Addition of Ga, Pb, and Li-Pb Materials to MELCOR Computer Model and Associated Enhancements

Eric Gracyalny

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FUSION TECHNOLOGY INSTITUTE

UNIVERSITY OF WISCONSIN

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Eric Gracyalny

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

http://fti.neep.wisc.edu

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Eric Gracyalny

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

Fusion Safety Program
Lockheed Martin Idaho Technologies
P.O. Box 1625
Idaho Falls ID 83415-3815

Under the supervision of

Dr. Kathy McCarthy
and
Brad Merrill

Base MELCOR Version: 1.8.3 PN
New MELCOR Version: 1.8.3 UD

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Contents

Acronyms

BH	Bottom Head (MELCOR module)
CAV	Cavity (MELCOR module)
COR	Core Behavior (MELCOR module)
CVH	Control Volume Hydrodynamics (MELCOR module)
EDF	External Data File (MELCOR module)
ESF	Engineered Safety Features (MELCOR module)
FDI	Fuel Dispersal Interaction (MELCOR module)
HPME	High Pressure Melt Ejection
HS	Heat Structure (MELCOR module)
ITER	International Thermonuclear Experimental Reactor
LPME	Low Pressure Melt Ejection
LWR	Light Water Reactor
MP	Material Properties (MELCOR module)
RN	Radionuclide Behavior (MELCOR module)
SPR	Containment Sprays (MELCOR module)
TF	Transfer Function (MELCOR module)
TP	Transfer Process (MELCOR module)

1. Introduction

This report summarizes the enhancements made to MELCOR [1] in order to adapt MELCOR to model a wider variety of liquid metal/water interaction scenarios expected for the ITER reactor project. In particular, the changes made to the Fuel Dispersal Interaction (FDI) module of MELCOR are discussed here. These changes primarily involve adding liquid metals specific to fusion systems to the Material Properties (MP) database in MELCOR and then allowing the FDI module to access these materials. Another enhancement was to make the low pressure melt ejection sequence found in the FDI package a truly 'stand alone' sequence. It is assumed that the reader has a basic understanding of what the MELCOR code is and how it works.

2. Original FDI Model

The FDI module in MELCOR is primarily a heat transfer package that models the interaction between ejected molten reactor fuel and the environment in the reactor cavity. This environment generally consists of air and possibly a water pool. There are three types of interactions considered by the FDI package:

1. low pressure melt ejection (LPME)
2. high pressure melt ejection (HPME)
3. steam explosions.

Although all coding for steam explosions is present in the FDI module it was disabled by the Sandia code developers pending further investigation. The LPME and HPME phenomena are named as such to differentiate between a low velocity melt ejection produced by a low pressure source, and a high velocity melt ejection produced by a high pressure source. The code determines which model should be used depending upon the velocity at which debris is ejected from the core. If this velocity exceeds the sensitivity coefficient of 10 m/s it is considered a HPME event, otherwise it is considered a LPME event.

2.1. Low Pressure Melt Ejection Model

The best way to visualize a LPME event is a water faucet barely turned on. A trickle of water falls into a sink and slowly spreads over the bottom. The LWR analogy is molten fuel spilling from the reactor vessel into the reactor cavity beneath the vessel. In the FDI model, energy is transferred from the debris to the water pool found in the cavity. No energy is transferred to the atmosphere. Furthermore, all transferred energy is used to boil the water with no sensible heating considered. If no water pool is present, the FDI package will do nothing but transfer the incoming mass to its destination. The LPME **does not** consider oxidation of fuel components.

Figure 1 depicts the possible flow paths in and out of the FDI package in MELCOR for a LPME event. Note that all mass leaving the FDI package **must** eventually be deposited to the Cavity (CAV) module.

