDOT)
.LT. 0.1) GO TO 977
IF (TLI .LT. TMELT) GO TO 976
IF (ICMB .EQ. 0 .OR. MOXP .GT. 0.01) GO TO 961
OXLB=OXLFS
ICMB=0
CMBRO=0.0
ROXLB=0.0
951 CONTINUE
IF (ILIT .EQ. 0 .OR. (LIT-LIBP) .GE. 0.01) GO TO 962
OXLB=LIT/RCMBO
ILIT=0
LIT=LIBP
CMBR=0.0
CMBRO=0.0
CMBRN=0.0
CMBRW=0.0
ROXLB=0.0
RNILB=0.0
RWALB=0.0
952 CONTINUE
IF (MNIP .GE. 0.0) GO TO 953
MNIP=0.0
ICMI=0
CMBRN=0.
RNILB=0.0
953 CONTINUE
IF (MWAP .GE. 0.0) GO TO 954
MWAP=0.0
CMBRW=0.0
RWALB=0.0
954 CONTINUE
CMBRH=3600.*(CMBRO+CMBRN+CMBRW)
IF (CMBRH .GE. 0.2 .OR. TIME .LE. 10.) GO TO 956
ICZ=0
CMBRO=0.0
CMBRN=0.0
CMBRW=0.0
CMBRH=0.0
ROXLB=0.0
RNILB=0.0
RWALB=0.0
955 CONTINUE
C
C.....

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C° CONVERT TEMP. TO DEG. F
C.....
C
  TSPPF=TSFP -460.
  TCZF=TCZ-460.
  TLIF=TLI-460.
  TGPFF=TGP-460.
  TSPF=TSP-460.
  TEHCPF=TEHCP-460.
  IF (.NOT. FLAG2) GO TO 980
  TGSF=TGS-460.
  TFSF=TFS-460.
  TSSF=TSS-460.
  TEHCSF=TEHCS-460.
980 CONTINUE
  IF (.NOT. FLAGPN) GO TO 961
  TPANF=TPAN-460.
  TINS1F=TINS1-460.
  TINS2F=TINS2-460.
961 CONTINUE
  IF (.NOT. FLAGW) GO TO 1001
  DO 1001 I=1,20
  TCF(I)=TC(I)-460.
1001 CONTINUE
  IF (.NOT. FLAGF) GO TO 1002
  DO 1002 I=1,20
  TBF(I)=TB(I)-460.
1002 CONTINUE
  TCONF=TCON-460.
  IF (FLAGDF) TLEADF=TLEAD-460.
C
C.....
C° TIME STEP CONTROL
C.....
C
  DT1=ABS(RELERR*TLI/Z21)
  DT2=ABS(RELERR*TGP/Z24)
  DT3=ABS(RELERR*TSP/Z26)
  IF (ILIT.EQ.0 .OR. ICZ.EQ.0) GO TO 966
  DT5=ABS(RELERR*TCZ/Z26)
  ZZ99=(CMBRH-CMBRHI)/DELT
  IF (ZZ99.EQ.0.) GO TO 966
  DT4=ABS(RELERR*CMBRH/ZZ99)
  CMBRHI=CMBRH
  IF (IPASS.EQ.1) DT4=1.E06
  GO TO 966
966 CONTINUE
  DT4=1.0E06
  DT5=1.0E06
966 CONTINUE
  IF (FLAGDF .AND. ZZPB .LT. 1.0E-15) ZZPB=1.0E-15
  IF (FLAGDF) DT6=ABS(RELERR*TLEAD/ZZPB)
  BILGE=AMINI(DT1,DT2,DT3,DT4,DT5)
  IF (FLAGDF) BILGE=AMINI(BILGE,DT6)
  BIL=(BILGE-DELT)/DELT
C THIS CONDITION IS TO REMOVE INSTABILITY DUE TO STEEP
C NITROGEN REACTION CURVE
  IF (TCZ .GT. 1900. .AND. ABS(BIL) .GT. 0.1) DELT=DELT+(BILGE-DELT)/10.
  IF (.NOT. (TCZ .GT. 1900. .AND. ABS(BIL) .GT. 0.1)) DELT=BILGE
C
  IF (TIME .LT. 8000.) DELOUT=50.
  IF (TIME .LT. 800.) DELOUT=20.
  IF (TIME .LT. 120.) DELOUT=5.0
  IF (TIME .LT. 26.) DELOUT=0.2
  IF (TIME .LE. 3.0) DELOUT=0.1
  IF (TIME .GE. 8000.) DELOUT=600.
C***** TEST CONDUCTION LIMITS ON TIME STEP ***
C LIMITING CONDUCTION RATE IS DETERMINED FROM POOL TO PAN
C (IF USING PAN OPTION) OTHERWISE FROM POOL TO STEEL LINER
C
  IF (FLAGPN) ALPHA2=((THKPAN+ZLI)/(ZLI/AKLI+THKPAN/KPAN))/
  ((RHLI*CPHI*ZLI+RHPAN*CPPAN+THKPAN)/(THKPAN+ZLI))

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IF (FLAGPN) PYU=0.075*(THKPAN+ZLI)**2/ALPHA2
IF (.NOT. FLAGPN) ALPHA2=((THFP+ZLI)/(ZLI/AKLI+THFP/KSTLFP))/
((RHLI*CPLI*ZLI+RHSFP*CPSFP*THFP)/(THFP*ZLI))
IF (.NOT. FLAGPN) PYU=0.075*(THFP+ZLI)**2/ALPHA2
IF (DELT .GT. PYU) DELT=PYU
C CONDUCTION TEST FOR POOL LAYERS IF USING DIFFUSION MODEL
IF (FLAGOF .AND. DELT .GT. PYUP) DELT=PYUP
C TESTING TWO CELL EXCHANGE RATE ON TIME STEP
IF (.NOT. FLAG2 .OR. ABS(XMDOT) .LT. 0.0001) GO TO 959
IF ((ABS(PAP-PAS)) .LT. .01 .AND. DELT .GT. .04) DELT=.04
DELM=HAIRP/ABS(XMDOT)/260.
DELS=HAIRS/ABS(XMDOT)/260.
IF (DELT .GT. DELM) DELT=DELM
IF (DELT .GT. DELS) DELT=DELS
959 CONTINUE
C AEROSOL REMOVAL TIME STEP CHECK
IF (DELT*STICK .GT. .40) DELT=.40/STICK
C
IF (DELT .GT. 3.0) DELT=3.0
C
IF (DELT.LT.DTMIN) DELT=DTMIN
IF (DELT .GT. DELOUT) DELT=DELOUT
C
C*****
C* OUTPUT SECTION *
C*****
C
IF (TIME.LT.TIMEO) GO TO 978
IF (FLAGSI) CALL SI
TIMEO=TIMEO+DELOUT
IF (IPAGE.LT.40) GO TO 974
WRITE (11,830) (NAME(I),I=1,80)
WRITE (12,830) (NAME(I),I=81,160)
WRITE (13,830) (NAME(I),I=161,240)
WRITE (14,830) (NAME(I),I=241,320)
830 FORMAT(' ',3(20A4.//),//,20A4)
974 CONTINUE
IF (IPAGE.GE.40) IPAGE=0
IPAGE=IPAGE+1
WRITE (11,826) TIME,DELT,TCZF,TLIF,TGPF,PAP,TSPF,TSFP
IF (FLAG2) WRITE (12,832) TIME,TGSF,TFSF,PAP,PAS,XMDOT
IF (.NOT. FLAG2) WRITE (12,832) TIME,LIBP,CMBRH,MOXP,MNIP,RN2
IF (FLAGPN) WRITE (13,832) TIME,TLIF,TPANF,TINS1F,TINS2F,PAP
IF (.NOT. FLAGPN) WRITE (13,832) TIME,MNIP,MOXP,RN2,CMBRH,LIBP
WRITE (14,832) TIME,XLIDOT,TLEADF,MLEAD,THPB,ZLI
826 FORMAT(3X,F9.1,F8.2,F10.2,F10.2,4(1X,F7.2),F8.2)
831 FORMAT(3X,F9.1,5F11.2)
832 FORMAT(3X,F9.1,5E13.4)
IF (FLAGSI) CALL SI
975 CONTINUE
IF (TIME.GT.TIMEF) GO TO 990
C***** RETURN TO TOP OF DYNAMIC CYCLE *****
GO TO 200
C
C*****
C* ERROR POINTERS *
C*****
C
976 CONTINUE
WRITE (11,836)
836 FORMAT(' POOL TEMP. HAS DROPPED TO LITHIUMS MELTING TEMP. ')
GO TO 990
977 CONTINUE
WRITE (11,836)
836 FORMAT(' CELL GAS TEMP. AND PRESS. HAVE RETURNED TO NORMAL ')
GO TO 990
978 CONTINUE
WRITE (11,837)
837 FORMAT(' LITHIUM TEMP. ABOVE BOILING POINT ')
837 FORMAT(1X,E12.4,E12.4)
838 FORMAT(1X,E12.4,E12.4)
GO TO 990
979 CONTINUE

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WRITE (11,839)
838 FORMAT(1X,'NO ROOT FOUND FOR SPRAY FIRE FOR TEMP.S LESS THAN ',
. '1 MILLION DEG. R')
. GO TO 990
980 CONTINUE
WRITE (11,839)
839 FORMAT (' SUSPENDED PAN OPTION CANNOT BE SELECTED CONCURRENT'/
. ' CONCRETE COMBUSTION OPTION')
. GO TO 990
984 CONTINUE
WRITE (11,844)
844 FORMAT (' SPRAY FIRE AND LITHIUM LEAD COMBUSTION ARE NOT',
. ' COMPATIBLE')
. GO TO 990
985 CONTINUE
WRITE (11,846)
845 FORMAT(' EXX IS NEGATIVE--CANNOT TAKE ROOT')
WRITE (11,846) TC2,CMBRH,ZZ6,ZZ8,RN2
846 FORMAT(' MESSED UP VARIABLES',5E10.3)
GO TO 990
986 CONTINUE
WRITE (11,847) STICK,BETA
847 FORMAT (' AEROSOL REMOVAL FRACTION IS TOO LARGE'/
. 'STICK = ',F12.4,' BETA = ',F12.4/)
. GO TO 990
987 CONTINUE
848 FORMAT(' LEAD LAYER THICKNESS IS GREATER THAN 2L1/3. DIFFUSION'/
. ' MODEL IS NO LONGER VALID'/)
990 CONTINUE
WRITE (11,867)
867 FORMAT(' PROGRAM EXECUTION STOPPED BY PROGRAM')
WRITE (11,868) DT1,DT2,DT3,DT4,DT6
868 FORMAT(' VALUES', 6E10.3)
close(unit=1)
close(unit=2)
close(unit=3)
close(unit=4)
close(unit=10)
close(unit=11)
close(unit=12)
close(unit=13)
close(unit=14)
CALL EXIT
END

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C THESE 3 SUBROUTINES ARE DESIGNED TO BE USED IN A MAIN PROGRAM WHICH
C SIMULATES A DYNAMIC SYSTEM EXPRESSED AS A SET OF ODE'S. THESE ODE'S
C MAY BE REEXPRESSED AS A SET OF INTEGRALS WHICH MUST BE INTEGRATED
C SIMULTANEOUSLY THROUGH THE DOMAIN OF INTEREST STARTING WITH THE APPROPRIATE
C INITIAL CONDITIONS. FOR EXAMPLE, THE FUNCTION Y MAY BE FOUND FROM THE
C SOLUTION OF  $dy/dt = \text{RATE} = F(Y,T)$  AND  $Y=Y_0$  AT  $T=T_0$ . THIS MAY BE
C REWRITTEN  $Y = \text{INTGRL}(Y_0, \text{RATE})$ . THE OPEN INTEGRAL OF RATE OVER T STARTING
C AT  $Y_0$ . A SET OF ODE'S MAY BE TREATED IN A SIMILAR MANNER.
C THE MAIN PROGRAM SHOULD CONSIST OF TWO MAIN PARTS, THE INITIALIZATION
C SECTION AND THE DYNAMIC SECTION. THE DYNAMIC SECTION IS FURTHER DIVIDED
C INTO INTEGRATION AND POST-INTEGRATION SECTIONS.
C THE INITIAL SECTION SHOULD BE USED FOR INPUT, CALCULATION OF NECESSARY
C CONSTANTS, AND FOR CALCULATING AND SETTING OF INITIAL CONDITIONS. IT
C SHOULD CONTAIN THE REAL INTGRL, COMMON, AND CALL INIT STATEMENTS.
C THE INTEGRATION SECTION SHOULD START WITH A NUMBERED CONTINUE
C STATEMENT AND END WITH THE CALL DYNAMI STATEMENT. IT SHOULD CONTAIN
C ALL CALCULATIONS OF PROGRAM VARIABLES AND NON-CONSTANT RATES. ALL INTGRL
C FUNCTION STATEMENTS SHOULD APPEAR IN A GROUP IMMEDIATELY PRECEDING THE
C CALL DYNAMI STATEMENT.
C THE INTEGRATION SECTION WILL BE LOOPED SEVERAL TIMES DURING EACH
C INTEGRATION STEP (SIMPSON'S RULE USES 4 LOOPS PER STEP, RUNGE-KUTTA USES

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12 CONTINUE
   ICOUNT=3
   RETURN 1
14 CONTINUE
   ICOUNT= 8
   RETURN 1
40 CONTINUE
   IPASS=1
   RETURN
   END
C   THIS SUBROUTINE INITIALIZES VARIABLES USED BY THE INTEGRATION ROUTINES.
C   IT SHOULD BE PLACED IN THE INITIALIZATION SECTION OF THE MAIN PROGRAM
C   BEFORE THE FIRST STATEMENT OF THE DYNAMIC SECTION.  SEE DYNAMI FOR VARIABLE
C   LIST AND INTEGRATION DESCRIPTION.
C
SUBROUTINE INIT
COMMON /INTGL/ IMETH,ICOUNT,ISTORE,INOIN,IPASS,DELT,
      XIC(101),A(501)
   IPASS=0
   ISTORE=0
   ICOUNT=1
   INOIN=0
   RETURN
   END
C   FUNCTION INTGRL PERFORMS THE ACTUAL INTEGRATIONS.  IN THE MAIN
C   PROGRAM, ALL INTGRL STATEMENTS SHOULD BE PLACED IN A GROUP AT THE END
C   OF THE INTEGRATION SECTION.  ALL RATE CALCULATIONS SHOULD PRECEDE THIS
C   GROUP AND IT SHOULD BE IMMEDIATELY FOLLOWED BY THE CALL DYNAMI STATEMENT.
C   FOR VARIABLE LIST AND DESCRIPTIONS SEE DYNAMI.
REAL FUNCTION INTGRL(XXIC,DXDT)
COMMON /INTGL/ IMETH,ICOUNT,ISTORE,INOIN,IPASS,DELT,
      XIC(101),A(501)
   IF (IPASS.EQ.0) GO TO 40
   ISTORE=ISTORE+1
   IF (IMETH.EQ.1) GO TO 10
C   SIMPSON'S RULE (DEFAULT) IMETH GREATER THAN 2
C
   IF (ICOUNT.EQ.4) GO TO 4
   IF (ICOUNT.EQ.3) GO TO 3
   IF (ICOUNT.EQ.2) GO TO 2
1 CONTINUE
   INOIN=INOIN+1
   IF (IPASS.EQ.1) XIC(INOIN)=XXIC
   A(ISTORE)=DXDT
   INTGRL=XIC(INOIN)+DELT*DXDT/2.
   A(500-ISTORE)=INTGRL
   RETURN
2 CONTINUE
   A(ISTORE)=DXDT
   INTGRL=A(500+INOIN-ISTORE)+DELT*DXDT/2.
   RETURN
3 CONTINUE
   INTGRL=XIC(ISTORE-2*INOIN)+DELT/6.*(A(ISTORE-2*INOIN)+4.*
      A(ISTORE-INOIN)+DXDT)
   XIC(ISTORE-2*INOIN)=INTGRL
   RETURN
4 CONTINUE
   INTGRL=XIC(ISTORE-3*INOIN)
   RETURN
C   RUNGE-KUTTA METHOD -FIXED STEP- IMETH=1
C
10 CONTINUE
   IF (ICOUNT.EQ.5) GO TO 15
   IF (ICOUNT.EQ.4) GO TO 14
   IF (ICOUNT.EQ.3) GO TO 13
   IF (ICOUNT.EQ.2) GO TO 12
11 CONTINUE
   INOIN=INOIN+1
   IF (IPASS.EQ.1) XIC(INOIN)=XXIC
   A(ISTORE)=DELT*DXDT

```

```

INTGRL=XIC(INOIN)+.5*A(ISTORE)
RETURN
12 CONTINUE
A(ISTORE)=DELTA*DXDT
INTGRL=XIC(ISTORE-INOIN)+.5*A(ISTORE)
RETURN
13 CONTINUE
A(ISTORE)=DELTA*DXDT
INTGRL=XIC(ISTORE-2*INOIN)+A(ISTORE)
RETURN
14 CONTINUE
AA=DELTA*OXDT
INTGRL=XIC(ISTORE-3*INOIN)+1./6.*(A(ISTORE-3*INOIN)+2.*
A(ISTORE-2*INOIN)+2.*A(ISTORE-INOIN)+AA)
XIC(ISTORE-3*INOIN)=INTGRL
RETURN
16 CONTINUE
INTGRL=XIC(ISTORE-4*INOIN)
RETURN
40 CONTINUE
INTGRL=XXIC
RETURN
END

```

C
C
C

```

FUNCTION AKEXX(T01,T02,RHOBAR)
GINBAR=32.2
TBAR=0.5*(T01+T02)
BBAR=1.0/TBAR
DBAR=((4.94E-05*TBAR+0.0188)/(RHOBAR*3600.))**.2
AKBAR=(0.014+1.92E-05*(TBAR-460.))/3600.
EXBAR=(GINBAR*BBAR*ABS(T01-T02)/DBAR)**.3333
AKEXX=AKBAR*EXBAR
RETURN
END

```

C
C
C
C

```

THIS FUNCTION IS FOR CALCULATING THE PARTIAL PRESSURE OF LITHIUM IN
LITHIUM-LEAD AS A FUNCTION OF CONCENTRATION
FUNCTION ACTVTY(XALI)
ALILN=8.835*(XALI**.219)-8.0
IF (ALILN .GT. 0.0) ALILN=0.0
ACTVTY=XALI*EXP(ALILN)
RETURN
END

```

C

C These subroutines are used to modularize litfire. they include the
C options of two cell geometry and pan geometry as well as floor and
C concrete combustion.

C

C this is the secondary cell subroutine.

```

SUBROUTINE CELL2
IMPLICIT REAL (K,L,M)
LOGICAL FLAGN,FLAGH,FLAGW,FLAGF,FLAG2
COMMON // NAME(320),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGDF,ICZ
COMMON /INTGL/ IMETH,ICOUNT,ISTORE,INOIN,IPASS,DELTA,
XIC(101),ZZZ(501)
COMMON /LITH/ AKLI,ASLI,CPLI,CSBLI,HB,LIBP,LIL,LILP,LIT,
RHLI,SPILL,TLI,TLII,ZLI
COMMON /STEEL/ CPSFP,CPSFS,CPSWP,CPSWS,ESTLFP,ESTLWP,KSTLFP,
KSTLFS,KSTLWP,KSTLWS,RHSFP,RHSFS,RHSWP,RHSWS
COMMON /MISC/ AFP,AFS,AWP,AWS,C7,C21,GIN,
HA,HINFAM,HINSAM,HTCPGP,QRADC,RADC,RCZW,
RHOAP,RLIW,RWPWS,SIGMA,TA,TC(20),TFS,
TFSZER,TGP,TGS,TGPZER,TSFP,TSP,TSS,
TSSZER,THFP,THFS,THWP,THWS,ZZS,ZZS,ZZS,ZZ1,ZZ7
COMMON /CONOP/ C8,CPCON,DT8DT(20),DTCDT(20),GAP,KCON,KGAP,
L(20),L1(20),NL,NL1,QRADB,RADB,RHCON,
SFLCR,TB(20),TBF(20),TBIC(20),TCF(20),
TCIC(20),THFC,THWC,TSFPI,TSPZER,XSFL

```



```

MNIS=MNIIS
MWAS=WWAS*RHOAIS*VS
MWAS=MWAIS
MOXIS=WOZS*RHOAIS*VS
MOXS=MOXIS
MAIS=WAS*RHOAIS*VS
MAS=MAIS
C***** CONVERSION TO FT. - LB. - SEC. *****
C
CRACK=CRACK/144.
KSTLWS=KSTLWS/3600.
KSTLFS=KSTLFS/3600.
N=3
RETURN
3 CONTINUE
C***** COMPUTE PHYSICAL PROPERTIES DEPENDENT ON TEMPERATURE *****
C***** CALCULATE AIR COMPOSITION AND SPECIFIC HEAT AT CONST. VOLUME *****
MAIRS=MOXS*MNIS+MWAS+MH2S+MAS
RHOAS=MAIRS/VS
FOXS=MOXS/MAIRS
FWAS=MWAS/MAIRS
FNIS=MNIS/MAIRS
CPO2S=(0.184+3.2E-06*TGS-1.36E04/(TGS*TGS))
CPMOXS=CPO2S*MOXS
CPN2S=(0.172+8.67E-06*TGS+1.02E-09*TGS*TGS)
CPMNIS=CPN2S*MNIS
CPLIOS=0.0602*TGS**0.326
CPLINS=0.3368+3.67E-04*TGS
CPMLOS=CPLIOS*MLIOS
HTCPGS=CPMOXS+CPMNIS+CPMLOS+CPAS*MAS+CPLINS*MLINS+CPLIH*MLIHS+
CPH2*MH2S+CPWA*MWAS
C***** CALCULATING RADIATIVE INTERCHANGE FACTORS *****
EMGS=1.-EXP(-(MLIOS/RHOLIO+MLINS/RHOLIN+MLIHS/RHOLIH))*2.27E06*CHS/
VS/RA)
IF (EMGS .LE. 0.005) EMGS=0.005
RIFPS=1./((1.-ESTLWP)/ESTLWP+(1.-ESTLWS)/ESTLWS*(AWP/AWS)+
(1.+AWP/AWS)/(1.+AWP/AWS*(1.-EMGS)))
RIFPGA=(ESTLWP*EMGS)/((1.-ESTLWP)*EMGS+ESTLWP)
RIFFPS=1./((1.-ESTLFP)/ESTLFP+(1.-ESTLFS)/ESTLFS*(AFP/AFS)+
(1.+AFP/AFS)/(1.+AFP/AFS*(1.-EMGS)))
RIFFGS=(ESTLFP*EMGS)/((1.-ESTLFP)*EMGS+ESTLFP)
RIFSCW=(ESTLWS*EMCONC)/(ESTLWS+EMCONC-ESTLWS*EMCONC)
RIFSCF=(ESTLFS*EMCONC)/(ESTLFS+EMCONC-ESTLFS*EMCONC)
C***** CALCULATING GAS HEAT TRANSFER COEFFICIENTS *****
C SECONDARY GAS TO SECONDARY EXTRANEIOUS HEAT CAPACITY
HEHCS=HINECS*AKEXX(TGS,TEHCS,RHOAS)
C SECONDARY STEEL LINER TO SECONDARY GAS
HSEC=HINGSS*AKEXX(TGS,TSS,RHOAS)
C PRIMARY STEEL WALL LINER TO SECONDARY CONTAINMENT GAS
HWPAS=HINPS*AKEXX(TSP,TGS,RHOAS)
C PRIMARY STEEL FLOOR LINER TO SECONDARY CONTAINMENT GAS
HFPAS=HINFGS*AKEXX(TSFP,TGS,RHOAS)
C SECONDARY STEEL FLOOR TO SECONDARY CELL GAS
HFGAS=HINFSG*AKEXX(TFS,TGS,RHOAS)
C SECONDARY STEEL LINER TO AMBIENT (SUPERCEDED BY CONCRETE TO AMBIENT
IF CONCRETE OPTION IN USE)
IF (.NOT. FLAGW) HA=HINSAM*AKEXX(TSS,TA,.074)
C SECONDARY STEEL FLOOR LINER TO AMBIENT
IF (.NOT. FLAGF) HAMF=HINFAM*AKEXX(TFS,TA,.074)
100 CONTINUE
C***** CALCULATING THERMAL DIFFUSIVITIES BETWEEN NODES *****
C11=KSTLWS*HA/(RHSWS*CPSWS*THWS*(KSTLWS+THWS*HA/2.))
C12=KSTLFS*HAMF/(RHSFS*CPSFS*AFS*(KSTLFS+THFS*HAMF/2.))
C14=KSTLFS*HFGAS/(RHSFS*CPSFS*THFS*(THFS*HFGAS/2.+KSTLFS))
C15=KSTLFS*HFGAS*AFS/HTCPGS/(THFS*HFGAS/2.+KSTLFS)
C18=KSTLFP*HFPAS/(RHSFP*CPSFP*THFP*(THFP*HFPAS/2.+KSTLFP))
C19=KSTLFP*HFPAS*AFP/HTCPGS/(THFP*HFPAS/2.+KSTLFP)
C20=KSTLWP*HWPAS/(RHSWP*CPSWP*THWP*(THWP*HWPAS/2.+KSTLWP))
C21=KSTLWS*HSEC/(RHSWS*CPSWS*THWS*(THWS*HSEC/2.+KSTLWS))
C22=KSTLWP*HWPAS*AWP/HTCPGS/(THWP*HWPAS/2.+KSTLWP)
C23=KSTLWS*HSEC*AWS/HTCPGS/(THWS*HSEC/2.+KSTLWS)
CEHCGS=HEHCS*AEHCS/HTCPGS

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CGSEHC=HEHCS*AEHCS/XMEHCS/CEHCS
C***** CALCULATING RADIATIVE HEAT TRANSFER BETWEEN NODES *****
QRADPS=SIGMA*AWP*(TSP**4-TSS**4)*RIFPS
RWPWS=QRADPS/(THWP*AWP*RHSWP*CPSWP)
RWSWP=QRADPS/(THWS*AWS*RHSWS*CPSWS)
QRADFS=SIGMA*AFP*(TSFP**4-TFS**4)*RIFFPS
RFPFS=QRADFS/(THFP*AFP*RHSFP*CPSFP)
RFSFP=QRADFS/(THFS*AFS*RHSFS*CPSFS)
QRADPG=SIGMA*AWP*(TSP**4-TGS**4)*RIFPGA
RWPAS=QRADPG/(THWP*AWP*RHSWP*CPSWP)
RSPGS=QRADPG/HTCPGS
QRADFG=SIGMA*AFP*(TSFP**4-TGS**4)*RIFFGS
RFPAS=QRADFG/(THFP*AFP*RHSFP*CPSFP)
RGASFP=QRADFG/HTCPGS
N=4
RETURN
4 CONTINUE
C***** CALCULATING RADIATION FROM OUTER STEEL LINERS *****
IF (.NOT. FLAGW) QRADC=SIGMA*AWS*(TSS**4-TA**4)*ESTLWS
IF (FLAGW) QRADC=SIGMA*AWS*(TSS**4-TC(1)**4)*RIFSCW
RADC=QRADC/(THWS*AWS*RHSWS*CPSWS)
IF (.NOT. FLAGF) QRADB=SIGMA*AFS*(TFS**4-TA**4)*ESTLFS
IF (FLAGF) QRADB=SIGMA*AFS*(TFS**4-TB(1)**4)*RIFSCF
RADB=QRADB/(THFS*AFS*RHSFS*CPSFS)
C* MODIFYING PRIMARY STEEL WALL AND FLOOR TEMPERATURE RATES OF CHANGE
ZZ5=ZZ5-C20*(TSP-TGS)-RWPWS-RWPAS
ZZ7=ZZ7+CSBLI*(TLI-TSFP)-C18*(TSFP-TGS)-RFPFS-RFPAS
CALCULATE EXTRANEIOUS HEAT CAPACITY TEMPERATURE RATE OF CHANGE
ZZ5=CGSEHC*(TGS-TEHCS)
CALCULATE OUTER CELL GAS TEMPERATURE RATE OF CHANGE DEG R/SEC
ZZ3=BREACKS+RSPGS+C22*(TSP-TGS)+C23*(TSS-TGS)+CEHCS*(TEHCS-TGS)
+C19*(TSFP-TGS)+RGASFP+C15*(TFS-TGS)
CALCULATE OUTER WALL STEEL TEMPERATURE RATE OF CHANGE DEG R/SEC
IF (.NOT. FLAGW) ZZS=C21*(TGS-TSS)-C11*(TSS-TA)+RWSWP-RADC
IF (FLAGW) ZZS=C21*(TGS-TSS)-C7*(TSS-TC(1))+RWSWP-RADC
CALCULATE OUTER FLOOR STEEL TEMPERATURE RATE OF CHANGE DEG R/SEC
IF (.NOT. FLAGW) ZZFS=C14*(TGS-TFS)-C12*(TFS-TA)+RFSFP-RADB
IF (FLAGW) ZZFS=C14*(TGS-TFS)-C8*(TFS-TB(1))+RFSFP-RADB
N=5
RETURN
5 CONTINUE
C*****
C** CALCULATING OVERPRESSURE **
C*****
XMAIRS=MOXS/32.+MNIS/28.+MWAS/18.+MAS/XMOLA
PAS=1545.*XMAIRS*TGS/144./VS
OVERPS=PAS-PASZER
C*****
C** CALCU. TOTAL LEAKAGE ***
C*****
LEAK=KLEAK*(ABS(PAS-14.7))**0.5
IF (PAS .LT. 14.7) LEAK=0.
IF (ABS(PAP-PAS) .LT. 0.0006 .AND. ISWICH .EQ. 1 .AND.
TIME .GT. TSWICH) CRACK=0.0
IF (CRACK .EQ. 0.0 .AND. ISWICH .EQ. 1) WRITE (11,816) TIME
815 FORMAT (' CELL PRESSURES HAVE EQUILIZED AT TIME = ',F11.2/
' CRACK SIZE HAS BEEN SET TO ZERO FOR REMAINDER OF CALCULATION')
IF (CRACK .EQ. 0.0) ISWICH=0
IF (CRACK .EQ. 0.0) GO TO 112
IF (ABS(PAP-PAS) .LT. 0.0006) GO TO 106
IF (PAP-PAS) 101,106,107
C***** FLOW OUT OF SECONDARY INTO PRIMARY *****
101 FOUTP=0.
IF (PAP/PAS .GE. 0.53) GO TO 103
C***** SONIC *****
IF (FLAGM) GO TO 102
C***** FIRST TIME SONIC *****C
WRITE (12,816)
IPAGE=IPAGE+1
FLAGM=.TRUE.
102 XMOOT=CD*CRACK*12.*SQRT(0.94*GIN*PAS*RHOAS)
GO TO 106

```

```

C***** SUBSONIC *****C
103 IF (.NOT. FLAGM) GO TO 104
C***** FIRST TIME BACK TO NORMAL SUBSONIC *****C
WRITE (12,817)
IPAGE=IPAGE+1
FLAGM=.FALSE.
104 XMDOT=CD*CRACK*SQRT(2.*GIN*(PAS-PAP)*RHOAS)*12.
105 FOUTS=XMDOT/MAIRS
RBREAK=XMDOT*(GAMMA*TGS-TGP)/(MAIRP*DELTA*XMDOT)
BREAKS=XMDOT*TGS*(1.-GAMMA)/(MAIRS*DELTA*XMDOT)
GO TO 112
C***** NO FLOW *****C
106 FOUTP=0.
FOUTS=0.
XMDOT=0.
RBREAK=0.
BREAKS=0.
GO TO 112
C***** FLOW OUT OF PRIMARY INTO SECONDARY *****C
107 FOUTS=0.
IF (PAS/PAP .GE. 0.53) GO TO 109
C***** SONIC *****C
IF (FLAGM) GO TO 108
C***** FIRST TIME SONIC *****C
WRITE (12,818)
IPAGE=IPAGE+1
FLAGM=.TRUE.
108 XMDOT=CD*CRACK*12.*SQRT(0.94*GIN*PAP*RHOAP)
GO TO 111
C***** SUBSONIC *****C
109 IF (.NOT. FLAGM) GO TO 110
C***** FIRST TIME BACK TO NORMAL SUBSONIC *****C
WRITE (12,817)
IPAGE=IPAGE+1
FLAGM=.FALSE.
110 XMDOT=CD*CRACK*SQRT(2.*GIN*(PAP-PAS)*RHOAP)*12.
111 FOUTP=ABS(XMDOT)/MAIRP
RBREAK=ABS(XMDOT)*TGP*(1.-GAMMA)/(MAIRP*DELTA*ABS(XMDOT))
BREAKS=ABS(XMDOT)*(GAMMA*TGP-TGS)/(MAIRS*DELTA*ABS(XMDOT))
XMDOT=0.-XMDOT
816 FORMAT (' FLOW BETWEEN PRIMARY AND SECONDARY HAS BECOME SONIC')
817 FORMAT(' FLOW BETWEEN PRIMARY AND SECONDARY HAS RETURNED TO SUBSONIC')
112 CONTINUE
FOUTI=FOUTS+LEAK
N=3
RETURN
END

```

C
C
C

C this is the pan geometry subroutine.

```

SUBROUTINE PAN
IMPLICIT REAL (K,L,M)
LOGICAL FLAGM
COMMON // NAME(320), FLAG2, FLAGAS, FLAGC, FLAGF, FLAGN,
FLAGPN, FLAGW, IPAGE, ISWICH, IAROSL, FLAGDF, ICZ
COMMON /LITH/ AKLI, ASLI, CPLI, CSBLI, HB, LIBP, LIL, LILP, LIT,
RHLI, SPILL, TLI, TLII, ZLI
COMMON /STEEL/ CPSFP, CPSFS, CPSWP, CPSWS, ESTLFP, ESTLWP, KSTLFP,
KSTLFS, KSTLWP, KSTLWS, RHSFP, RHSFS, RHSWP, RHSWS
COMMON /MISC/ AFP, AFS, AWP, AWS, C7, C21, GIN,
HA, HINFAM, HINSAM, HTCPCP, QRAOC, RADC, RCZW,
RHOAP, RLIW, RWPWS, SIGMA, TA, TC(20), TFS,
TFSZER, TGP, TGS, TGPZER, TSFP, TSP, TSS,
TSSZER, THFP, THFS, THWP, THWS, ZZES, ZZS, ZZI, ZZT
COMMON /PANOP/ AINS, APAN, BREDTH, CLIST, CPINS, CPPAN, EMGP, FPG, FPW,
KPAN, RHINS, RHPAN, THKIN1, THKIN2, THKPAN,
TINS1, TINS1F, TINS1I, TINS2, TINS2F, TINS2I,
TPAN, TPANF, TPANZO, ZZ2, ZZ4, ZZ8, ZZ9

```

C

IF (FLAGN) N=1

```

GO TO (1,2,3)N
1 CONTINUE
C
C***** READ IN PAN GEOMETRY PARAMETERS *****
C (ONLY IF USING PAN OPTION)
C
READ (3,701) KPAN,RHPAN,CPPAN,RHINS,CPINS,EMINS
READ (3,701) TPANZO,APAN,BREDTH,AINS,HINGPF
READ (3,701) THKPAN,THKIN1,THKIN2
C
WRITE (10,800) TPANZO,APAN,CPPAN,THKPAN,BREDTH,KPAN,RHPAN
WRITE (10,801) THKIN1,THKIN2,AINS,RHINS,CPINS,EMINS,HINGPF
C
700 FORMAT(20A4)
701 FORMAT(8F12.4)
800 FORMAT(///,' DATA FOR SUSPENDED PAN OPTIONAL GEOMETRY:',/,1X,
.41(1H-),//T10,'TPANZO =',F12.4,T36,'APAN =',F12.4,T60,
.'CPPAN =',F12.4//T10,'THKPAN =',F12.4,T36,'BREDTH =',F12.4//T10,
.'KPAN =',F12.4,T36,'RHPAN =',F12.4//)
801 FORMAT(//T10,'THKIN1 =',F12.4,T36,'THKIN2 =',F12.4,T60,'AINS =',
.F12.4//T10,'RHINS =',F12.4,T36,'CPINS =',F12.4,T60,
.'EMINS =',F12.4//T10,'HINGPF =',F12.4//)
C
N=2
RETURN
2 CONTINUE
C***** INITIALIZE PAN GEOMETRY VARIABLES *****
FPG=0.29
FPW=0.384
TINS1=0.8*(TPANZO+TGPZER)
TINS2=TGPZER
TINS1=TINS1
TINS2=TINS2
C CONVERT THERMAL CONDUCTIVITY OF LI PAN TO BTU/SEC-FT-DEG R
KPAN=KPAN/3600.
N=3
RETURN
3 CONTINUE
C
C***** COMPUTE PHYSICAL PROPERTIES DEPENDENT ON TEMPERATURE *****
C
C***** RADIATIVE INTERCHANGE FACTORS *****
RIFPAS=1./((1.-EMINS)/EMINS+(1.-ESTLFP)/ESTLFP*AINS/AFP+
.(AINS/AFP+1.)/(1.+AINS/AFP*(1.-EMGP)))
RIFPAG=EMINS*EMGP/(EMINS*EMGP+EMINS*EMGP)
C
C***** CALCULATING GAS HEAT TRANSFER COEFFICIENTS *****
HFPGP=HINGPF*AKEXX(TGP,TSFP,RHOAP)
C
C***** CALCULATIONS WITH SUSPENDED LITHIUM SPILL PAN *****
C
HPAN=0.714*HB
AHT=ASLI+ZLI*BREDTH
TET1=0.0025*(TINS1-400.)-2.8
KIN1=(.70892+.36584*TET1+.04565*TET1**2-.00791*TET1**3)/43200.
TET2=0.0025*(TINS2-400.)-2.8
KIN2=(.70892+.36584*TET2+.04565*TET2**2-.00791*TET2**3)/43200.
YPAGAS=AINS/(THKIN2/2./KIN2+1./HPAN)
C2=YPAGAS/HTCPGP
C13=YPAGAS/(RHINS*AINS*THKIN2*CPINS)
C16=KSTLFP*HFPGP/(RHSFP*CPSFP*THFP*(THFP*HFPGP/2.+KSTLFP))
C17=KSTLFP*HFPGP*AFP/HTCPGP/(THFP*HFPGP/2.+KSTLFP)
QRADS=SIGMA*AINS*(TINS2**4-TSFP**4)*RIFPAS
QRADCG=SIGMA*AINS*(TINS2**4-TGP**4)*RIFPAG
RPAINT=QRADS/(RHSFP*AFP*THFP*CPSFP)
RSTPAN=QRADS/(RHINS*AINS*THKIN2*CPINS)
RGASPA=QRADCG/(RHINS*AINS*THKIN2*CPINS)
RPAGAS=QRADCG/HTCPGP
CLIPAN=2.*AHT/(LIL*CPLI)/(ZLI/AKLI+THKPAN/KPAN)
CPANLI=2.*AHT/(RHPAN*APAN*THKPAN*CPPAN)/(ZLI/AKLI+THKPAN/KPAN)
CPIN1=2./(RHPAN*APAN*THKPAN*CPPAN)/(THKPAN/KPAN/APAN+THKIN1/
KIN1/AINS)