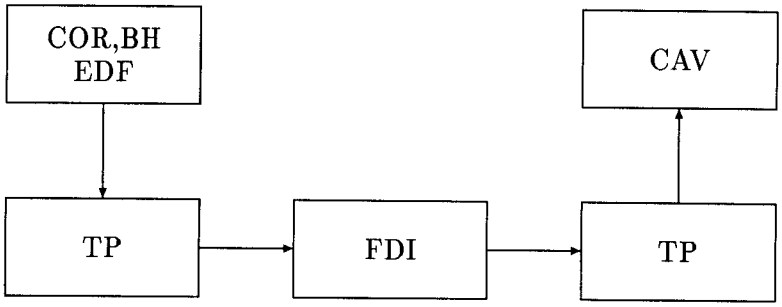

Figure 1. LPME Flow Paths

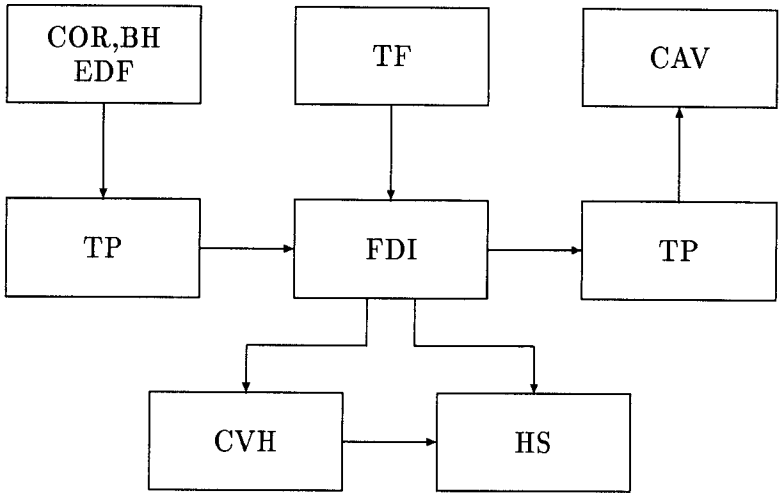

Figure 2. HPME Flow Paths

2.2. High Pressure Melt Ejection Model

Using the faucet analogy above, a HPME would be best described by a faucet turned all the way on. The velocity of the stream is so high that the jet breaks up into droplets which are dispersed in the atmosphere above the sink and may actually settle on the sides of the sink instead of the sink bottom. The HPME is a simple and straightforward model that distributes mass to a variety of volumes and structures using first-order rate equations with user defined time constants. Mass can be deposited to either an atmosphere, which then settles to a surface, or to a surface directly. Unlike the LPME, the HPME can transfer energy to the atmosphere via a phenomenon called Direct Containment Heating. Also, the HPME considers the oxidation of fuel debris; however, this is controlled by first-order rate equations. Although the HPME model may seem robust at first, everything is modeled with a first-order rate equation which depends upon user defined constants.

Figure 2 depicts the possible flow paths in and out of the FDI package in MELCOR for a HPME

event. The primary differences with the LPME flowpaths are a) incoming mass can be specified with a Tabular Function (TF) and b) outgoing mass can be deposited directly to a Heat Structure (HS). The CVH flowpath represents mass deposition to the atmosphere.

2.3. Other Features

There are some other characteristics of the FDI module that should be mentioned. The FDI module will switch between the LPME and HPME models when appropriate, provided that input for both models is supplied. When a switch occurs, mass undergoing one phenomenon will not be transferred to the other model. For example, when a switch from HPME to LPME occurs direct containment heating continues in the HPME until the debris mass in the atmosphere settles out.

Only five (5) core materials can be transferred from the TP package to the FDI module (1) UO_2, (2) Zr, (3) steel, (4) ZrO_2, (5) steel oxide. These are the only materials the LPME model considers. These are also the only materials that can be sent to the CAV package regardless of which FDI model is utilized.

When a Tabular Function is used to send mass to the FDI package in a HPME event, other materials may be included in addition to the five mentioned above: (1) B_4C, (2) silver-indium-cadmium, (3) U, (4) Al (5) Al_2O_3, (6) Cd. None of these materials may be passed to the CAV package, however.

A characteristic that may in fact be a bug in MELCOR is that when the velocity of the melt ejection is input by External Data File (EDF), it **does not** undergo linear interpolation as do the other values. Instead it is a step function that is a function of the next data point. As an example, given the following input for time and velocity in an EDF

Time	Velocity
0.0	20.0
1000.0	10.0
2000.0	5.0
5000.0	1.0

the velocity will be 10.0 between 0 and 1000 seconds, 5.0 between 1000 and 2000 seconds and 1.0 between 2000 and 5000 seconds.