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CIN1PN=2./((RHINS*AINS*THKIN1*CPINS))/(THKPAN/KPAN/APAN+THKIN1/
KIN1/AINS)
CIN12=2./((RHINS*CPINS*THKIN1)/(THKIN1/KIN1+THKIN2/KIN2)
CIN21=CIN12*THKIN1/THKIN2
C*****MODIFYING PRIMARY CELL TEMPERATURE RATES OF CHANGE DUE TO PAN *****
ZZ1=ZZ1+CLIST*(TLI-TSFP)-CLIPAN*(TLI-TPAN)
ZZ4=ZZ4+C2*(TINS2-TGP)+RPAGAS+C17*(TSFP-TGP)
ZZ7=ZZ7-CSBLI*(TLI-TSFP)+C16*(TGP-TSFP)+RPNST
C
C***** CALCULATE LI SPILL PAN TEMP. RATE OF CHANGE DEG R/SEC *****
ZZ2=CPANLI*(TLI-TPAN)+CPINI*(TINS1-TPAN)
C CALCULATE INSULATION TEMPERATURE RATE OF CHANGE
ZZ8=CIN1PN*(TPAN-TINS1)+CIN12*(TINS2-TINS1)
ZZ9=CIN21*(TINS1-TINS2)+C13*(TGP-TINS2)-RSTPAN-RGASPA
RETURN
END
C this is the wall concrete subroutine
SUBROUTINE CONCW
IMPLICIT REAL (K,L,M)
DIMENSION C4(20)
LOGICAL FLAGN,FLAG2
COMMON // NAME(320), FLAG2, FLAGAS, FLAGC, FLAGF, FLAGN,
FLAGPN, FLAGW, IPAGE, ISWICH, IAROSL, FLAGDF, ICZ
COMMON /LITH/ AKLI, ASLI, CPLI, CSBLI, HB, LIBP, LIL, LILP, LIT,
RMLI, SPILL, TLI, TLII, ZLI
COMMON /STEEL/ CPSFP, CPSFS, CPSWP, CPSWS, ESTLFP, ESTLWP, KSTLFP,
KSTLFS, KSTLWP, KSTLWS, RHSFP, RHSFS, RHSWP, RHSWS
COMMON /MISC/ AFP, AFS, AWP, AWS, C7, C21, GIN,
HA, HINFAM, HINSAM, HTCPCP, ORADC, RADC, RCZW,
RHOAP, RLW, RWPWS, SIGMA, TA, TC(20), TFS,
TFSZER, TGP, TGS, TGPZER, TSFP, TSP, TSS,
TSSZER, THFP, THFS, THWP, THWS, ZZES, ZZS, ZZS, ZZ1, ZZ7
COMMON /INTGL/ IMETH, ICOUNT, ISTORE, INOIN, IPASS, DELT,
XIC(101), ZZZ(501)
COMMON /CONOP/ C8, CPCON, DTBOT(20), DTC(20), GAP, KCON, KGAP,
L(20), L1(20), NL, NL1, ORADB, RADB, RHCON,
SFLCR, TB(20), TBF(20), TBIC(20), TCF(20),
TCIC(20), THFC, THWC, TSFPI, TSPZER, XSFL
C
IF (FLAGN) N=1
GO TO (1,2,3)N
1 CONTINUE
NLM1=NL-1
C***** INITIALIZE WALL CONCRETE VARIABLES *****
DATA C3, C5, C7, RADCC/4*0.0/
IF (FLAG2) GO TO 100
AWS=AWP
CPSWS=CPSWP
KSTLWS=KSTLWP
RHSWS=RHSWP
THWS=THWP
TSSZER=TSPZER
100 CONTINUE
DO 1001 IAM=1,20
C4(IAM)=0.
1001 DTC(IAM)=0.
DO 1002 I=1, NL
TCIC(I)=TSSZER
TC(I)=TSSZER
1002 L(I)=THWC*L(I)
N=2
RETURN
2 CONTINUE
C***** CALCULATING GAS HEAT TRANSFER COEFFICIENT FROM OUTERMOST *****
C CONCRETE NODE TO AMBIENT
TCNL=TC(NL)
HA=HINSAM*AKEXX(TCNL, TA, .074)
C ***** CALCULATING THERMAL DIFFUSIVITIES BETWEEN NODES *****
USUBA=KCON*HA/(KCON+HA*L(NL)/2.)
B=L(1)/(KCON*2.)+GAP/KGAP+THWS/(KSTLWS*2.)
C3=1./((B*L(1))*RHCON*CPCON)
DO 1004 I=1, NLM1

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C4(I)=2.*KCON/(RHCON*CPCON*L(I)*(L(I)+L(I+1)))
1004 CONTINUE
C5=USUBA/(RHCON*CPCON*L(NL))
C7=1./(B*THWS*RHSWS*CPSWS)
N=3
RETURN
3 CONTINUE
IF (.NOT. FLAG2) TSS=TSP
RADCC=QRADC/(L(1)*AWS*RHCON*CPCON)
C***** WALL CONCRETE TEMPERATURE CHANGE *****
DTCOT(1)=C3*(TSS-TC(1))+C4(1)*(TC(2)-TC(1))*RADCC
DTCOT(NL)=C4(NLM1)*(TC(NLM1)-TC(NL))-C6*(TC(NL)-TA)
DO 1006 I=2,NLM1
1006 DTCOT(I)=C4(I)*(TC(I+1)-TC(I))+C4(I-1)*(TC(I-1)-TC(I))
N=2
RETURN
END

C
C
C this is the floor concrete subroutine
SUBROUTINE CONCF
IMPLICIT REAL (K,L,M)
DIMENSION C10(20)
LOGICAL FLAGN
COMMON // NAME(320), FLAG2, FLAGAS, FLAGC, FLAGF, FLAGN,
. FLAGPN, FLAGW, IPAGE, ISWICH, IAROSL, FLAGDF, ICZ
COMMON /LITH/ AKLI, ASLI, CPLI, CSBLI, HB, LIBP, LIL, LILP, LIT,
. RHLI, SPILL, TLI, TLII, ZLI
COMMON /STEEL/ CPSFP, CPSFS, CPSWP, CPSWS, ESTLFP, ESTLWP, KSTLFP,
. KSTLFS, KSTLWP, KSTLWS, RHSFP, RHSFS, RHSWP, RHSWS
COMMON /MISC/ AFP, AFS, AWP, AWS, C7, C21, GIM,
. HA, HINFAM, HINSAM, HTCGRP, QRADC, RADCC, RCZW,
. RHOAP, RLIW, RWPWS, SIGMA, TA, TC(20), TFS,
. TFSZER, TGP, TGS, TGPZER, TSFP, TSP, TSS,
. TSSZER, THFP, THFS, THWP, THWS, ZZES, ZZS, ZZ1, ZZ7
COMMON /INTGL/ IMETH, ICOUNT, ISTORE, INOIN, IPASS, DELT,
. XIC(101), ZZZ(501)
COMMON /CONOP/ C8, CPCON, DTBDT(20), DTCOT(20), GAP, KCON, KGAP,
. L(20), LI(20), NL, NLM1, QRADB, RAD8, RHCON,
. SFLCR, TB(20), TBF(20), TBIC(20), TCF(20),
. TCIC(20), THFC, THWC, TSFPI, TSPZER, XSFL

C
IF (FLAGN) N=1
GO TO (1,2,3)N
1 CONTINUE
IF (FLAG2) GO TO 100
AFS=AFP
CPSFS=CPSFP
KSTLFS=KSTLFP
RHSFS=RHSFP
THFS=THFP
TFSZER=TSFPI
100 CONTINUE
NLM1=NLI-1
C***** INITIALIZE FLOOR CONCRETE VARIABLES *****
DATA C8,C9,RADCB/3*0.0/

C
DO 1001 IAM=1,20
C10(IAM)=0.
1001 DTBDT(IAM)=0.
DO 1003 I=1,NLM1
TBIC(I)=TFSZER
TB(I)=TFSZER
1003 LI(I)=THFC*LI(I)
N=2
RETURN

C
2 CONTINUE
C ***** CALCULATING THERMAL DIFFUSIVITIES BETWEEN NODES *****
BB=L1(1)/(KCON*2.)*GAP/KGAP+THFS/(KSTLFS*2.)
C8=1./(BB*THFS*RHSFS*CPSFS)
C9=1./(BB*L1(1)*RHCON*CPCON)

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DO 1005 I=1,NL1M1
C10(I)=2.*KCON/(RHCON*CPCON*L1(I)*(L1(I)+L1(I+1)))
1005 CONTINUE
N=3
RETURN
3 CONTINUE
IF (.NOT. FLAG2) TFS=TSFP
RADCB=QRADB/(L1(1)*AFS*RHCON*CPCON)
C***** FLOOR CONCRETE TEMPERATURE CHANGE
DTBDT(1)=C9*(TFS-TB(1))+C10(1)*(TB(2)-TB(1))+RADCB
DTBDT(NL1)=C10(NL1M1)*(TB(NL1M1)-TB(NL1))
DO 1007 IB=2,NL1M1
1007 DTBDT(IB)=C10(IB)*(TB(IB+1)-TB(IB))+C10(IB-1)*(TB(IB-1)-TB(IB))
N=2
RETURN
END

C
C
C This is the gas injection subroutine
SUBROUTINE INJEC
IMPLICIT REAL (X,L,M)
LOGICAL FLAGN,FLAGAS
COMMON // NAME(320),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGDF,ICZ
COMMON /INJOP/ DP1,DP2,DP3,MNIINJ,MOXINJ,TIME,VP
COMMON /MISC/ AFP,AFS,AWP,AWS,C7,C21,GIN,
HA,HINFAM,HINSAM,HTCPGP,QRADC,RADC,RCZW,
RHOAP,RLIW,RWPWS,SIGMA,TA,TC(20),TFS,
TFSZER,TGP,TGS,TGPZER,TSFP,TSP,TSS,
TSSZER,THFP,THFS,THWP,THWS,ZZES,ZZS,ZZS,ZZ1,ZZ7
C
C IF (FLAGN) N=1
GO TO (1,2)N
1 CONTINUE

C
C***** READ IN GAS INJECTION VARIABLES *****
C (ONLY IF USING GAS INJECTION OPTION)
READ (4,700) TONE,TTWO,TTHREE,DP1,DP2,DP3,FCT1,FCT2,FCT3
700 FORMAT (3F10.2,6F8.4)

C
WRITE (10,800) TONE,TTWO,TTHREE,DP1,DP2,DP3,FCT1,FCT2,FCT3
800 FORMAT (////' DATA FOR GAS INJECTION MODELING:',/,1X,31(1H-),
//T10,'TONE = ',F12.4,T35,'TTWO = ',F12.4,T60,'TTHREE = ',F12.4
//T10,'DP1 = ',F12.4,T35,'DP2 = ',F12.4,T60,'DP3 = ',F12.4
//T10,'FCT1 = ',F12.4,T35,'FCT2 = ',F12.4,T60,'FCT3 = ',F12.4)

C
INJEC1=0
INJEC2=0
INJEC3=0
N=2
RETURN
2 CONTINUE
C***** INJECTION OF NITROGEN AND OXYGEN TO MODEL MEDL EXPERIMENT ***
IF (TIME .LT. TONE .OR. TIME .GT. (TONE+60.)) GO TO 100
IF (INJEC1 .EQ. 0 .AND. DP1 .GT. 0.0) WRITE (11,801) TONE,DP1
801 FORMAT (//' INJECTION OF GAS AT TIME = ',F8.0,' TO RAISE
PRESSURE BY',F8.4,' PSI.')
INJEC1=1
MOINJ1=2.9822*VP/TGP*DP1*(1.0-FCT1)
MNIINJ1=2.6094*VP/TGP*DP1*FCT1
MOXINJ1=MOINJ1/60.
MNIINJ1=MNIINJ1/60.
100 CONTINUE
IF (TIME .LT. TTWO .OR. TIME .GT. (TTWO+60.)) GO TO 101
IF (INJEC2 .EQ. 0 .AND. DP2 .GT. 0.0) WRITE (11,801) TTWO,DP2
INJEC2=1
MOINJ2=2.9822*VP/TGP*DP2*(1.0-FCT2)
MNIINJ2=2.6094*VP/TGP*DP2*FCT2
MOXINJ2=MOINJ2/60.
MNIINJ2=MNIINJ2/60.
101 CONTINUE
IF (TIME .LT. TTHREE .OR. TIME .GT. (TTHREE+60.)) GO TO 102

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IF (INJEC3 .EQ. 0 .AND. DP3 .GT. 0.0) WRITE (11,801) TTHREE,DP3
INJEC3=1
MOINJ3=2.9822*VP/TGP*DP3*(1.0-FCT3)
MNINJ3=2.6094*VP/TGP*DP3*FCT3
MOXINJ=MOINJ3/60.
MNIINJ=MNINJ3/60.
102 CONTINUE
IF (TIME .GT. (TTHREE+60.)) FLAGAS=.FALSE.
RETURN
END

C
C
C
Cthis is the concrete combustion subroutine
SUBROUTINE COMCC
IMPLICIT REAL (K,L,M)
LOGICAL FLAGN,FLAGO
COMMON // NAME(320),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGOF,ICZ
COMMON /LITH/ AKLI,ASLI,CPLI,CSBLI,HB,LIBP,LIL,LILP,LIT,
RHLI,SPILL,TLI,TLII,ZLI
COMMON /MISC/ AFP,AFS,AMP,AWS,C7,C21,GIN,
HA,HINFAM,HINSAM,HTCPGP,QRADC,RADC,RCZM,
RHOAP,RLTW,RWPWS,SIGMA,TA,TC(20),TFS,
TFSZER,TGP,TGS,TGPZER,TSFP,TSP,TSS,
TSSZER,THFP,THFS,THWP,THWS,ZZES,ZZS,ZZS,ZZ1,ZZ7
COMMON /CONOP/ C8,CPCON,DT8DT(20),DTCOT(20),GAP,KCON,KGAP,
L(20),L1(20),NL,NL1,QRADB,RADB,RHCON,
SFLCR,TB(20),TBF(20),TBIC(20),TCF(20),
TCIC(20),THFC,THWC,TSFPI,TSPZER,XSFL
COMMON /CCOP/ CMBRO,CRACON,DCOCZ,H2LEFT,QCCONC,RCMBO,RCMBW,
RELESE,TCIGNI,TCON,TCONF,XMH2OI,ZZC,ZZD,ZZDIN

C
IF (FLAGN) N=1
GO TO (1,2,3)N
1 CONTINUE
C***** READ IN CONCRETE COMBUSTION PARAMETERS *****
READ (3,700) ZZDIN,QCCONC,CRACON,XMH2OI,TCIGNI,RCMBC
700 FORMAT (6F12.4)
C
WRITE (10,800) ZZDIN,QCCONC,CRACON,XMH2OI,TCIGNI,RCMBC
800 FORMAT ('/' CONCRETE COMBUSTION INPUT DATA' /1X,30(1H-)//T10,
'ZZDIN = ',F12.4,T35,'QCCONC = ',F12.4,T60,'CRACON = ',F12.4//
.T10,'XMH2OI = ',F12.4,T35,'TCIGNI = ',F12.4,T60,'RCMBC = ',F12.4//)
C
N=2
RETURN
2 CONTINUE
DATA CCOCZ,CCOCZP,CCOZCO,CPCOCZ,RELESE,ZZC/6*0.0/
ZZD=ZZDIN
TCON=TSFPI
DCOCZ=0.01
XMCOCZ=1.0
FLAGD=.FALSE.
H2LEFT=XMH2OI
VCONC=AFP*L1(1)
N=3
RETURN
3 CONTINUE
C WATER RELEASE FROM CONCRETE --- CORRELATION BASED ON DRYING TESTS
C OF MAGNITITE. SEE R.D. PEAK "CACECO A CONTAINMENT ANALYSIS CODE-
C USERS GUIDE"
RELESE=0.
IF (TB(1) .GE. 658.5 .AND. TB(1) .LT. 1960.) WATER=(1.-EXP(28.207
+TB(1)*(-0.0721+TB(1)*(6.96E-05-TB(1)*2.26E-08)))/11.7)*XMH2OI
C "WATER" IS THE AMOUNT THAT SHOULD BE LEFT AT TB(1) IN UNITS OF LBS./FT**3
IF (TB(1) .GE. 658.5 .AND. (H2LEFT-WATER) .GT. 0. .AND. TB(1)
.LT. 1960.) RELESE=(H2LEFT-WATER)*VCONC/30.
IF (TB(1) .GE. 1960. .AND. H2LEFT .GT. 0.) RELESE=H2LEFT*VCONC/30.
C IN OTHER WORDS THE RELEASE RATE OF WATER IS SUCH THAT THE DIFFERENCE
C BETWEEN THE ACTUAL AMOUNT AND THE CORRECT AMOUNT ( ACCORDING TO THE
C CORRELATION USED) IS GIVEN OFF IN THIRTY SECONDS.

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C***** CALCULATE THERMAL DIFFUSIVITIES *****
XMCOCZ=DCOCZ*CRACON*RHCOM
CPCOCZ=2.*CRACON*KCON*AKLI/(KCON*ZLI+AKLI*DCOCZ)/XMCOCZ
CCOCZP=2.*CRACON*KCON*AKLI/(KCON*ZLI+AKLI*DCOCZ)/LIL
CCOCZ=2.*CRACON*KCON/(DCOCZ+L1(1))/XMCOCZ
CCOZCO=2.*CRACON*KCON/(DCOCZ+L1(1))/(RHCOM*CPCON*L1(1)*AFP)
C FLAGD IS TRUE WHEN CONCRETE COMBUSTION STOPS
FLAGD=.FALSE.
IF (LILP .LT. 0.1 .OR. TCON .LT. TCIGNI) FLAGD=.TRUE.
ZZD=ZZDIN
IF (FLAGD) ZZD=0.0
ZZC=CPCOCZ*(TLI-TCON)+CCOCZ*(TB(1)-TCON)+ZZD*CRACON*QCCONC*RHCOM
/XMCOCZ/CPCON+RELESE*QCW*RCMBW/XMCOCZ/CPCON
ZZ1=ZZ1+CCOCZP*(TCON-TLI)
DTBDT(1)=DTBDT(1)+CCOCZO*(TCON-TB(1))
CMBRO=RELESE*RCMBO+ZZD*CRACON*RHCOM*RCMBC
N=3
RETURN
END

C
C
C THIS IS THE LITHIUM LEAD COMBUSTION SUBROUTINE
C
C
SUBROUTINE LIPB
IMPLICIT REAL (K,L,M)
LOGICAL FLAGN,FLAGL
COMMON /LITH/ AKLI,ASLI,CPLI,CSBLI,HB,LIPB,LIL,LILP,LIT,
RHLI,SPILL,TLI,TLII,ZLI
COMMON // NAME(32),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGDF,ICZ
COMMON /LEAD/ CPLEAD,KLEAD,RHLEAD,MLIPB,XALLOY,ATML,ATMPB,CMBR
COMMON /PBPOOL/ DMPBDT,ZZPB,MLEAD,TLEADI,XWLI,DFLIPB,XLIDOT,
THPB,TLEADF

C
IF (FLAGN) N=1
GO TO (1,2,3)N
1 CONTINUE

C
C***** READ IN LEAD PARAMETERS *****
C
READ (3,701) CPLEAD,KLEAD,RHLEAD,ALLOYI,QDISS
C
WRITE (10,800) CPLEAD,KLEAD,RHLEAD,ALLOYI,QDISS
C
701 FORMAT (6F12.4)
800 FORMAT(//,' DATA FOR LITHIUM LEAD COMBUSTION OPTION: ',/,1X,40(1H-),
/,/T10,'CPLEAD =',F12.4,T35,'KLEAD =',F12.4,T60,'RHLEAD =',F12.4//
,T10,'ALLOYI =',F12.4,T35,'QDISS =',F12.4//)
C
KLEAD=KLEAD/3600.
DFLIPB=DFLIPB/1.0E08
ATMLPB=SPILL/(6.941*ALLOYI+(1.-ALLOYI)*207.2)
ATMPB=(1.-ALLOYI)*ATMLPB
ATMLI=ALLOYI*ATMLPB
MLIPBI=SPILL
SPILL=ATMLPB*6.941*ALLOYI
C
WRITE (10,801) SPILL
801 FORMAT(' MODIFIED PARAMETERS FOR LITHIUM IN LITHIUM LEAD POOL ',/,
.1X,52(1H-),//T10,' AMOUNT OF LITHIUM AVAILABLE FOR COMBUSTION =',
F12.4//T10,' THICKNESS OF LIPB POOL IS LESS THAN ZLI ABOVE AND ',/
T35,' IS CALCULATED IN PROGRAM')
N=2
RETURN
C
2 CONTINUE
C***** MODIFYING LITHIUM POOL PROPERTIES TO INCLUDE LEAD *****
C
IF (FLAGDF) GO TO 100
MLIPB=MLIPBI-LIPB
XMLIPB=MLIPBI-LIT+LILP