3. MELCOR Enhancements

3.1. Material Properties Package

The changes made to the Material Properties package are rather straightforward. Three materials that may be used in ITER test modules were added to the database. These new materials are gallium, lead and lithium lead ($Li_{17}Pb_{83}$). The properties used within MELCOR are listed in Appendix A. Parties interested in adding materials of their own to MELCOR should see Appendix B for the procedure. Any of these properties may be overridden by using Tabular Function input as described in the Material Properties Users' Guide.

3.2. Fuel Dispersal Interaction Package

The modifications made to the FDI module lie in two areas: 1) allowing the LPME model to deposit mass to something other than the CAV package, 2) allowing the FDI module to use the new materials added to the MP package.

3.2.1. LPME Mass to a Heat Structure

The first modification allows the LPME model to send mass to a heat structure instead of a cavity. This was done to make the LPME model a 'stand alone' sequence within MELCOR similar to the HPME model, and because no phenomenon that is simulated by the CAV package is expected to occur in ITER. This modification was made at the point in the LPME code where mass is transferred to the CAV package. Instead of sending mass to the CAV package, it is transferred to a limited version of the HPME model that is contained in a new subroutine called FDIHIL. This subroutine is limited with respect to the full blown HPME sequence in that debris can only be sent to a heat structure, not an atmosphere. Furthermore no oxidation reactions are considered. The only thing done in FDIHIL is to deposit the fuel debris (liquid metal droplets) on a heat structure and to calculate the energy transfer associated with that debris.

The user specifies which deposition surface the FDI model should use in the FDI MELGEN input. This is done by simply entering the HS number instead of the CAV number for the NFDCAV field on line FDInn00. When a heat structure is used instead of a cavity, then the NFDTPI field on the same line has no meaning, but still must be input. Please refer to the Fuel Dispersal Interaction Users' Guide for further information. Due to coding convention **mass must be deposited to the left hand side of a heat structure.** If mass settles on the right hand side of a heat structure errors will occur.

3.2.2. Accessibility of New Materials from the FDI Package

Allowing the FDI package to access the new materials (Ga, Pb, Li-Pb) was a surprisingly simple procedure. It involved adding indices to certain arrays found throughout the FDI code. The precise method used will not be explained here due to the difficulties in describing the process. Instead a discussion on how to access these new materials is provided.

If mass is entering the FDI package via Tabular Function (HPME only) the user may simply enter the name of the material in the MELGEN input file on the FDInnii input lines (see FDI Users' Guide). The names these materials go by in MELCOR are:

- GALLIUM
- LEAD
- LITHIUM-LEAD.

The original 11 materials are still usable.

If mass is entering the FDI package via Transfer Process (TP), then the new materials can only be added if an EDF is used. This restriction could be lifted with further enhancements. The channel definitions for the EDF are:

Column	Parameter	Column	Parameter
1	Time (s)	11	Fuel temperature (K)
2	Integral mass of UO_2 (kg)	12	Diameter of vessel breach (m)
3	Integral mass of Zr (kg)	13	Fuel ejection velocity (m/s)
4	Integral mass of steel (kg)	14	Fraction of Fe in steel (-)
5	Integral mass of ZrO_2 (kg)	15	Fraction of Cr in steel (-)
6	Integral mass of steel oxide (kg)	16	Fraction of Ni in steel (-)
7	Integral mass of Ga (kg)	17	Fraction of FeO in steel oxide (-)
8	Integral mass of Pb (kg)	18	Fraction of CrO in steel oxide (-)
9	Integral mass of Li-Pb (kg)	19	Fraction of NiO in steel oxide (-)
10	Blank		

Because more input channels are required for sending mass to the FDI module through a Transfer Process in this new version of MELCOR, **old input decks that utilize the FDI module will not work properly**. Some minor corrections are required in TP input to upgrade previous inputs. Generally this involves increasing the values of NMSIN and NMSOT from 5 to 8 and defining a translation matrix (see Transfer Process Users' Guide).