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ATML=ATMLI-LIBP/8.941
IF (ATML .LE. 0.0) ATML=0.0
XALLOY=ATML/(ATML+ATMPB)
GO TO 110
100 CONTINUE
MLIPB=MLIPBI-LIBP-MLEAD
IF (MLIPB .LT. 0.0) MLIPB=0.0
XMLIPB=MLIPB
ATML=ATMLI*MLIPB/MLIPBI
XALLOY=ALLOYI
110 CONTINUE
XWLI=XALLOY*8.941/(XALLOY*8.941+(1.-XALLOY)*207.2)
AKLI=XWLI*AKLI+(1.-XWLI)*KLEAD-0.72*ABS(AKLI-KLEAD)*XWLI*(1.-XWLI)
CPLI=XALLOY*CPLI+(1.-XALLOY)*CPLEAD
RHLI=XALLOY*RHLI+(1.-XALLOY)*RHLEAD+332.6*XALLOY*(1.-XALLOY)**0.64
ZLI=XMLIPB/RHLI/ASLI
IF ((MLIPB .LT. 0.1*MLIPBI) .AND. (ALPHA*DELT .GT. ZLI*ZLI .OR.
. XMLIPB .LT. 1.0)) FLAGL=.TRUE.
IF (FLAGL) LIL=MLIPBI/10.
IF (.NOT. FLAGL) LIL=XMLIPB
N=3
RETURN
C
3 CONTINUE
C***** MODIFYING POOL TEMP RATE OF CHANGE TO INCLUDE HEAT OF LITHIUM *****
C DISSOCIATION FROM LEAD
Z21=Z21-QDISS*CMBR*ASLI/(LIL*CPLI)
N=2
RETURN
END
C
C
C THIS IS THE LITHIUM LEAD DIFFUSION MODEL SUBROUTINE.
C
SUBROUTINE LIDIFF
IMPLICIT REAL (K,L,M)
LOGICAL FLAGN,FLAGPB
COMMON // NAME(320),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
. FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGDF,ICZ
COMMON /LITH/ AKLI,ASLI,CPLI,CSBLI,HB,LIBP,LIL,LILP,LIT,
. RHLI,SPILL,TLI,TLII,ZLI
COMMON /LEAD/ CPLEAD,KLEAD,RHLEAD,MLIPB,XALLOY,ATML,ATMPB,CMBR
COMMON /INJOP/ DP1,DP2,DP3,MNINJ,MOXINJ,TIME,VP
COMMON /PBPOOL/ DHPBOT,ZZPB,MLEAD,TLEADI,XWLI,DFLIPB,XLIDOT,
. THPB,TLEADF
COMMON /STEEL/ CPSFP,CPSFS,CPSWP,CPSWS,ESTLFP,ESTLWP,KSTLFP,
. KSTLFS,KSTLWP,KSTLWS,RHSFP,RHSFS,RHSP,RHSWS
COMMON /MISC/ AFP,AFS,AWP,AWS,C7,C21,GIN,
. HA,HINFAM,HINSAM,HTCPGP,QRADC,RADC,RCZW,
. RHOAP,RLIW,RPWWS,SIGMA,TA,TC(20),TFS,
. TFSZER,TGP,TGS,TGPZER,TSFP,TSP,TSS,
. TSSZER,THFP,THFS,THWP,THWS,ZZES,ZZB,ZZS,ZZ1,ZZ7
COMMON /PANOP/ AINS,APAN,BREDTH,CLIST,CPINS,CPPAN,EMGP,FPG,FPW,
. KPAN,RHINS,RHPAN,THKIN1,THKIN2,THKPAN,
. TINS1,TINS1F,TINS1I,TINS2,TINS2F,TINS2I,
. TPAN,TPANF,TPANZO,ZZ2,ZZ4,ZZB,ZZB
COMMON /UNITS/ AEHCP,BETA,CHP,CMBRH,CPAP,CPEHCP,MAP,MNIP,
. MOXP,MWAP,PAPZER,QCN,QCO,QCO1,QCO2,QCW,QVAP,
. TCZ,TCZF,TCZI,TEHCP,TEHCPF,TEHCZP,TGPF,
. TLIF,TMELT,TSFPF,TSPF,TVAP,XMEHCP
COMMON /INTGL/ IMETH,ICOUNT,ISTORE,INOIN,IPASS,DELT,
. XIC(101),ZZZ(501)
COMMON /PBDIF/ CCZP,CGLI,CLIG,CPCZ,CPMCZ,DFILM,KFILM,PYUP,
. QRADP,RCZP,RGLI,RIFCZP,RIFPG,RIFPW,RLIG,RWLI,
. TLEAD,YAPC2,ZZB
C
IF (FLAGN) N=1
GO TO (1,2,3)N
1 CONTINUE
TLEADI=TLII
ZZPB=0.
N=2

```

```

RETURN
C
2 CONTINUE
THPB=MLEAD/RHLEAD/ASLI
IF (THPB .LT. 1.0E-16) THPB=1.0E-16
DFLIPB=6.5E-08*EXP(-1224./TLI)
XLIDOT=DFLIPB*RHLI*XWLI/THPB
DMPBDT=(1.-XALLOY)/XALLOY*CMBR*ASLI*207.2/8.941
N=3
RETURN
3 CONTINUE
C
ZLI1=.667*ZLI
ZLI2=.333*ZLI
KLIPB1=(MLEAD*KLEAD+.333*LIL*AKLI)/(MLEAD+.223*LIL)
CPLPB1=(MLEAD*CPLEAD+.333*LIL*CPLI)
THPB1=ZLI2+THPB
C
C***** MODIFY POOL, COMBUSTION ZONE AND PRIMARY CELL TEMP RATES OF CHANGE
100 CONTINUE
IF (ICZ .EQ. 0) GO TO 110
ZZ1=ZZ1-CCZP*(TCZ-TLI)-RCZP+QVAP*CMBR*ASLI*CCZP/YAPCZ+RWLI+RGLI
ZZ4=ZZ4-RLIG
ZZ5=ZZ5-RLIW
ZZ6=ZZ6+CPCZ*(TCZ-TLI)+QRADP/CPMCZ
C
CCLIPB=2.*ASLI*KLIPB1*AKLI/
(.667*LIL*CPLI*(ZLI1*KLIPB1+THPB1*AKLI))
CCPBLI=2.*KLIPB1*AKLI*ASLI/(CPLPB1*(ZLI1*KLIPB1+THPB1*AKLI))
YAPCZ=KFILM*KLIPB1*ASLI/(DFILM*KLIPB1+KFILM*THPB1/2.)
CPCZ=YAPCZ/CPMCZ
CCZP=YAPCZ/CPLPB1
QRADP=SIGMA*ASLI*(TLEAD**4-TLEAD**4)*RIFCZP
RCZP=QRADP/CPLPB1
QRADY=SIGMA*ASLI*(TLEAD**4-TSP**4)*RIFPW
QRADZ=SIGMA*ASLI*(TLEAD**4-TGP**4)*RIFPG
RLIW=QRADY/(THWP*AWP*RHSWP*CPSWP)
RWLI=QRADY/CPLPB1
RGLI=QRADZ/CPLPB1
RLIG=QRADZ/HTCPGP
C
ZZPB=CCZP*(TCZ-TLEAD)+RCZP+QVAP*CMBR*ASLI/CPLPB1
-RWLI-RGLI-CCPBLI*(TLEAD-TLI)
ZZ1=ZZ1+CCLIPB*(TLEAD-TLI)
ZZ4=ZZ4+RLIG
ZZ5=ZZ5+RLIW
ZZ6=ZZ6-QRADP/CPMCZ-CPCZ*(TCZ-TLEAD)
GO TO 120
110 CONTINUE
C***** MODIFY TEMPS WITHOUT COMBUSTION ZONE MODELING *****
ZZ1=ZZ1-CGLI*(TGP-TLI)+RWLI+RGLI
ZZ4=ZZ4-CLIG*(TLI-TGP)-RLIG
ZZ5=ZZ5-RLIW
C
YALIG=KLIPB1*HB*ASLI/(KLIPB1+HB*THPB1/2.)
CLIG=YALIG/HTCPGP
QRADW=SIGMA*ASLI*(TLEAD**4-TSP**4)*RIFPW
QRADG=SIGMA*ASLI*(TLEAD**4-TGP**4)*RIFPG
RLIW=QRADW/(THWP*AWP*RHSWP*CPSWP)
RWLI=QRADW/CPLPB1
RGLI=QRADG/CPLPB1
RLIG=QRADG/HTCPGP
CGLI=YALIG/CPLPB1
CCLIPB=2.*ASLI*KLIPB1*AKLI/
(.667*LIL*CPLI*(ZLI1*KLIPB1+THPB1*AKLI))
CCPBLI=2.*KLIPB1*ASLI*AKLI/(CPLPB1*(ZLI1*KLIPB1+THPB1*AKLI))
C
ZZPB=CGLI*(TGP-TLEAD)-RWLI-RGLI-CCPBLI*(TLEAD-TLI)
ZZ1=ZZ1+CCLIPB*(TLEAD-TLI)
ZZ4=ZZ4+CLIG*(TLEAD-TGP)+RLIG
ZZ5=ZZ5-RLIW
ZZ6=(TLI-TCZ)/DELT

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120 CONTINUE
ALPHAP=((THPB1+ZLI1)/(ZLI1/AKLI+THPB1/KLIPB1))/
      (((RHLI*CPLI*ZLI1)+(CPLPB1/ASLI))/(THPB1+ZLI1))
PYUP=0.075*(THPB1+ZLI1)**2/ALPHAP
N=2
RETURN
END

```

C
C this is the System International unit conversion subroutine allowing
C the input and output to be prepared and written in SI units.

```

SUBROUTINE SI
IMPLICIT REAL (K,L,M)
LOGICAL FLAGW,FLAGF,FLAG2,FLAGPN,FLAGC,FLAGAS,FLAGN
COMMON // NAME(320),FLAG2,FLAGAS,FLAGC,FLAGF,FLAGN,
      FLAGPN,FLAGW,IPAGE,ISWICH,IAROSL,FLAGOF,ICZ
COMMON /LITH/ AKLI,ASLI,CPLI,CSBLI,HB,LIBP,LIL,LILP,LIT,
      RHLI,SPILL,TLI,TLII,ZLI
COMMON /STEEL/ CPSFP,CPSFS,CPSWP,CPSWS,ESTLFP,ESTLWP,KSTLFP,
      KSTLFS,KSTLWP,KSTLWS,RHSFP,RHSFS,RHSWP,RHSWS
COMMON /MISC/ AFP,AFS,AWP,AWS,C7,C21,GIN,
      HA,HINFAM,HINSAM,HTCPGP,QRADC,RADC,RCZW,
      RHOAP,RLIW,RWPWS,SIGMA,TA,TC(20),TFS,
      TFSZER,TGP,TGS,TGPZER,TSFP,TSP,TSS,
      TSSZER,THFP,THFS,THWP,THWS,ZZES,ZZS,ZZS,ZZ1,ZZ7
COMMON /INJOP/ DP1,DP2,DP3,MNIINJ,MOXINJ,TIME,VP
COMMON /PANOP/ AINS,APAN,BREDTH,CLIST,CPINS,CPPAN,EMGP,FPG,FPW,
      KPAN,RHINS,RHPAN,TKIN1,TKIN2,THKPAN,
      TINS1,TINS1F,TINS1I,TINS2,TINS2F,TINS2I,
      TPAN,TPANF,TPANZO,ZZ2,ZZ4,ZZ8,ZZ9
COMMON /CONOP/ C8,CPCON,DTBDT(20),DTCDT(20),GAP,KCON,KGAP,
      L(20),L1(20),NL,NL1,QRADB,RADB,RHCON,
      SFLCR,TB(20),TBF(20),TBIC(20),TCF(20),
      TCIC(20),THFC,THWC,TSFPI,TSPZER,XSFL
COMMON /CCOP/ CMBRO,CRACON,DCOCZ,H2LEFT,QCCONC,RCMBO,RCHBW,
      RELESE,TCIGNI,TCON,TCONF,XMH2OI,ZZC,ZZD,ZZDIN
COMMON /PBPOOL/ DMPBDT,ZZPB,MLEAD,TLEADI,XWLI,DFLIPB,XLIDOT,
      THPB,TLEADF
COMMON /PBDIF/ CCZP,CGLI,CLIG,CPCZ,CPMCZ,DFILM,KFILM,PYUP,
      QRADP,RCZP,RGLI,RIFCZP,RIFPG,RIFPW,RLIG,RWLI,
      TLEAD,YAPCZ,ZZ6
COMMON /SECOF/ AEHCS,C11,C20,CHS,CPEHCS,CPH2,CPLIN,CPWA,CRACK,
      FOUTP,FOUTS,FOUTT,HINFGS,HINFSG,HINGSS,HINPS,KLEAK,
      LEAK,MAIRP,MAIRS,MAIS,MAS,MH2S,MLIHS,MLINIS,MLINS,
      MLIOTS,MLIOS,MNIIS,MNIS,MOXIS,MOXS,MWAIS,
      MWAS,PAP,PAS,PASZER,RA,RBREAK,RHOLIH,
      RHOLIN,RHOLIO,RWPGAS,TEHCS,TEHCSF,TEHCZS,TGSF,
      TFSF,TGSZER,TSSF,VS,XMDOT,XMEHCS,XMOLA,ZZ3,ZZFS
COMMON /UNITS/ AEHCP,BETA,CHP,CMBRH,CPAP,CPEHCP,MAP,MNIP,
      MOXP,MWAP,PAPZER,QCN,QCO,QCO1,QCO2,QCW,QVAP,
      TCZ,TCZF,TCZI,TEHCP,TEHCPF,TEHCZP,TGPF,
      TLIF,TMELT,TSFPF,TSPF,TVAP,XMEHCP

```

C
IF (FLAGN) N=2
GO TO (1,2,3)N
1 CONTINUE
AEHCP=AEHCP*10.765
AFP=AFP*10.765
AKLI=AKLI*0.57803
ASLI=ASLI*10.765
AWP=AWP*10.765
CHP=CHP*3.281
CPAP=CPAP*2.389E-04
CPCON=CPCON*2.389E-04
CPEHCP=CPEHCP*2.389E-04
CPLI=CPLI*2.389E-04
CPSFP=CPSFP*2.389E-04
CPSWP=CPSWP*2.389E-04
GAP=GAP*3.281
KLEAK=KLEAK*0.03771
KCON=KCON*0.57803
KGAP=KGAP*0.57803
KSTLFP=KSTLFP*0.57803

KSTLWP-KSTLWP*0.57803
PAPZER-PAPZER*1.450E-01
QCN=QCN*4.311E-01
QCO=QCO*4.311E-01
QCO1=QCO1*4.311E-01
QCO2=QCO2*4.311E-01
QCW=QCW*4.311E-01
QVAP=QVAP*4.311E-01
RHCON=RHCON*0.062428
RHLI=RHLI*0.062428
RHOLI=RHOLI*0.062428
RHOLIN=RHOLIN*0.062428
RHOLIO=RHOLIO*0.062428
RHSFP=RHSFP*0.062428
RHSWP=RHSWP*0.062428
SPILL=SPILL*2.2046
TA=TA*1.8
TCZI=TCZI*1.8
TEHCZP=TEHCZP*1.8
TGPZER=TGPZER*1.8
THFC=THFC*3.281
THWC=THWC*3.281
THFP=THFP*3.281
THWP=THWP*3.281
TLII=TLII*1.8
TMELT=TMELT*1.8
TSFPI=TSFPI*1.8
TSPZER=TSPZER*1.8
TVAP=TVAP*1.8
VP=VP*35.32
XMEHCP=XMEHCP*2.2046
ZLI=ZLI*3.281

C

IF (.NOT. FLAG2) GO TO 100
AEHCS=AEHCS*10.765
AFS=AFS*10.765
AWS=AWS*10.765
CHS=CHS*3.281
CPAS=CPAS*2.389E-04
CPEHCS=CPEHCS*2.389E-04
CPSFS=CPSFS*2.389E-04
CPSWS=CPSWS*2.389E-04
CRACK=CRACK*0.1560
KSTLFS=KSTLFS*0.57803
KSTLWS=KSTLWS*0.57803
PASZER=PASZER*1.450E-01
RHSFS=RHSFS*0.062428
RHSWS=RHSWS*0.062428
TEHCZS=TEHCZS*1.8
TFSZER=TFSZER*1.8
TGSZER=TGSZER*1.8
THFS=THFS*3.281
THWS=THWS*3.281
TSSZER=TSSZER*1.8
VS=VS*35.32
XMEHCS=XMEHCS*2.2046
100 CONTINUE

C

IF (.NOT. FLAGPN) GO TO 101
AINS=AINS*10.765
APAN=APAN*10.765
BREDTH=BREDTH*3.281
CPINS=CPINS*2.389E-04
CPPAN=CPPAN*2.389E-04
KPAN=KPAN*0.57803
RHINS=RHINS*0.062428
RHPAN=RHPAN*0.062428
THKIN1=THKIN1*3.281
THKIN2=THKIN2*3.281
THKPAN=THKPAN*3.281
TPANZO=TPANZO*1.8
101 CONTINUE

```

C
  IF (IBLOW .NE. 1) GO TO 102
  BLOWV=BLOWV*2119.2
  CPAB=CPAB*2.389E-04
  EXHSTV=EXHSTV*2119.2
  TBLOW=TBLOW*1.8
102 CONTINUE
  IF (ISFLC .EQ. 1) SFLCR=SFLCR*9.476E-04
  IF (IESC .EQ. 1) ESCR=ESCR*9.476E-04
C
  IF (IAROSL .EQ. 1) BETA=BETA/3.281
C
  IF (.NOT. FLAGC) GO TO 103
  CRACON=CRACON*10.786
  QCCONC=QCCONC*4.311E-01
  TCIGNI=TCIGNI*1.8
  XMH2OI=XMH2OI*2.2046
  ZZDIN=ZZDIN*3.281
103 CONTINUE
C
  IF (.NOT. FLAGAS) GO TO 104
  DP1=DP1*1.450E-01
  DP2=DP2*1.450E-01
  DP3=DP3*1.450E-01
104 CONTINUE
C
  N=2
  RETURN
  2 CONTINUE
C
C*** THIS STEP CONVERTS OUTPUT VARIABLES TO SI ***
C
  CMBRN=CMBRN*4.8824
  LIBP=LIBP/2.2046
  MAP=MAP/2.2046
  MNIP=MNIP/2.2046
  MOXP=MOXP/2.2046
  MWAP=MWAP/2.2046
  PAP=PAP/1.450E-01
  TCZF=TCZF/1.8-273.
  TEHCPF=TEHCP/1.8-273.
  TGP=TEHCP/1.8-273.
  TLI=TLI/1.8-273.
  TSFP=TSFP/1.8-273.
  TSP=TSFP/1.8-273.
  ZLI=ZLI/3.281
  IF (.NOT. FLAG2) GO TO 106
  PAS=PAS/1.450E-01
  TEHCSF=TEHCS/1.8-273.
  TGSF=TGS/1.8-273.
  TFSF=TFS/1.8-273.
  TSSF=TSS/1.8-273.
  XMDOT=XMDOT/2.2046
106 CONTINUE
  IF (FLAGPN) TPANF=TPAN/1.8-273.
  IF (FLAGPN) TINS1F=TINS1/1.8-273.
  IF (FLAGPN) TINS2F=TINS2/1.8-273.
  IF (FLAGC) TCONF=TCON/1.8-273.
  IF (.NOT. FLAGDF) GO TO 110
  MLEAD=MLEAD/2.2046
  THPB=THPB/3.281
  TLEADF=TLEAD/1.8-273.
  XLIDOT=XLIDOT*4.8824*3600.
110 CONTINUE
  IF (.NOT. FLAGW) GO TO 1001
  DO 1001 I=1,20
  TCF(I)=TC(I)/1.8-273.
1001 CONTINUE
  IF (.NOT. FLAGF) GO TO 1002
  DO 1002 I=1,20
  TBF(I)=TB(I)/1.8-273.
1002 CONTINUE

```

```
      N=3
      RETURN
3 CONTINUE
C
C**** THIS STEP CONVERTS OUTPUT FROM SI TO ENGLISH AFTER ****
C      OUTPUT IS PRINTED SO THAT PROGRAM CAN CALCULATE
C      THINGS IN ENGLISH AGAIN. NOT NEEDED FOR OUTPUT TEMPS.
C
      CMBRH=CMBRH/4.8824
      LIBP=LIBP*2.2046
      MAP=MAP*2.2046
      MNIP=MNIP*2.2046
      MOXP=MOXP*2.2046
      MWAP=MWAP*2.2046
      PAP=PAP*1.450E-01
      ZLI=ZLI*3.281
      IF (FLAG2) PAS=PAS*1.450E-01
      IF (FLAG2) XMDOT=XMDOT*2.2046
      IF (FLAGDF) XLIDOT=XLIDOT/3600./4.8824
      IF (FLAGDF) MLEAD=MLEAD*2.2046
      IF (FLAGDF) THPB=THPB*3.281
      N=2
      RETURN
      END
```

APPENDIX E

Sample Input/Output for LITFIRE

LA-5 HEDL TEST LI-1:PB-4 THESIS RUNS
 USING VERSION OF LITFIRE: "LITFIR"
 DATE: 28 AUGUST, 1982

TIME	DLCT	TCZF	TLIF	TGPF	PAP	TSPF	TSFPF
1 1 1 0 0 0 1 0 0 0 0 0 1 0							
5 5							
.20	.20	.20	.20	.20			
.20	.20	.20	.20	.20			
30086.00	66.70		0.1247	39.90			
543.0	12300.000	5100.0		0.120	0.00		
00.0840	00.0840	0.0000		0.015	0.00		
0.85	0.1200	30.00		497.5498	5600.00		0.0580
0.85	0.1200	30.00		497.5498	4000.00		0.0580
0.2	0.9960	33.80		30.00			
0.9	0.2550	0.0227		144.00			
124.00	86.9400	160.00		0.04	0.90		0.100
18510.0	0.0	4080.0		13784.0			
0.8764	0.0	1.487		0.383	6.93		
815.0	2916.0	8431.0		0.0			
0.12	0.12	0.120		0.070	0.07		0.07
0.07	0.07						
21.650	220.00	0.0000		0.050	5.0		
1140.0	549.175	546.96		546.0	540.53		1140.0
16.433	0.2316	0.0062		0.0094			
00030000000.20000009935.0000000000.00600002000.0000							

THIS OUTPUT CORRESPONDS TO ONE CELL GEOMETRY
 HEDL TEST CASE: LA-5
 DATE: 17 AUGUST 1982

TIME	TGSF	TFSF	PAP	PAS	XNDOT
250000.00	44.00	14.7	534.00	534.00	534.00
00.00	00.000	0.232	00.0000	0.1247	
534.1	1.0	00.00	1.00	0.0	
0.85	0.1200	30.00	497.5498	20960.10	0.0260
0.85	0.1200	30.00	497.5498	88.00	0.0260
350.00					

THIS IS THE PAN OUTPUT FILE TESTING LIPB CODE
 HEDL TEST CASE: LA-5
 DATE: 24 AUGUST 1982

TIME	TLIF	TPANF	TIHS1F	TIHS2F	PAP
0000013.00000000490.00000000000.12000000010.00000000000.20000000000.9000					
535.00	35.29	16.50	14.15	.000	
0.0157	0.1667	0.0833			
0.0350	9.30	708.00	0.2000	3315.0	10.7600

CONCRETE NODAL TEMPERATURE PROFILES.

TIME	TBF(1)	TBF(2)	TBF(3)	TBF(4)	TBF(5)
0000100.0000					

UWMAK-III TWO CELL TEST CASES WITH CRACK=0.01 CM**2
 USING VERSION OF LITFIRE: "AKEXX" IN SI UNITS
 DATE: 12 august, 1982

TIME	DELT	TCZF	TLIF	TGPF	PAP	TSPF	TSBF
0.0	0.10	320.00	320.00	250.00	101.40	250.00	250.00
0.1	0.10	320.00	320.00	250.00	101.40	250.00	260.01
0.2	0.10	320.00	319.99	250.00	101.40	250.00	250.01
0.3	0.10	319.99	319.99	250.00	101.40	249.99	250.02
0.4	0.10	319.99	319.99	250.00	101.40	249.99	260.03
0.5	0.10	319.99	319.98	250.00	101.40	249.99	250.04
0.6	0.10	319.98	319.98	250.00	101.40	249.99	250.04
0.7	0.10	319.98	319.98	250.00	101.40	249.98	250.05
0.8	0.10	319.98	319.97	250.00	101.40	249.98	250.06
0.9	0.10	319.97	319.97	260.01	101.40	249.98	250.07
1.0	0.10	319.97	319.97	250.01	101.40	249.98	250.07
1.1	0.10	319.97	319.96	260.01	101.40	249.98	250.08
1.2	0.10	319.96	319.96	250.01	101.40	249.97	250.09
1.3	0.10	319.96	319.96	250.01	101.40	249.97	250.10
1.4	0.10	319.96	319.96	250.01	101.40	249.97	250.10
1.5	0.10	319.96	319.95	250.01	101.40	249.97	250.11
1.6	0.10	319.95	319.95	250.01	101.40	249.97	250.12
1.7	0.10	319.95	319.95	250.01	101.40	249.96	250.13
1.8	0.10	319.95	319.94	250.01	101.40	249.96	250.13
1.9	0.10	319.94	319.94	250.01	101.40	249.96	250.14
2.0	0.10	319.94	319.94	250.01	101.40	249.96	250.15
2.1	0.10	319.94	319.93	250.02	101.40	249.95	250.16
2.2	0.10	319.93	319.93	250.02	101.40	249.95	250.16
2.3	0.10	319.93	319.93	250.02	101.40	249.95	250.17
2.4	0.10	319.93	319.92	250.02	101.40	249.95	250.18
2.5	0.10	319.92	319.92	250.02	101.40	249.95	250.19
2.6	0.10	319.92	319.92	250.02	101.40	249.94	250.19
2.7	0.10	319.92	319.91	250.02	101.40	249.94	250.20
2.8	0.10	319.91	319.91	250.02	101.40	249.94	250.21
2.9	0.10	319.91	319.91	250.03	101.40	249.94	250.22
3.0	1.00	319.91	319.90	250.03	101.41	249.93	250.22
4.0	1.00	319.89	319.87	250.04	101.41	249.91	250.30
5.0	1.00	319.87	319.84	250.06	101.41	249.89	250.37
6.0	1.00	319.84	319.81	250.08	101.42	249.87	250.44
7.0	1.00	319.81	319.78	250.10	101.42	249.85	250.52
8.0	1.00	319.78	319.75	250.13	101.43	249.83	250.59
9.0	1.00	319.75	319.71	250.16	101.43	249.80	250.66
10.0	1.00	319.71	319.68	250.19	101.44	249.78	250.74
11.0	0.03	319.60	319.65	250.22	101.44	249.76	250.81
12.0	0.06	345.67	319.62	250.27	101.44	249.74	250.88

UWMAK-III TWO CELL TEST CASES WITH CRACK=0.01 CM**2
 USING VERSION OF LITFIRE: "AKEXX" IN SI UNITS
 DATE: 12 august, 1982

TIME	DELT	TCZF	TLIF	TGPF	PAP	TSPF	TSBF
13.0	0.07	359.26	319.59	250.32	101.45	249.72	250.96
14.0	0.08	368.12	319.57	250.39	101.45	249.70	251.03
15.1	0.08	374.71	319.56	250.47	101.46	249.67	251.11
16.0	0.09	379.72	319.55	250.56	101.47	249.65	251.17
17.0	0.10	384.55	319.53	250.65	101.48	249.63	251.25
18.0	0.10	388.93	319.52	250.75	101.48	249.61	251.32
19.1	0.11	393.40	319.51	250.87	101.50	249.59	251.39
20.1	0.12	397.56	319.51	250.99	101.51	249.57	251.47
21.1	0.12	401.39	319.50	251.11	101.52	249.55	251.54
22.1	0.13	405.37	319.50	251.24	101.53	249.53	251.61
23.1	0.14	409.51	319.49	251.39	101.55	249.51	251.68
24.1	0.14	413.27	319.49	251.54	101.56	249.49	251.75
25.1	0.15	417.18	319.49	251.71	101.58	249.46	251.83
30.2	0.19	435.67	319.50	252.63	101.67	249.36	252.18
35.1	0.22	452.73	319.54	253.74	101.79	249.26	252.53
40.1	0.26	469.50	319.60	255.09	101.94	249.16	252.88
45.2	0.30	485.35	319.69	256.64	102.11	249.06	253.23
50.0	0.34	499.66	319.80	258.28	102.30	248.96	253.56
55.1	0.39	513.96	319.93	260.18	102.51	248.86	253.91
60.4	0.43	528.07	320.09	262.23	102.75	248.76	254.27

THIS OUTPUT CORRESPONDS TO TWO CELL GEOMETRY
 TEST CASE: UWMAK-III LARGE SPILL COMPARISON.
 DATE: 12 august 1982

TIME	TGSF	TSSF	PAP	PAS	XMDOT
0.0	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.1	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.2	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.3	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.4	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.5	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.6	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.7	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.8	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
0.9	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.0	0.2700E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.1	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.2	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.3	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.4	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.5	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.6	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.7	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.8	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
1.9	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.0	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.1	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.2	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.3	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.4	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.5	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.6	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.7	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.8	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
2.9	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
3.0	0.2701E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
4.0	0.2702E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
5.0	0.2702E+02	0.2700E+02	0.1014E+03	0.1014E+03	0.0000E+00
6.0	0.2703E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.2792E-05
7.0	0.2703E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.3411E-05
8.0	0.2704E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.4016E-05
9.0	0.2704E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.4609E-05
10.0	0.2705E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.5192E-05
11.0	0.2705E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.5766E-05
12.0	0.2706E+02	0.2700E+02	0.1014E+03	0.1014E+03	-0.5796E-05

THIS OUTPUT CORRESPONDS TO TWO CELL GEOMETRY
 TEST CASE: UWMAK-III LARGE SPILL COMPARISON.
 DATE: 12 august 1982

TIME	TGSF	TSSF	PAP	PAS	XMDOT
13.0	0.2706E+02	0.2701E+02	0.1014E+03	0.1014E+03	-0.6051E-05
14.0	0.2707E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.6447E-05
15.1	0.2707E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.6936E-05
16.0	0.2708E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.7436E-05
17.0	0.2708E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.8016E-05
18.0	0.2709E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.8613E-05
19.1	0.2709E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.9280E-05
20.1	0.2710E+02	0.2701E+02	0.1016E+03	0.1014E+03	-0.9943E-05
21.1	0.2710E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.1059E-04
22.1	0.2711E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.1128E-04
23.1	0.2711E+02	0.2701E+02	0.1015E+03	0.1014E+03	-0.1203E-04
24.1	0.2712E+02	0.2701E+02	0.1016E+03	0.1014E+03	-0.1273E-04
25.1	0.2712E+02	0.2701E+02	0.1016E+03	0.1014E+03	-0.1348E-04
30.2	0.2715E+02	0.2701E+02	0.1017E+03	0.1014E+03	-0.1729E-04
35.1	0.2717E+02	0.2701E+02	0.1018E+03	0.1015E+03	-0.2113E-04
40.1	0.2719E+02	0.2702E+02	0.1019E+03	0.1015E+03	-0.2516E-04
45.2	0.2722E+02	0.2702E+02	0.1021E+03	0.1015E+03	-0.2919E-04
50.0	0.2724E+02	0.2702E+02	0.1023E+03	0.1015E+03	-0.3298E-04
55.1	0.2727E+02	0.2702E+02	0.1025E+03	0.1015E+03	-0.3689E-04
60.4	0.2729E+02	0.2702E+02	0.1028E+03	0.1015E+03	-0.4085E-04

THIS IS THE PAN OUTPUT FILE
 UWMK-III SPILL TWO CELL CODE
 DATE: 7 august 1982

TIME	MNIP	MOXP	RN2	CMBRH	LTBP
0.0	0.4909E+03	0.1480E+03	0.0000E+00	0.8042E-03	0.0000E+00
0.1	0.4909E+03	0.1480E+03	0.0000E+00	0.1151E-01	0.0000E+00
0.2	0.4909E+03	0.1480E+03	0.0000E+00	0.2218E-01	0.0000E+00
0.3	0.4909E+03	0.1480E+03	0.0000E+00	0.3282E-01	0.0000E+00
0.4	0.4909E+03	0.1480E+03	0.0000E+00	0.4342E-01	0.0000E+00
0.5	0.4909E+03	0.1480E+03	0.0000E+00	0.5398E-01	0.0000E+00
0.6	0.4909E+03	0.1480E+03	0.0000E+00	0.6451E-01	0.0000E+00
0.7	0.4909E+03	0.1480E+03	0.0000E+00	0.7500E-01	0.0000E+00
0.8	0.4909E+03	0.1480E+03	0.0000E+00	0.8546E-01	0.0000E+00
0.9	0.4909E+03	0.1480E+03	0.0000E+00	0.9588E-01	0.0000E+00
1.0	0.4909E+03	0.1480E+03	0.0000E+00	0.1063E+00	0.0000E+00
1.1	0.4909E+03	0.1480E+03	0.0000E+00	0.1166E+00	0.0000E+00
1.2	0.4909E+03	0.1480E+03	0.0000E+00	0.1269E+00	0.0000E+00
1.3	0.4909E+03	0.1480E+03	0.0000E+00	0.1372E+00	0.0000E+00
1.4	0.4909E+03	0.1480E+03	0.0000E+00	0.1475E+00	0.0000E+00
1.5	0.4909E+03	0.1480E+03	0.0000E+00	0.1577E+00	0.0000E+00
1.6	0.4909E+03	0.1480E+03	0.0000E+00	0.1679E+00	0.0000E+00
1.7	0.4909E+03	0.1480E+03	0.0000E+00	0.1780E+00	0.0000E+00
1.8	0.4909E+03	0.1480E+03	0.0000E+00	0.1881E+00	0.0000E+00
1.9	0.4909E+03	0.1480E+03	0.0000E+00	0.1982E+00	0.0000E+00
2.0	0.4909E+03	0.1480E+03	0.0000E+00	0.2082E+00	0.0000E+00
2.1	0.4909E+03	0.1480E+03	0.0000E+00	0.2183E+00	0.0000E+00
2.2	0.4909E+03	0.1480E+03	0.0000E+00	0.2282E+00	0.0000E+00
2.3	0.4909E+03	0.1480E+03	0.0000E+00	0.2382E+00	0.0000E+00
2.4	0.4909E+03	0.1480E+03	0.0000E+00	0.2481E+00	0.0000E+00
2.5	0.4909E+03	0.1480E+03	0.0000E+00	0.2580E+00	0.0000E+00
2.6	0.4909E+03	0.1480E+03	0.0000E+00	0.2678E+00	0.0000E+00
2.7	0.4909E+03	0.1480E+03	0.0000E+00	0.2776E+00	0.0000E+00
2.8	0.4909E+03	0.1480E+03	0.0000E+00	0.2874E+00	0.0000E+00
2.9	0.4909E+03	0.1480E+03	0.0000E+00	0.2971E+00	0.0000E+00
3.0	0.4909E+03	0.1480E+03	0.0000E+00	0.3068E+00	0.0000E+00
4.0	0.4909E+03	0.1480E+03	0.0000E+00	0.4025E+00	0.0000E+00
5.0	0.4909E+03	0.1430E+03	0.0000E+00	0.4950E+00	0.0000E+00
6.0	0.4909E+03	0.1480E+03	0.0000E+00	0.5844E+00	0.0000E+00
7.0	0.4909E+03	0.1480E+03	0.0000E+00	0.6709E+00	0.0000E+00
8.0	0.4909E+03	0.1480E+03	0.0000E+00	0.7544E+00	0.0000E+00
9.0	0.4909E+03	0.1480E+03	0.0000E+00	0.8352E+00	0.0000E+00
10.0	0.4909E+03	0.1480E+03	0.0000E+00	0.9133E+00	0.0000E+00
11.0	0.4909E+03	0.1480E+03	0.2693E-01	0.9887E+00	0.0000E+00
12.0	0.4909E+03	0.1479E+03	0.3099E-01	0.1091E+01	0.4383E-01

THIS IS THE PAN OUTPUT FILE
 UWMK-III SPILL TWO CELL CODE
 DATE: 7 august 1982

TIME	MNIP	MOXP	RN2	CMBRH	LTBP
13.0	0.4909E+03	0.1479E+03	0.3330E-01	0.1194E+01	0.9149E-01
14.0	0.4909E+03	0.1478E+03	0.3487E-01	0.1298E+01	0.1446E+00
15.1	0.4909E+03	0.1478E+03	0.3609E-01	0.1403E+01	0.2029E+00
16.0	0.4909E+03	0.1477E+03	0.3704E-01	0.1499E+01	0.2601E+00
17.0	0.4909E+03	0.1476E+03	0.3797E-01	0.1600E+01	0.3258E+00
18.0	0.4908E+03	0.1476E+03	0.3884E-01	0.1699E+01	0.3940E+00
19.1	0.4908E+03	0.1475E+03	0.3975E-01	0.1804E+01	0.4712E+00
20.1	0.4908E+03	0.1474E+03	0.4062E-01	0.1903E+01	0.5497E+00
21.1	0.4908E+03	0.1474E+03	0.4143E-01	0.1997E+01	0.6273E+00
22.1	0.4908E+03	0.1473E+03	0.4228E-01	0.2094E+01	0.7133E+00
23.1	0.4908E+03	0.1472E+03	0.4319E-01	0.2197E+01	0.8085E+00
24.1	0.4908E+03	0.1471E+03	0.4403E-01	0.2291E+01	0.9003E+00
25.1	0.4908E+03	0.1470E+03	0.4492E-01	0.2389E+01	0.1001E+01
30.2	0.4907E+03	0.1465E+03	0.4934E-01	0.2858E+01	0.1552E+01
35.1	0.4906E+03	0.1460E+03	0.5377E-01	0.3298E+01	0.2180E+01
40.1	0.4905E+03	0.1453E+03	0.5848E-01	0.3739E+01	0.2924E+01
45.2	0.4902E+03	0.1446E+03	0.6329E-01	0.4163E+01	0.3757E+01
50.0	0.4902E+03	0.1439E+03	0.6795E-01	0.4553E+01	0.4631E+01
55.1	0.4900E+03	0.1431E+03	0.7295E-01	0.4950E+01	0.5636E+01
60.4	0.4897E+03	0.1422E+03	0.7823E-01	0.5349E+01	0.6772E+01

APPENDIX F

LITFIRE Glossary

C
 C
 C ACTVY CALCULATES ACTIVITY OF LITHIUM IN LIPB
 C AEHCP SURFACE AREA OF PRIMARY EXTRANEIOUS HEAT CAPACITY FT2.
 C AEHCS SURFACE AREA OF SECONDARY EXTRANEIOUS HEAT CAPACITY FT2.
 C AFP AREA OF THE PRIMARY STEEL FLOOR THAT IS OF INTEREST IN HEAT
 C TRANSFER CALCULATIONS. USUALLY EQUAL TO "ASLI" WHEN
 C LITHIUM IS SPILLED DIRECTLY ONTO FLOOR.
 C AFS SURFACE AREA OF SECONDARY STEEL FLOOR LINER FT2.
 C AHT SURFACE AREA OR HEAT TRANSFER BETWEEN LITHIUM POOL AND PAN FT2.
 C AINS OUTSIDE EXPOSED AREA OF INSULATING LAYER ON PAN (FT2)
 C AKLEAD THERMAL CONDUCTIVITY OF LEAD BTU/FT.-SEC. DEG. F
 C INPUT AS BTU/FT. HR. DEG. F
 C AKLI THERMAL CONDUCTIVITY OF LITHIUM BTU/FT.-SEC. DEG. F
 C INPUT AS BTU/FT. HR. DEG. F
 C AK1,AK2,AK3ES,AK3EP,AK4H,AK5 PROD. OF THERMAL COND. AND PRANDTL NO.
 C BTU/SEC-FT-DEG. F SEE RELATED FILM TEMPS. "T"
 C ALLOY1 INITIAL ATOM PERCENT OF LI IN LIPB SPILLED
 C ALPHA USED IN DETERMINING IF LIPB SHOULD BE FIXED AT A MINIMUM
 C EQUAL TO AKLI/(RHLI*CPLI)
 C ALPHA2 USED IN DETERMINING PYU TESTS CONDUCTION LIMIT OF THE PAN OR
 C STEEL LINER ON TIM STEP
 C AMIN1 A FORTRAN SUPPLIED STATEMENT THAT DETERMINES THE MINIMUM
 C VALUE OF THE ARGUMENTS LISTED.
 C AMLI ATOMIC MASS OF BREEDER
 C AMPB ATOMIC MASS OF ALLOY METAL
 C APAN PAN EXTERNAL AREA FOR HEAT TRANSFER
 C ARE SURFACE AREA OF BREEDER ELEMENT
 C ASLI SURFACE AREA OF LITHIUM FT2
 C ATI INNER SURFACE AREA OF COOLANT TUBES IN ELEMENT
 C ATO OUTER SURFACE AREA OF COOLANT TUBES IN ELEMENT
 C ANP PRIMARY CONTAINMENT EXPOSED WALL AREA FT2
 C AWS SECONDARY CONTAINMENT EXPOSED WALL AREA FT2
 C B USED IN CALC. THERMAL RESIST. OF LINER-GAP-CONC. FT.
 C BB ANALOGOUS TO B , ONLY FOR FLOOR CONCRETE
 C B1,B2,B3EP,B3ES,B4,B4H,B5 COEFFICIENT OF GAS EXPANSION 1/DEG. F
 C SEE RELATED FILM TEMPS. "T"
 C BETA THE INVERSE STICKING COEFFICIENT FOR PARTICLES IMPACTING
 C ON A WALL SEC.
 C BIL FRACTION CHANGE BETWEEN BILGE AND DELT USED IN DETERMINING
 C MINIMUM TIME STEP.
 C BILGE EQUAL TO THE MINIMUM VALUE OF DT1, DT2, DT3, DT4, OR DT6
 C USED IN CALCULATING THE TIME STEP
 C BLIN TIME AFTER SPILL AT WHICH INERT GAS FLOODING AND
 C EXHAUST BEGINS SEC
 C BLOUT TIME AFTER SPILL AT WHICH FLOODING AND EXHAUST STOPS SEC
 C BLOWR INERT GAS INPUT RATE LB/SEC
 C BLOWV INERT GAS INPUT RATE FT3/MIN
 C BREAKS OUTER CELL TEMP. RATE OF CHANGE DUE TO CELL GAS LEAKAGE
 C BREOTH LENGTH AROUND THE SIDE OF THE SPILL PAN IN FEET
 C
 C**** "C" IS THE INITIAL USED FOR INDICATING A THERMAL DIFFUSIVITY. I.E., A
 C CONDUCTIVITY BETWEEN TWO NODES DIVIDED BY THE HEAT CAPACITY OF ONE OF
 C THOSE NODES
 C C1 CONTAINMENT GAS TO WALL STEEL IN GAS
 C C2 PAN TO CONT GAS IN GAS
 C C3 STEEL LINER TO CONCRETE WALL IN WALL
 C C4(I) CONCRETE NODE I TO NODE I+1 IN WALL CONCRETE
 C C5 CONCRETE WALL TO AMBIENT IN CONCRETE
 C C6 CONTAINMENT GAS TO WALL STEEL IN STEEL
 C C7 STEEL LINER TO CONCRETE WALL IN STEEL
 C C8 STEEL LINER TO CONCRETE FLOOR IN STEEL
 C C9 STEEL LINER TO CONCRETE FLOOR IN CONCRETE
 C C10(I) CONCRETE FLOOR NODE I TO NODE I+1 IN FLOOR CONCRETE
 C C11 STEEL WALL LINER TO AMBIENT (NO CONCRETE OPTION) IN STEEL
 C C12 STEEL FLOOR LINER TO AMBIENT (NO CONCRETE OPTION) IN STEEL
 C C13 PAN TO GAS IN PAN
 C C14 SECONDARY STEEL FLOOR TO SECONDARY GAS IN STEEL
 C C15 SECONDARY STEEL FLOOR TO SECONDARY GAS IN GAS
 C C16 PRIMARY STEEL FLOOR TO PRIMARY GAS IN STEEL
 C C17 PRIMARY STEEL FLOOR TO PRIMARY GAS IN GAS
 C C18 PRIMARY STEEL FLOOR TO SECONDARY GAS IN STEEL

C C19 PRIMARY STEEL FLOOR TO SECONDARY GAS IN GAS
C C20 PRIMARY STEEL WALL TO SECONDARY GAS IN STEEL
C C21 SECONDARY STEEL LINER TO SECONDARY CELL GAS IN STEEL
C C22 PRIMARY STEEL WALL TO SECONDARY GAS IN GAS
C C23 SECONDARY STEEL LINER TO SECONDARY CELL GAS IN GAS
C CCZ AMOUNT OF HEAT BEING DEVELOPED IN THE COMB. ZONE (BTU/SEC)
C CCZG COMBUSTION ZONE TO CONTAINMENT GAS IN GAS
C CCZP POOL TO COMBUSTION ZONE IN POOL
C CD COEFFICIENT OF DISCHARGE (NEAR UNITY)
C CEHCGP THERMAL DIFFUSIVITY BETWEEN PRIMARY EXTR. HEAT CAPACITY
AND PRIMARY GAS IN PRIMARY GAS
C CEHCGS THERMAL DIFFUSIVITY BETWEEN SECONDARY EXTR. HEAT CAPACITY
AND SECONDARY GAS IN SECONDARY GAS
C CF THERMAL IMPEDANCE BETWEEN BREEDER ELEMENTS IN INNER ELEMENT
C CGCZ COMBUSTION ZONE TO CONTAINMENT GAS IN COMBUSTION ZONE
C CGLI POOL TO CONTAINMENT GAS (NO COMBUSTION) IN POOL
C CGPEHC THERMAL DIFFUSIVITY BETWEEN PRIMARY GAS AND PRIMARY
EXTRANEIOUS HEAT CAPACITY IN EXTR. HEAT CAPACITY
C CGSEHC THERMAL DIFFUSIVITY BETWEEN SECONDARY GAS AND SECONDARY
EXTRANEIOUS HEAT CAPACITY IN EXTR. HEAT CAPACITY
C CHP PRIMARY CONTAINMENT HEIGHT FT
C CHS SECONDARY CONTAINMENT HEIGHT FT
C CIN1PN STEEL PAN TO INNER INSULATION IN INSULATION
C CIN12 INNER TO OUTER INSULATION IN INNER INSULATION
C CIN21 INNER TO OUTER INSULATION IN OUTER INSULATION
C CLIG POOL TO CONTAINMENT GAS (NO COMBUSTION) IN GAS
C CLIPAN POOL TO SPILL PAN IN POOL (SUSP PAN OPTION)
C CLIST LITHIUM POOL TO FLOOR STEEL IN LITHIUM
C CMBR TOTAL COMBUSTION RATE LB. LI/SEC.-FT2
C CMBRH TOTAL COMBUSTION RATE LB. LI/HR.-FT2
C CMBRHI INITIAL COMBUSTION RATE LB. LI/HR.-FT2
C CMBRN COMB. RATE FOR NITROGEN REACTION LB. LI/SEC.-FT2
C CMBRO COMB. RATE FOR OXYGEN REACTION LB. LI/SEC.-FT2
C CMBRW COMB. RATE FOR WATER VAPOR REACTION LB. LI/SEC.-FT2
C CPA INERT GAS SPECIFIC HEAT BTU/LB.-DEG. F
C CPAB SPEC. HEAT OF FLOODING GAS BTU/LB.-DEG. F
C CPANLI POOL TO PAN IN PAN
C CPAP SPECIFIC HEAT OF PRIMARY CELL INERT GAS (BTU/LB DEG F)
C CPAS SPECIFIC HEAT OF SECONDARY CELL INERT GAS (BTU/LB DEG F)
C CPCOM HEAT CAPACITY OF FLOOR AND WALL CONCRETE
C CPCZ LITHIUM POOL TO COMBUSTION ZONE IN COMBUSTION ZONE
C CPEHCP SPECIFIC HEAT OF PRIMARY EXTRANEIOUS HEAT CAPACITY (BTU/LB DEG F)
C CPENC S SPECIFIC HEAT OF SECONDARY EXTRANEIOUS HEAT CAPACITY (BTU/LB DEG F)
C CPFAC used in calculating cpl1 (cpfac=.004938**t11-6.20741)
C CPHZ SPECIFIC HEAT OF HYDROGEN GAS
SET TO 3.76 BTU/LB.-DEG. F. IN PROGRAM
C CPINS SPECIFIC HEAT OF INSULATION BTU/LB DEG F
C CPLEAD SPECIFIC HEAT OF PURE LEAD
C CPLI SPECIFIC HEAT OF LI BTU/LB. -DEG. F
C CPLIH SPECIFIC HEAT OF LITH. HYDROXIDE IN CONT.
SET TO 0.67 BTU/LB.-DEG. F IN PROGRAM.
C CPLIN SPECIFIC HEAT OF LITHIUM NITRIDE BTU/LB.-DEG. F
C CPLIMP SPECIFIC HEAT OF LITH. NITRIDE IN PRIMARY CONT. BTU/LB.-DEG. F
C CPLINS SPECIFIC HEAT OF LITH. NITRIDE IN SECONDARY CONT. BTU/LB.-DEG. F
C CPLIO SPECIFIC HEAT OF LITHIUM OXIDE BTU/LB.-DEG. F
C CPLIOH SPECIFIC HEAT OF LIOH BTU/LB.-MOLE F
C CPLIOP SPECIFIC HEAT OF LITHIUM OXIDE IN PRIMARY BTU/LB.-DEG F.
C CPLIOS SPECIFIC HEAT OF LITHIUM OXIDE IN SECONDARY BTU/LB.-DEG F.
C CPLII MEAN HEAT CAPACITY OF BREEDER AS SOLID BTU/LB MOLE-R
C CPM CZ EFFECTIVE HEAT CAPACITY OF COMB. ZONE BTU/DEG F
C CPMH2 HEAT CAPACITY OF HYDROGEN IN CONTAINMENT BTU/DEG. F
C CPMLOS HEAT CAP. OF LITHIUM OXIDE IN PRIMARY CONT. BTU/DEG. F
C CPMLOP HEAT CAP. OF LITHIUM OXIDE IN SECONDARY CONT. BTU/DEG. F
C CPMNIP HEAT CAPACITY OF NITROGEN IN PRIMARY CONT. BTU/DEG. F
C CPMNIS HEAT CAPACITY OF NITROGEN IN SECONDARY CONT. BTU/DEG. F
C CPMOXP HEAT CAPACITY OF OXYGEN IN PRIMARY CONTAINMENT BTU/DEG. F
C CPMOXS HEAT CAPACITY OF OXYGEN IN SECONDARY CONTAINMENT BTU/DEG. F
C CPMKA HEAT CAP. OF WATER VAP. IN CONTAINMENT BTU/DEG. F
C CPN1N1 THERMAL DIFFUSIVITY OF STEEL PAN TO INNER INSULATION IN PAN
C CPN2P SPECIFIC HEAT OF NITROGEN GAS IN PRIMARY CONT. BTU/LB.-DEG F.
C CPN2S SPECIFIC HEAT OF NITROGEN GAS IN SECONDARY CONT. BTU/LB.-DEG F.
C CPO2P SPECIFIC HEAT OF OXYGEN GAS IN PRIMARY CONT. BTU/LB.-DEG F.

C CPO2S SPECIFIC HEAT OF OXYGEN GAS IN SECONDARY CONT. BTU/LB-DEG F.
C CPPAN SPECIFIC HEAT OF SPILL PAN BTU/LB-DEG F
C CPPB HEAT CAPACITY OF ALLOY METAL IN BREEDER ZONE BTU/LB-F
C CPPB1 MEAN HEAT CAPACITY OF ALLOY METAL SOLID BTU/LB-MOLE-R
C CPPL LIQUID HEAT CAPACITY OF ALLOY METAL BTU/LB R
C CPPZ HEAT CAPACITY OF ALLOY METAL IN REACTION ZONE BTU/LM F
C CPSTL HEAT CAPACITY OF STEEL LINER (BTU/LB-DEG F)
C CPWA SPEC. HEAT OF WATER VAPOR (SET TO 0.44 BTU/LB.-DEG. F)
C CP1 USED TO CALCULATE CP CHANGE OF ALLOY METAL BTU/LB R
C CP2 USED TO CALCULATE CP CHANGE OF ALLOY METAL BTU/LB R
C CRACON AREA OF CONCRETE EXPOSED TO LITHIUM IN CONCRETE
C COMBUSTION MODEL FT**2
C CRACK AREA OF ORRIFICE BETWEEN PRIMARY AND SECONDARY CONTAINMENTS
C THE UNITS OF CRACK ARE SQUARE INCHES!!! CONVERTED TO FT2 IN
C PROGRAM
C CSBLI THERMAL DIFFUSIVITY OF LITHIUM POOL TO FLOOR STEEL IN STEEL
C CT THERMAL IMPEDANCE BETWEEN BREEDER ELEMENTS IN OUTER ELEMENT
C DELH STANDARD HEAT OF HYDROLYSIS OF BREEDER BTU/LB MOLE
C DELMP FRACTIONAL EXCHANGE RATE OF PRIMARY GAS (IN SEC) USED IN
C DETERMINING THE MINIMUM TIME STEP
C DELMS FRACTIONAL EXCHANGE RATE OF SECONDARY GAS (IN SEC) USED IN
C DETERMINING THE MINIMUM TIME STEP
C DELOUT OUT TIME STEP SEC.
C DELT INTEGRATION TIME STEP SEC.
C DFILM LITHIUM VAPOR FILM THICKNESS FT
C DFLIPB DIFFUSION COEFFICIENT FOR LITHIUM THROUGH LEAD FT**2/SEC
C DIFF DIFFUSION COEFF. TO COMB. ZONE FT2/SEC.
C DIFFLI LITHIUM VAPOR DIFFUSION COEFFICIENT FT2/SEC
C DMPBDT MASS RATE OF CHANGE OF LEAD IN LEAD LAYER LB/SEC
C DPROD ENTHALPY CHANGE OF REACTION PRODUCTS IN REACTION ZONE
C DP1,DP2,DP3 PSIA INCREASE IN CONTAINMENT PRESSURE DUE TO EACH INJECT
C DREAC ENTHALPY CHANGE OF REACTANTS IN REACTION ZONE
C DTRDT(I) CONC. FLOOR TEMP. RATE OF CHANGE, NODE I DEG. F/SEC.
C DTCDT(I) CONC. WALL TEMP. RATE OF CHANGE, NODE I DEG. F/SEC.
C DTMIN MINIMUM TIME STEP TO BE USED SEC.
C DT1...DT4 USED IN CALCULATING TIME STEP SEC.
C DT1 POOL TIME STEP (TEMP./RATE OF CHANGE OF TEMP.)
C DT2 CONT. GAS TIME STEP
C DT3 STEEL WALL TIME STEP
C DT4 COMBUSTION RATE TIME STEP
C DT5 COMBUSTION ZONE TEMP. TIME STEP
C DYNAMI SUBROUTINE USED IN CONTROLLING INTEGRATION LOOPS
C D1,D2,D3EP,D3ES,D4,D4H,D5 KINCHATIC VISCOSITY OF CELL GAS (SQUARED)
C (FT4/SEC2) SEE RELATED FILM TEMPS "T"
C EFILM FILM DEPTH OF DEPLETED ZONE ABOVE COMB. ZONE (IN INCHES)
C EMCONC THERMAL EMISSIVITY OF CONCRETE
C EMCZ THERMAL EMISSIVITY OF COMBUSTION ZONE
C EMF USED IN FIXING MINIMUM THERMAL EMISSIVITY OF LI POOL
C SET EQUAL TO .9 IN PROGRAM
C EMGP THERMAL EMISSIVITY OF PRIMARY CELL GAS
C MINIMUM VALUE OF .005 IN PROGRAM
C EMGS THERMAL EMISSIVITY OF SECONDARY CELL GAS
C MINIMUM VALUE OF .006 IN PROGRAM
C EMINS THERMAL EMISSIVITY OF INSULATION AROUND PAN
C EMLI THERMAL EMISSIVITY OF LITHIUM POOL
C EMSTL THERMAL EMISSIVITY OF STEEL LINER
C ESCR HEAT REMOVAL RATE BY EMERGENCY SPACE COOLING BTU/SEC
C ESCTIN TIME AFTER SPILL WHEN ESCR BEGINS SEC
C EXHSTR RATE OF CONTAINMENT GAS EXHAUST LB/SEC
C EXHSTV RATE OF CONTAINMENT GAS EXHAUST FT3/SEC
C EXX USED IN CALC. MASS & HEAT TRANSF. COEFF. 1/FT3
C EX1,EX2,EX3EP,EX3ES,EX4H,EX5 USED IN CALCULATING MASS
C & HEAT TRANSF. COEFF. 1/FT SEE RELATED FILM TEMPS "T"
C FCT1,FCT2,FCT3 FRACTION OF NITROGEN PRESENT IN EACH INJECTION(BY NO.)
C FF1,FF2 USED IN HEAT BALANCE EQS. FOR SPRAY FIRE BTU
C FMLEAK FRACT. OF MASS LEAKED OUT OF CONTAINMENT
C FMLEFT FRACTION OF MASS STILL WITHIN CONTAINMENT
C FNIP WT. FRACTION OF NITROGEN IN PRIMARY CELL GAS
C FNIS WT. FRACTION OF NITROGEN IN SECONDARY CELL GAS
C FOUTP LOSS RATE OF PRIMARY CONT. GAS WHICH EITHER LEAKS OR IS EXHAUSTED
C FOUTS LOSS RATE OF SECONDARY CONT. GAS WHICH EITHER LEAKS OR IS EXHAUSTED
C FOUTT TOTAL LEAKAGE FROM OUTERMOST CONTAINMENT (FOUTS+LEAK)

C FOXP WT. FRACTION OF OXYGEN IN PRIMARY CELL GAS
C FOXS WT. FRACTION OF OXYGEN IN SECONDARY CELL GAS
C FPG RADIATIVE VIEW FACTOR FROM POOL TO GAS (1.0 IF NO PAN, 0.23 IF PAN)
C FPW RAD. VIEW FACTOR FROM POOL TO WALL (1.0 IF NO PAN, 0.384 IF PAN)
C FRA FRACTION OF COMBUSTION PRODUCTS EVOLVED INTO CELL GAS
C FWAP WT. FRACTION OF WATER VAPOR IN PRIMARY CELL GAS
C FWAS WT. FRACTION OF WATER VAPOR IN SECONDARY CELL GAS
C GAP AIR GAP BETWEEN STEEL LINER AND CONCRETE FLOOR (INPUT AS FT.)
C GAMMA RATIO OF SPECIFIC HEATS C_p/C_v (SET = 1.4)
C GIN GRAVITATIONAL CONSTANT 32.2 FT/SEC**2
C HGWP INTERIOR FILM COEF. BTU/SEC-FT**2-DEG. F
C HA EXTERIOR FILM COEF. BTU/SEC. FT**2-DEG. F
C HB HEAT TRANSFER COEFFICIENT TO POOL BTU/SEC-FT2-DEG F
C HBINF EQUILIBRIUM VALUE OF HB
C HCO HEAT TRANSFER COEFFICIENT OF BOILING WATER BTU/SEC-FT**2-DEG F.
C HEHCP HEAT TRANSFER COEFFICIENT OF PRIMARY CELL EXTRANEIOUS HEAT
CAPACITY TO PRIMARY GAS BTU/SEC-FT**2-DEG F.
C HEHCS HEAT TRANSFER COEFFICIENT OF SECONDARY CELL EXTRANEIOUS HEAT
CAPACITY TO SECONDARY CELL GAS BTU/SEC-FT**2-DEG F.
C HF GAS TRANSPORT COEFF. TO POOL FT/SEC.
C HFPGP HEAT TRANSFER COEFFICIENT FROM PRIMARY FLOOR STEEL TO
PRIMARY CELL GAS BTU/SEC-FT**2-DEG F.
C HFPGAS HEAT TRANSFER COEFFICIENT FROM PRIMARY FLOOR STEEL TO
SECONDARY CELL GAS BTU/SEC-FT**2-DEG F.
C HFINF EQUILIBRIUM VALUE OF HF
C HIN CORRELATION FOR HEAT TRANSFER COEFFICIENT (H, HB, HF)
C HINECP CORRELATION FOR HEAT TRANSFER COEFFICIENT FOR PRIMARY
CELL EXTRANEIOUS HEAT CAPACITY DIMENSIONLESS
C HINECS CORRELATION FOR HEAT TRANSFER COEFFICIENT FOR SECONDARY
CELL EXTRANEIOUS HEAT CAPACITY DIMENSIONLESS
C HINGGS CORRELATION FOR HEAT TRANSFER COEFFICIENT (HFPGAS)
C HINGSP CORRELATION FOR HEAT TRANSFER COEFFICIENT (HGWP)
C HINGSS CORRELATION FOR HEAT TRANSFER COEFFICIENT (HSEC)
C HINPS CORRELATION FOR HEAT TRANSFER COEFFICIENT (HWPAS)
C HINBAM CORRELATION FOR HEAT TRANSFER COEFFICIENT (HAWBAM)
C HINSAM CORRELATION FOR HEAT TRANSFER COEFFICIENT (HA)
C HPAN HEAT TRANSFER COEFFICIENT TO PAN BTU/SEC-FT**2-DEG F.
C HSEC HEAT TRANSFER COEFFICIENT FROM SECONDARY STEEL WALL LINER
TO SECONDARY CELL GAS BTU/SEC-FT**2-DEG F.
C HTCPCP HEAT CAPACITY OF PRIMARY CONTAINMENT ATMOSPHERE BTU/DEG.F
C HTCPCS HEAT CAPACITY OF SECONDARY CONTAINMENT ATMOSPHERE BTU/DEG.F
C HWPAS HEAT TRANSFER COEFFICIENT FROM PRIMARY STEEL WALL TO
SECONDARY CELL GAS BTU/SEC-FT**2-DEG F.
C I GENERAL PURPOSE DO LOOP INDEX
C IAM DO LOOP INDEX FOR FLOOR AND WALL CONCRETE NODE INITIALIZATION
C IB DO LOOP INDEX USED FOR FLOOR CONCRETE ITERATIONS
C INIT INITIALIZING SUBROUTINE FOR INTEGRATION CALCULATIONS
C INJEC1, INJEC2, INJEC3 FLAGS FOR GAS INJECTION ... INJEC-1 INDICATES
THAT THE PARTICULAR INJECTION HAS OCCURRED
C INTGRL ARITHMETIC STATEMENT FUNCTION FOR FINDING INTEGRALS
C IPAGE NUMBER OF OUTPUT LINES PER PAGE (BETWEEN HEADINGS)
C IPASS SEE SUBROUTINE VARIABLE LIST
C J1=1 IF LITHIUM IS BREEDER
C J2=1 IF HYDROGEN IS EVOLVED
C KLEAK LEAK RATE CONSTANT FROM CONTAINMENT (INCHES/((LB**0.5)*SEC))
C NOTE: UNITS HAVE BEEN INFERRED FROM THE PROGRAM AND MAY NOT
BE CORRECT. REFERENCE INPUT VALUE: 2.588E(-09)
C KCON THERMAL CONDUCTIVITY OF THE FLOOR AND WALL CONCRETE
CONVERTED TO BTU/SEC-FT-DEG F IN PROGRAM
C KFILM THERM. COND. OF LI POOL/COMB. ZONE FILM BTU/SEC-FT-F
C KGAP THERMAL COND. OF THE AIR GAP BETWEEN THE LINER AND CONCRETE
CONVERTED TO BTU/SEC-FT-DEG F IN PROGRAM
C KIN1 THERMAL CONDUCTIVITY OF INNER INSULATION - CALC. IN PROGRAM
C KIN2 THERMAL CONDUCTIVITY OF OUTER INSULATION - CALC. IN PROGRAM
C KPAN THERMAL CONDUCTIVITY OF LI PAN BTU/HR-FT-DEG F
CONVERTED TO BTU/SEC-FT-DEG F IN PROGRAM
C KSTL THERMAL CONDUCTIVITY OF THE STEEL LINER (BTU/HR-FT-DEG F)
CONVERTED TO BTU/SEC-FT-DEG F IN PROGRAM
C L CONCRETE WALL ELEMENT THICKNESS FT.
C LBN DISTANCE BETWEEN TWO BREEDER ELEMENTS
C LEAK CELL GAS LEAKAGE RATE FROM OUTERMOST CONTAINMENT 1/SEC.
C LEAKO INITIAL CELL GAS LEAKAGE RATE FROM OUTERMOST CONTAINMENT 1/SEC.

C LIBP LITHIUM BURNED IN POOL FIRE LB.
C LIL AMOUNT OF LI LEFT IN POOL , BUT NOT ALLOWED TO BE LESS
C THAN LIT/10 FOR NUMERICAL STABILITY IN HEAT TRANSFER CALC.
C LILNT AMOUNT OF LITHIUM NITRIDE IN POOL LB.
C LILOX AMOUNT OF LITHIUM OXIDE IN POOL LB.
C LILP TRUE AMOUNT OF LITHIUM IN POOL (LB)
C LIS LITHIUM USED IN SPRAY FIRE LB.
C LIT MASS OF LITHIUM IN POOL INITIALLY LB.
C LI CONCRETE FLOOR ELEMENT THICKNESS FT.
C MAIP INITIAL MASS OF INERT GAS IN PRIMARY CONTAINMENT (LB)
C MAIS INITIAL MASS OF INERT GAS IN SECONDARY CONTAINMENT (LB)
C MAIRP WT. OF PRIMARY CELL GAS LB.
C MAIRS WT. OF SECONDARY CELL GAS LB.
C MAP WT. OF INERT GAS IN PRIMARY CELL LB.
C MAS WT. OF INERT GAS IN SECONDARY CELL LB.
C MB MASS OF BREEDER ELEMENT LB MOLE
C MCZ REACTION ZONE MASS LB MOLES
C MCZ1 INITIAL REACTION ZONE MASS LB MOLE
C MH2P WT. OF HYDROGEN IN PRIMARY CONT. CELL GAS LB.
C MH2S WT. OF HYDROGEN IN SECONDARY CONT. CELL GAS LB.
C MLEAD MASS OF LEAD IN LEAD LAYER ABOVE LIBP POOL LB.
C MLHP WT. OF LITHIUM HYDROXIDE IN PRIMARY CONT. GAS LB.
C MLHS WT. OF LITHIUM HYDROXIDE IN SECONDARY CONT. GAS LB.
C MLINIP INITIAL MASS OF LITHIUM NITRIDE IN PRIMARY CONT. LB
C MLINIS INITIAL MASS OF LITHIUM NITRIDE IN SECONDARY CONT. LB
C MLINP WT. OF LITHIUM NITRIDE IN PRIMARY CONT. GAS CELL LB.
C MLINS WT. OF LITHIUM NITRIDE IN SECONDARY CONT. GAS CELL LB.
C MLI0H MASS OF LIOH PRODUCT IN LB MOLES
C MLI0IP INITIAL MASS OF LITHIUM OXIDE IN PRIMARY CONT. LB
C MLI0IS INITIAL MASS OF LITHIUM OXIDE IN SECONDARY CONT. LB
C MLIOP WEIGHT OF LITHIUM OXIDE IN PRIMARY CELL GAS. ALL OF THE
C SPRAY FIRE PRODUCT REMAINS IN THE CELL GAS. A FRACTION
C OF THE PRODUCTS FROM THE POOL FIRE IS ADDED LB.
C MLIOS WT. OF LITHIUM OXIDE IN SECONDARY CELL GAS. LB. (ZERO)
C MNINJ RATE OF INJECTION OF NITROGEN DURING A 60 SEC INTERVAL
C USED TO MODEL HEDL PROCEDURE (LB/SEC)
C MNIIP INITIAL WEIGHT OF NITROGEN IN PRIMARY CONTAINMENT LB
C MNIIS INITIAL WEIGHT OF NITROGEN IN SECONDARY CONTAINMENT LB
C MNIP WEIGHT OF NITROGEN IN PRIMARY CONT. CELL GAS LB.
C MNIS WEIGHT OF NITROGEN IN SECONDARY CONT. CELL GAS LB.
C MNINJ1,MNINJ2,MNINJ3 MASS OF NITROGEN INJECTED (LBS)
C MOINJ1,MOINJ2,MOINJ3 MASS OF OXYGEN INJECTED (LBS.)
C MOXINJ RATE OF INJECTION OF OXYGEN USED TO MODEL HEDL EXPERIMENTAL
C PROCEDURE. OCCURS DURING A 60 SEC. INTERVAL(LB./SEC.)
C MOXIP INITIAL WEIGHT OF OXYGEN IN PRIMARY CONT. LB.
C MOXIS INITIAL WEIGHT OF OXYGEN IN SECONDARY CONT. LB.
C MOXP WEIGHT OF OXYGEN IN PRIMARY CELL GAS LB.
C MOXS WEIGHT OF OXYGEN IN SECONDARY CELL GAS LB.
C MPB MASS OF ALLOY METAL PRODUCT IN LB MOLES
C MWAP WEIGHT OF WAT. VAP. IN PRIMARY CONTAINMENT CELL GAS LB.
C MWAS WEIGHT OF WAT. VAP. IN SECONDARY CONTAINMENT CELL GAS LB.
C MWAIP INITIAL MASS OF WATER VAPOR IN PRIMARY CONT. CELL GAS LB
C MWAIS INITIAL MASS OF WATER VAPOR IN SECONDARY CONT. CELL GAS LB
C N INDICE USED TO TRANSFER CONTROL IN SUBROUTINES
C NA NUMBER OF ELEMENTS IN BREEDER ZONE
C NAME(I) INPUT CONTAINING PROGRAM TITLE AND HEADING
C NL NUMBER OF CONCRETE WALL NODES
C NL1 NUMBER OF CONCRETE FLOOR NODES
C NLM1,NL1M1 WALL AND FLOOR CONCRETE NUMBER OF NODES MINUS ONE
C NUMCTD NUMBER OF COOLANT TUBES DAMAGED
C OUTINT FRACTION OF THE OUTERMOST CONTAINMENT GAS LEAKED TO AMBIENT
C OVERP CONTAINMENT OVER PRESSURE PSIG
C OVERPP PRIMARY CONTAINMENT OVERPRESSURE PSIG
C OVERPS SECONDARY CONTAINMENT OVERPRESSURE PSIG
C OXLB OXYGEN BURNED LB.
C OXLB1 OXYGEN BURNED INITIALLY LB.
C OXLF5 OXYGEN LEFT AFTER SPRAY FIRE LB.
C PAP GAS PRESSURE IN PRIMARY CELL PSIA
C PAPZR INITIAL PRIMARY CELL PRESSURE PSIA
C PAS GAS PRESSURE IN SECONDARY CELL PSIA
C PASZR INITIAL SECONDARY CELL PRESSURE PSIA
C PAZERO INITIAL CELL PRESSURE PSIA

C PBMELT MELTING POINT OF ALLOY METAL R
 C PERCEN PERCENTAGE BY NUMBER OF PEROXIDE (VS. MONOXIDE) FORMED IN
 C COMBUSTION
 C PLIV PARTIAL PRESSURE OF LITHIUM VAPOR PSIA
 C PYU USED IN SETTING THE MINIMUM TIME STEP CALCULATED FROM
 C CONDUCTION RATE FROM PAN OR STEEL LINER FROM POOL
 C PZEROP PRIMARY CONTAINMENT PRESSURE AFTER SPRAY FIRE
 C QC FORCED CONVECTIVE COOLING HEAT FLOW
 C QCCONC HEAT OF COMB. FOR CONCRETE REACTION BTU/LB. LI
 C QCN HEAT OF COMB. FOR NITROGEN REACTION BTU/LB. LI
 C QCO HEAT OF COMBUSTION FOR OXYGEN REACTION BTU/LB. LI
 C QCO1 HEAT OF COMBUSTION FOR MONOXIDE REACTION BTU/LB. LI
 C QCO2 HEAT OF COMBUSTION FOR PEROXIDE REACTION BTU/LB. LI
 C QCW HEAT OF COMB. FOR REACTION WITH WATER VAPOR BTU/LB. LI
 C QIN HEAT ADDITION TO CELL GAS FROM SPRAY FIRE BTU
 C QLION LATENT HEAT OF MELTING FOR LION BTU/LB-MOLE
 C QMELT HEAT OF FUSION OF BREEDER BTU/LB MOLE
 C QMELTP HEAT OF FUSION OF ALLOY METAL BYU/LB MOLE
 C QOUT1,2,3,4 USED IN HEAT BALANCE EQS. FOR SPRAY FIRE BTU
 C QRAD INDICATES A RADIATIVE HEAT FLOW BTU/SEC
 C QRAOB FROM STEEL FLOOR (PAN) TO FLOOR CONC. OR TO AMBIENT
 C QRADC FROM STEEL WALL TO WALL CONCRETE OR TO AMBIENT
 C QRADCG FROM SPILL PAN TO CELL GAS
 C QRADFS FROM PRIMARY STEEL FLOOR TO SECONDARY STEEL WALL
 C QRADG FROM LI POOL TO GAS (NO COMB.) OR FROM COMB ZONE TO CELL GAS
 C QRADP FROM COMB. ZONE TO LITHIUM POOL (COMB. ZONE MODEL ONLY)
 C QRADPG FROM PRIMARY STEEL WALL TO SECONDARY CELL GAS
 C QRADPS FROM PRIMARY STEEL WALL TO SECONDARY STEEL WALL
 C QRADS FROM SPILL PAN TO STEEL FLOOR
 C QRADW FROM COMB ZONE TO WALL STEEL OR FROM LI POOL TO WALL STEEL
 C QVAP HEAT OF VAPORIZATION OF LITHIUM BTU/LB
 C QWA HEAT OF REACTION OF BREEDER WITH WATER
 C RA MEAN RADIUS OF COMBUSTION PRODUCT PARTICLES MICRONS
 C RAREA SURFACE AREA OF REACTION ZONE
 C
 C THE SYMBOL "R" DESIGNATES A TEMPERATURE RATE OF CHANGE IN SOME NODE
 C DUE TO RADIATION HEAT TRANSFER BETWEEN THAT NODE AND SOME OTHER NODE
 C RADB IN FLOOR STEEL DUE TO RAD. TO FLOOR CONC. OR TO AMBIENT
 C RADC IN WALL STEEL DUE TO RAD. TO CONCRETE OR TO AMBIENT
 C RADCB IN FLOOR CONCRETE FROM STEEL FLOOR (PAN)
 C RADCC IN WALL CONCRETE FROM STEEL WALL
 C RBREAK TEMP. RATE OF CHANGE OF PRIMARY CELL GAS DUE TO GAS LEAKAGE
 C RCBH2 STOICH. COMB. RATIO FOR H2O VAPOR REACT. LB. LI/LB. H2
 C RCBN STOICH. COMB. RATIO OF NITROGEN REACT. LB. LI / LB. N
 C RCMB0 STOICH. COMB. RATIO FOR OXYGEN REACTION LB. LI/LB. O
 C RCMB01 STOICH. COMB. RATIO FOR MONOXIDE REACTION LB. LI/LB. O
 C RCMB02 STOICH. COMB. RATIO FOR PEROXIDE REACTION LB. LI/LB. O
 C RCBW STOICH. COMB. RATIO FOR WAT. VAP. REACT. LB. LI/LB. H2O
 C RCZG IN GAS FROM COMBUSTION ZONE
 C RCZP IN LITHIUM POOL FROM COMBUSTION ZONE
 C RCZW IN WALL STEEL FROM COMBUSTION ZONE
 C RELERR MAXIMUM ALLOWABLE FRACTIONAL TEMP. CHANGE ACROSS A SINGLE
 C INTEGRATION STEP. USED TO VARY TIME STEP.
 C RGASPA IN PAN DUE TO RAD. TO CONTAINMENT GAS
 C RGLI IN POOL DUE TO RAD. TO GAS (NO COMB)
 C RHCON DENSITY OF FLOOR AND WALL CONCRETE
 C RHINS DENSITY OF INSULATING LAYER ON PAN
 C RHLEAD DENSITY OF PURE LEAD LB./FT**3
 C RHLI DENSITY OF LITHIUM LB. / FT3
 C RHOAIP INITIAL DENSITY OF PRIMARY CELL GAS LB/FT3
 C RHOAIS INITIAL DENSITY OF SECONDARY CELL GAS LB/FT3
 C RHOAP DENSITY PRIMARY CELL GAS LB/FT3
 C RHOAS DENSITY SECONDARY CELL GAS LB/FT3
 C RHOLIH DENSITY OF LITHIUM HYDROXIDE LB/FT3
 C RHOLIN DENSITY OF LITHIUM NITRIDE LB/FT3
 C RHOLIO DENSITY OF LITHIUM OXIDE LB/FT3
 C RHO LIV LITHIUM VAPOR DENSITY ABOVE POOL LB/FT3
 C RHPAN DENSITY OF LI SPILL PAN LBS/FT**3
 C RHPB DENSITY OF ALLOY METAL LB-MOLE/FT3
 C RHSTL DENSITY OF STEEL LINER (LB/FT3)
 C RIFCZG RADIATIVE INTERCHANGE FACTOR BETWEEN COMB. ZONE AND THE
 C PRIMARY CELL GAS

C RIFCZP RADIATIVE INTERCHANGE FACTOR BETWEEN COMB. ZONE AND
C THE POOL SURFACE
C RIFCZW RADIATIVE INTERCHANGE FACTOR BETWEEN COMB. ZONE AND
C CONTAINMENT WALLS
C RIFFPS RADIATIVE INTERCHANGE FACTOR BETWEEN PRIMARY STEEL FLOOR
C AND SECONDARY STEEL FLOOR
C RIFPAG RADIATIVE INTERCHANGE FACTOR PAN TO GAS
C RIFPAS RADIATIVE INTERCHANGE FACTOR PAN TO STEEL FLOOR
C RIFPG RAD. INT. FAC. BETWEEN POOL AND PRIMARY CELL GAS
C RIFPGA RAD. INT. FAC. BETWEEN PRIMARY STEEL WALL AND SECONDARY GAS
C RIFPS RAD. INT. FAC. BETWEEN PRIMARY AND SECONDARY CELLS
C RIFPW RAD. INT. FACT. BETWEEN POOL AND WALL
C RIFSLC RADIATIVE INTERCHANGE FACTOR BETWEEN STEEL LINER
C AND CONCRETE SURFACE
C RIN UNIVERSAL GAS CONSTANT 1545 FT. LBF./LB.MOLE-DEG. F
C RINP PRIMARY CELL RIM
C RINS SECONDARY CELL RIM
C RLIG IN GAS DUE TO RAD. FROM POOL (NO COMBUSTION)
C RLIW IN WALL STEEL FROM LITHIUM POOL (NO COMB)
C RNILB RATE OF NITROGEN CONSUMPTION LB./SEC
C RMZ DEGREE TO WHICH NITROGEN-LI REACTION OCCURS. VALUE IS
C BETWEEN ZERO AND ONE (=0 FOR NO REACTION, =1 FOR COMPLETE)
C ROXLB RATE OF OXYGEN CONSUMPTION BY POOL FIRE LB./SEC.
C RPAGAS IN CELL GAS DUE TO RAD. FROM LI PAN
C RPANST IN WALL STEEL DUE TO RAD. FROM LITHIUM PAN
C RRAD INITIAL RADIUS OF REACTION ZONE FT
C RSTPAN IN PAN DUE TO RAD. TO FLOOR STEEL
C
C RTLI,RTG,RADB,RADW,RADCB,RADCW VARIOUS RATES OF TEMP.
C CHANGE OF NODES DEG. F/SEC.
C
C RVOL INITIAL REACTION ZONE VOLUME FT3
C RVOL1 REACTION ZONE VOLUME FT3
C RWALB RATE OF WATER VAPOR CONSUMPTION LB./SEC
C
C RWCZ,RCZW,RCZG,RADB,RADW,RADCB,RADCW,RLIW,RGLI,RLIG,RSPGS,RWLI,RWPGAS,
C RWPWS,RWSWP VARIOUS RATES OF TEMP. CHANGE OF NODES DEG. F/SEC
C
C RWLI IN LITHIUM POOL FROM RAD. TO WALL STEEL (NO COMB)
C R1 COEFFICIENT OF BREEDER IN WATER REACTION EQUATION
C R2 COEFFICIENT OF ALLOY METAL IN WATER REACTION EQUATION
C SFLCR HEAT REMOVAL RATE BY EMERGENCY COOLING OF STEEL
C FLOOR LINER BTU/SEC
C SFLEND TIME AFTER SPILL WHEN SFLCR ENDS SEC
C SFLTND TIME AFTER SPILL WHEN SFLCR BEGINS SEC
C SIGMA STEPHAN-BOLTZMAN CONSTANT1713E-8 BTU/FT**2/HR/R**4
C SPILL TOTAL WEIGHT OF LITHIUM SPILLED LB.
C SPRAY WEIGHT FRACTION OF LITHIUM CONSUMED IN THE SPRAY FIRE
C STICK RATE AT WHICH AEROSOLS ARE REMOVED FROM PRIMARY DUE TO
C STICKING TO THE WALL. IF STICK>1.0 EXECUTION IS STOPPED
C STICK MAY BE DECREASED BY INCREASING "BETA".
C TA AMBIENT TEMPERATURE DEG. F
C TAU TIME CONSTANT FOR TRANSIENT NATURAL CONVECTION should
C be time dependent see marks mail for explanation.
C TAUCZ USED TO MODEL COMBUSTION ZONE-POOL COUPLING IN THE RADIATIVE
C INTERCHANGE FACTORS INSTEAD OF (1.-EMCZ) (DIMENSIONLESS)
C TB(I) TEMP. OF ITH NODE OF CONCRETE FLOOR DEG. R
C TBIC(I) INITIAL TEMP. OF ITH NODE OF CONCRETE FLOOR DEG. R
C TBF, TCF, TGF, ETC. CORRESPONDING TEMP. IN DEGREES FAHRENHEIT
C TBLow INERT GAS INLET TEMP. DEG. R
C TC(I) TEMP. OF ITH NODE OF CONCRETE WALL DEG. R
C TCIC(I) INITIAL TEMP. OF ITH NODE OF CONCRETE WALL DEG. R
C TCIGNI IGNITION TEMPERATURE OF CONCRETE LITHIUM REACTION
C IN CONCRETE COMBUSTION MODEL DEG R.
C TCON CONCRETE COMBUSTION ZONE TEMPERATURE IN
C CONCRETE COMBUSTION MODEL DEG R.
C TCONF CONCRETE COMBUSTION ZONE TEMPERATURE IN
C CONCRETE COMBUSTION MODEL DEG F.
C TCZ COMBUSTION ZONE TEMPERATURE DEG R
C TCZF COMBUSTION ZONE TEMP. DEG F.
C TCZI INITIAL VALUE OF COMB. ZONE TEMP. DEG R
C TE EQUILIBRIUM TEMP. RESULTING FROM SPRAY FIRE DEG. R

C TEHCP TEMP. OF PRIMARY EXTRANEIOUS HEAT CAPACITY NODE DEG R.
C TEHCPF TEMP. OF PRIMARY EXTRANEIOUS HEAT CAPACITY NODE DEG F.
C TEHCS TEMP. OF SECONDARY EXTRANEIOUS HEAT CAPACITY NODE DEG R.
C TEHCSF TEMP. OF SECONDARY EXTRANEIOUS HEAT CAPACITY NODE DEG F.
C TEHCZP INITIAL TEMP. OF PRIMARY EXTRANEIOUS HEAT CAPACITY NODE DEG R.
C TEHCZS INITIAL TEMP. OF SECONDARY EXTRANEIOUS HEAT CAPACITY NODE DEG R.
C TET1 USED IN CALCULATING THERMAL CONDUCTIVITY OF INNER
C PAN INSULATION SEE KIN1
C TET2 USED IN CALCULATING THERMAL CONDUCTIVITY OF OUTER
C PAN INSULATION SEE KIN2
C TEZ AVERAGE OF COMBUSTION ZONE TEMP. AND LITHIUM POOL TEMP.
C USED IN TEST FOR COMBUSTION CONDITION
C TFEFF NORMALIZED TEMP. OF LI POOL/COMB. ZONE FILM
C TGF CONTAINMENT GAS TEMP. IN FARENHEIT
C TGP PRIMARY CELL GAS TEMP. AFTER SPRAY FIRE DEG. R.
C TGPF PRIMARY CELL GAS TEMP. DEG F.
C TGPZER INITIAL PRIMARY CELL GAS TEMP. DEG. R.
C TGS SECONDARY CONT. CELL GAS TEMP. DEG R.
C TGSF SECONDARY CONT. CELL GAS TEMP. DEG F.
C TGSZER INITIAL SECONDARY CELL GAS TEMP. DEG. R.
C THFC CONCRETE FLOOR THICKNESS INPUT AS FT.
C THFP PRIMARY STEEL FLOOR THICKNESS INPUT AS FT.
C THFS SECONDARY STEEL FLOOR THICKNESS INPUT AS FT.
C THKIN1 INNER INSULATION THICKNESS INPUT AS FT.
C THKIN2 OUTER INSULATION THICKNESS INPUT AS FT.
C THKPAN SPILL PAN THICKNESS IN FEET (INPUT AS FT.)
C THPB THICKNESS OF LEAD LAYER ABOVE LIPB POOL
C THWC CONCRETE WALL THICKNESS INPUT AS FT.
C THWP PRIMARY STEEL WALL THICKNESS INPUT AS FT.
C THWS SECONDARY STEEL WALL THICKNESS INPUT AS FT.
C TIME TIME AFTER SPILL HAS OCCURRED SEC.
C TIMEF STOP INTEGRATION TIME SEC.
C TIMEO OUTPUT TIME INDICATOR SEC.
C TINS1 TEMP. OF INNER NODE OF INSULATION DEG R.
C TINS1F TEMP. OF INNER NODE OF INSULATION DEG F.
C TINS1I INITIAL TEMP. OF INNER NODE OF INSULATION DEG R.
C TINS2 TEMP. OF OUTER NODE OF INSULATION DEG R.
C TINS2F TEMP. OF OUTER NODE OF INSULATION DEG F.
C TINS2I INITIAL TEMP. OF OUTER NODE OF INSULATION DEG R.
C TLEAD TEMP. OF LEAD LAYER IN POOL DEG R.
C TLEADF TEMP. OF LEAD LAYER IN POOL DEG F.
C TLEADI INITIAL TEMP. OF LEAD LAYER IN POOL DEG R.
C TLI LITHIUM TEMP. IN POOL DEG. R.
C TLIBS LITHIUM TEMPERATURE BEFORE SPRAY FIRE DEG R.
C TLI F LITHIUM POOL TEMP. IN FARENHEIT
C TLIJ INITIAL LITHIUM POOL TEMP. (DEG R)
C TLI O INITIAL LITHIUM POOL TEMP. DEG. R.
C TMELT MELTING TEMP. OF LITHIUM DEG. R.
C TN TEMPERATURE OF BREEDER ZONE ELEMENT DEG R.
C TO TEMP. OF CELL GAS BEFORE SPHAY FIRE DEG. R.
C TONE.TTWO.TTHREE TIME IN SECONDS AT WHICH EACH INJECTION OCCURS
C TPAN LITHIUM PAN TEMP (DEG R) SUSP PAN OPTION
C TPANF LITHIUM PAN TEMP (DEG F)
C TPANZO INITIAL PAN TEMPERATURE IN DEGREES R
C TSFP PRIMARY STEEL FLOOR LINER TEMP. DEG. R
C TSFPF PRIMARY FLOOR STEEL LINER TEMPERATURE DEG F.
C TSFPI INITIAL PRIMARY STEEL FLOOR LINER TEMP. DEG.R
C TSFSI INITIAL SECONDARY CELL FLOOR LINER TEMP. DEG R.
C TSP PRIMARY CELL STEEL WALL LINER TEMP. DEG R.
C TSPF PRIMARY CELL STEEL WALL LINER TEMP. DEG F.
C TSPZER INITIAL PRIMARY CELL STEEL WALL LINER TEMP. DEG. R.
C TSS SECONDARY CELL STEEL WALL LINER TEMP. DEG. R.
C TSSF SECONDARY CELL STEEL WALL LINER TEMP. DEG. F.
C TSSZER INITIAL SECONDARY CELL STEEL WALL LINER TEMP. DEG. R
C TVAP BOILING POINT OF LITHIUM DEG. R
C T1 FILM TEMP. BETWEEN PRIMARY CELL GAS AND POOL DEG. R
C T2 FILM TEMP. BETWEEN PRIMARY CELL GAS AND STEEL WALL LINER DEG. R
C T3EP FILM TEMP. BETWEEN PRIMARY CELL GAS AND EXTR. HEAT CAP. DEG R.
C T3ES FILM TEMP. BETWEEN SECONDARY CELL GAS AND EXTR. HEAT CAP. DEG R.
C T4 FILM TEMP. BETWEEN SECONDARY GAS AND SECONDARY STEEL WALL DEG R.
C T4H FILM TEMP. BETWEEN AMBIENT AND OUTSIDE STEEL OR CONCRETE WALL
C DEPENDING IF THERE IS CONCRETE PRESENT DEG R.

C T6 FILM TEMP. BETWEEN PRIMARY STEEL WALL AND SECONDARY GAS DEG R.
 C T6 FILM TEMP. BETWEEN SECONDARY CELL GAS AND PRIMARY FLOOR DEG R.
 C T7 FILM TEMP. BETWEEN AMBIENT AND OUTSIDE STEEL FLOOR OR CONCRETE
 C FLOOR DEPENDING IF THERE IS CONCRETE PRESENT DEG R.
 C USUBA HEAT TRANSF. COEFF., CONTAINMENT-AMBIENT BTU/SEC-FT²-DEG. F
 C VCONC VOLUME OF CONCRETE IN FIRST NODE OF CONCRETE IN THE CONCRETE
 C COMBUSTION MODEL FT³
 C VP PRIMARY CONTAINMENT CELL FREE VOLUME FT³
 C VS SECONDARY CONTAINMENT CELL FREE VOLUME FT³
 C VOL VOLUME OF BREEDER ELEMENT
 C WAB WEIGHT FRACTION OF INERT GAS IN FLOODING GAS
 C WAP WT. FRACTION OF INERT GAS IN PRIMARY ATMOSPHERE
 C WAS WT. FRACTION OF INERT GAS IN SECONDARY ATMOSPHERE
 C WATER AMOUNT OF WATER THAT SHOULD BE LEFT IN CONCRETE TOP NODE
 C ACCORDING TO THE CORRELATION USED LBS/FT³
 C WFP THICKNESS OF PRIMARY FLOOR STEEL LINER (INPUT AS FT.)
 C WN2P WEIGHT FRACTION OF NITROGEN IN PRIMARY ATMOSPHERE
 C WN2S WEIGHT FRACTION OF NITROGEN IN SECONDARY ATMOSPHERE
 C WN2B WEIGHT FRACTION OF NITROGEN IN FLOODING GAS
 C WO2P WEIGHT FRACTION OF OXYGEN IN PRIMARY ATMOSPHERE
 C WO2S WEIGHT FRACTION OF OXYGEN IN SECONDARY ATMOSPHERE
 C WO2B WEIGHT FRACTION OF OXYGEN IN FLOODING GAS
 C WP THICKNESS OF PRIMARY STEEL POOL LINER (INPUT AS FT.)
 C WS THICKNESS OF SECONDARY STEEL POOL LINER (INPUT AS FT.)
 C WWAB WT. FRACTION OF WATER VAPOR IN FLOODING GAS
 C WWAP WEIGHT FRACTION OF WATER VAPOR IN PRIMARY CONTAINMENT ATMOSPHERE
 C WWAS WEIGHT FRACTION OF WATER VAPOR IN SECONDARY CONTAINMENT ATMOSPHERE
 C XALLOY ATOM PERCENT LITHIUM IN LIPB POOL
 C XBLOW USED IN CONJUNCTION WITH IBLOW
 C XESC USED IN CONJUNCTION WITH IESC
 C XLI WEIGHT FRACTION OF LITHIUM IN LIPB ALLOY
 C XLIDOT MASS FLOW RATE OF LITHIUM THROUGH LEAD LAYER ABOVE LIPB POOL LB/SEC
 C XMAIRP AMOUNT OF GAS IN PRIMARY CONTAINMENT AFTER SPRAY LB.-MOLES
 C XMAIRS AMOUNT OF GAS IN SECONDARY CONTAINMENT AFTER SPRAY LB.-MOLES
 C XMDOT MASS FLOW RATE OF GAS BETWEEN PRIMARY AND SECONDARY CONT. (LB./SEC)
 C XMEHCP MASS OF PRIMARY EXTRANEOUS HEAT CAPACITY Lbm.
 C XMEHCS MASS OF SECONDARY EXTRANEOUS HEAT CAPACITY Lbm.
 C XMH2OI INITIAL MASS OF WATER IN CONCRETE IN CONCRETE COMBUSTION
 C OPTION Lbm.
 C XMOLP MOL. WEIGHT OF PRIMARY CONTAINMENT GAS LB./LB.-MOLE
 C XMOLS MOL. WEIGHT OF SECONDARY CONTAINMENT GAS LB./LB.-MOLE
 C XMOLA MOLECULAR WT. OF INERT GAS LB./LB.-MOLE
 C XMOLAR MOL. WT. OF INERT FLOODING GAS
 C XPB WEIGHT FRACTION OF ALLOY METAL
 C XSFL INDICATES EMERGENCY COOLING OF FLOOR STEEL
 C XSFL=0. FOR NO COOLING , XSFL=1. FOR COOLING
 C (1/SEC.)
 C YALICZ EFFECTIVE THERMAL ADMITTANCE, FILM-COMB. ZONE BTU/SEC-DEG. F
 C YALIG EFFECTIVE THERMAL ADMITTANCE, POOL-CELL GAS BTU/SEC-DEG. F
 C YAPCZ EFFECTIVE THERMAL ADMITTANCE POOL-COMB. ZONE BTU/SEC-DEG F
 C YPAGAS EFFECTIVE THERMAL ADMITTANCE PAN-PRIMARY CELL GAS BTU/SEC-DEG F
 C ZLI THICKNESS OF LITHIUM NODE FT.
 C ZP USED TO DETERMINE EMLI IF EMLI.LT.0.9
 C ZZ TEMPERATURE RATE OF CHANGE IN BREEDER ELEMENT
 C ZZ1 POOL TEMP. RATE OF CHANGE DEG. F/SEC.
 C ZZ2 LI SPILL PAN TEMP. RATE OF CHANGE (DEG R/SEC)
 C ZZ3 SECONDARY CELL GAS TEMPERATURE RATE OF CHANGE (DEG. R/SEC)
 C ZZ4 PRIMARY CELL GAS TEMP. RATE OF CHANGE DEG. F/SEC.
 C ZZ5 STEEL WALL LINER TEMP. RATE OF CHANGE DEG. F/SEC.
 C ZZ6 COMB. ZONE TEMP. RATE OF CHANGE DEG. F/SEC
 C ZZ7 FLOOR STRUCTURE TEMP. RATE OF CHANGE DEG. F/SEC.
 C ZZ8 INNER INSULATION TEMP. RATE OF CHANGE (SUSP. PAN OPTION)
 C ZZ9 OUTER INSULATION TEMP. RATE OF CHANGE (SUSP. PAN OPTION)
 C ZZ99 USED TO ENSURE POSITIVE COMBUSTION RATE
 C ZZEP PRIMARY CELL EXTRANEOUS HEAT CAPACITY TEMP. RATE OF CHANGE
 C DEG R./SEC
 C ZZES SECONDARY CELL EXTRANEOUS HEAT CAPACITY TEMP. RATE OF CHANGE
 C DEG R./SEC
 C ZZPB LEAD LAYER ABOVE LIPB POOL TEMPERATURE RATE OF CHANGE DEG R/SEC
 C ZZS SECONDARY CONTAINMENT CELL STEEL WALL TEMPERATURE RATE OF
 C CHANGE DEG R./SEC
 C

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C   PROGRAM DECISION FLAGS
C
C   IAROSL= 1 AEROSOL REMOVAL FROM PRIMARY CONTAINMENT DUE TO AEROSOL
C           STICKING TO THE WALL.
C           = 0 NO AEROSOL REMOVAL.
C
C   IBLOW = 1 FLOOD CONTASINMENT WITH INERT GAS
C           = 0 NO CONTAINMENT FLOODING
C
C   ICMB = 0 NO OXYGEN LEFT AFTER SPRAY FIRE.
C           = 1 THERE IS STILL OXYGEN LEFT AFTER SPRAY FIRE.
C           SET INITIALLY TO 1 AND THEN RESET TO 0 WHEN THE
C           PROGRAM CALCULATES THAT THE OXYGEN HAS RUN OUT.
C
C   ICNI = 1 NITROGEN REACTIONS POSSIBLE.
C           = 0 NITROGEN REACTIONS NOT POSSIBLE.
C
C   ICZ = 1 COMBUSTION ZONE MODEL USED
C           = 0 COMBUSTION ZONE MODEL NOT USED
C
C   IESC = 1 EMERGENCY SPACE COOLING OPTION
C           = 0 NO EMERGENCY SPACE COOLING
C
C   ILIT = 0 NO LITHIUM LEFT TO BURN.
C           = 1 LITHIUM LEFT TO BURN (INITIAL CONDITION).
C
C   IMETH = 1 RUNGE-KUTTA METHOD OF INTEGRATION USED.
C           = 3 SIMPSON'S RULE METHOD OF INTEGRATION USED.
C
C   ISFLC = 1 EMERGENCY COOLING OF STEEL FLOOR LINER OPTION
C           = 0 NO EMERGENCY COOLING OF STEEL FLOOR LINER
C
C   ISWICH= 1 CRACK SIZE BECOMES ZERO AFTER INNER AND OUTER CELL
C           PRESSURES EQUILIBRATE IN TWO CELL CALCULATION.
C           = 0 CRACK SIZE REMAINS CONSTANT.
C
C   FLAG2 = .TRUE. TWO CELL CALCULATION (DEFAULTS TO 1 CELL IF FALSE)
C
C   FLAGAS= .TRUE. INJECTIONS OF DRY GAS DURING RUN
C
C   FLAGC = .TRUE. CONCRETE COMBUSTION (BREACH OF STEEL LINER)
C
C   FLAGD = .TRUE. CONCRETE COMBUSTION HAS STOPPED
C
C   FLAGDF= .TRUE. LIPB LAYERED POOL COMBUSTION MODEL IN USE
C
C   FLAGF = .TRUE. FLOOR CONCRETE
C
C   FLAGL = .TRUE. LILP IS FIXED AT A MINIMUM
C
C   FLAGM = .TRUE. SONIC FLOW BETWEEN CONTAINMENTS (CALCULATED IN PROGRAM)
C
C   FLAGN = .TRUE. SETS N=1 IN SUBROUTINES IN ORDER TO PROPERLY TRANSFER
C           FLOW THROUGH SUBROUTINES
C
C   FLAGPB= .TRUE. LIPB POOL COMBUSTION MODEL IN USE
C
C   FLAGPN= .TRUE. YES ON SUSPENDED PAN GEOMETRY
C
C   FLAGSI= .TRUE. IF USER WISHES INPUT/OUTPUT IN SI UNITS
C
C   FLAGW = .TRUE. WALL CONCRETE

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