4. Benchmark Calculations

This section demonstrates the behavior of the original FDI package and how the enhancements have effected this behavior. First, a demonstration of both the LPME and HPME models before modification is presented. Next, the ability of the LPME to send mass to a heat structure is demonstrated. Finally, the behavior of the new materials in the FDI package is analyzed.

The initial conditions for all test problems are the same. The FDI volume is a cube five meters on a side at a pressure of 1 atmosphere and 300°K. A water pool 0.5 meters in height is also present. The atmosphere contains 80% N_2, 20% O_2 at 50% relative humidity. The fuel melt enters the FDI volume at a temperature of 2550°K. For LWR materials, the flow rates of debris entering the FDI volume are 27 kg/s of UO_2, 4.56 kg/s of Zr and 16.76 kg/s of steel. The duration of each simulation is 2000 seconds.

4.1. Base Cases

Figures 3 – 6 show some figures of merit for the base case LPME model simulation given the conditions above. Over time the water in the pool is vaporized into steam. It should be noted that this conversion is primarily due to the effect of the CAV package, not the FDI package. The FDI module only accounts for about 1000 kg of steam. The debris temperature in Figure 6 is meant to give an indication of the temperature change that fuel undergoes as it passes through the FDI package. Recall that the incoming fuel temperature is 2550°K.

Figures 7 – 10 show the same information, but for a HPME event. The time constants for oxidation and heat transfer were both 0.1 seconds while the time constant for debris settling from the atmosphere to the heat structure was 50 seconds. The destination of the debris entering the FDI package was evenly split between the atmosphere and the heat structure. The continual downward trend in total mass in the volume is due to the constant oxidation of zirconium and steel by steam. This behavior is not seen in the LPME simulation because oxidation is not coded in the LPME

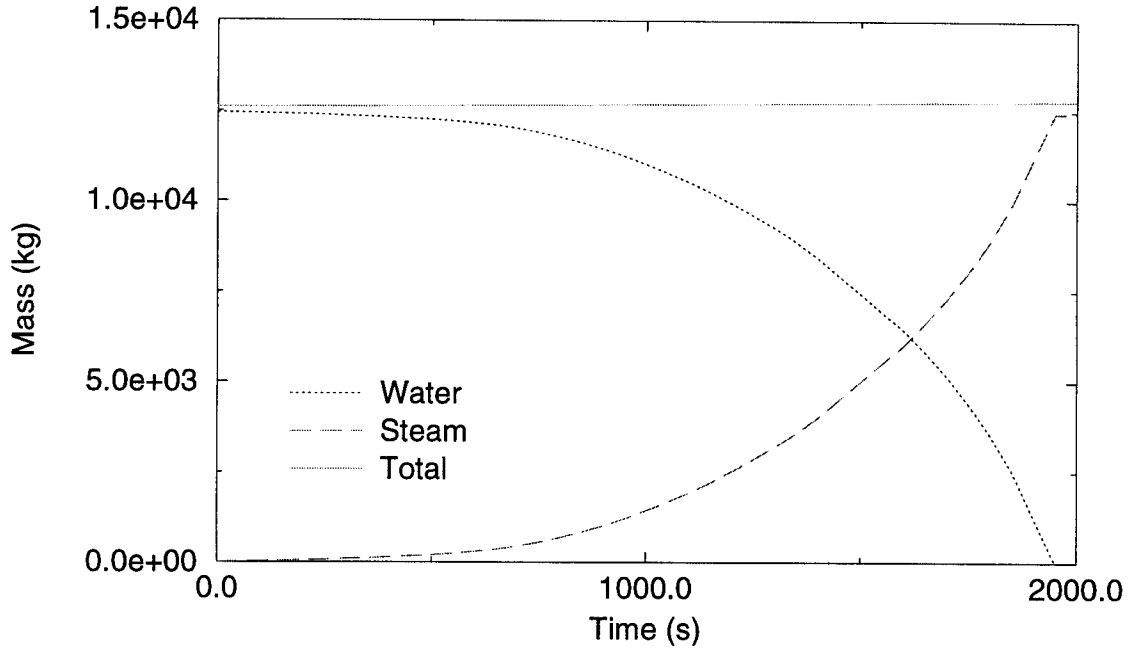

Figure 3. LPME Base Case - Volume Masses

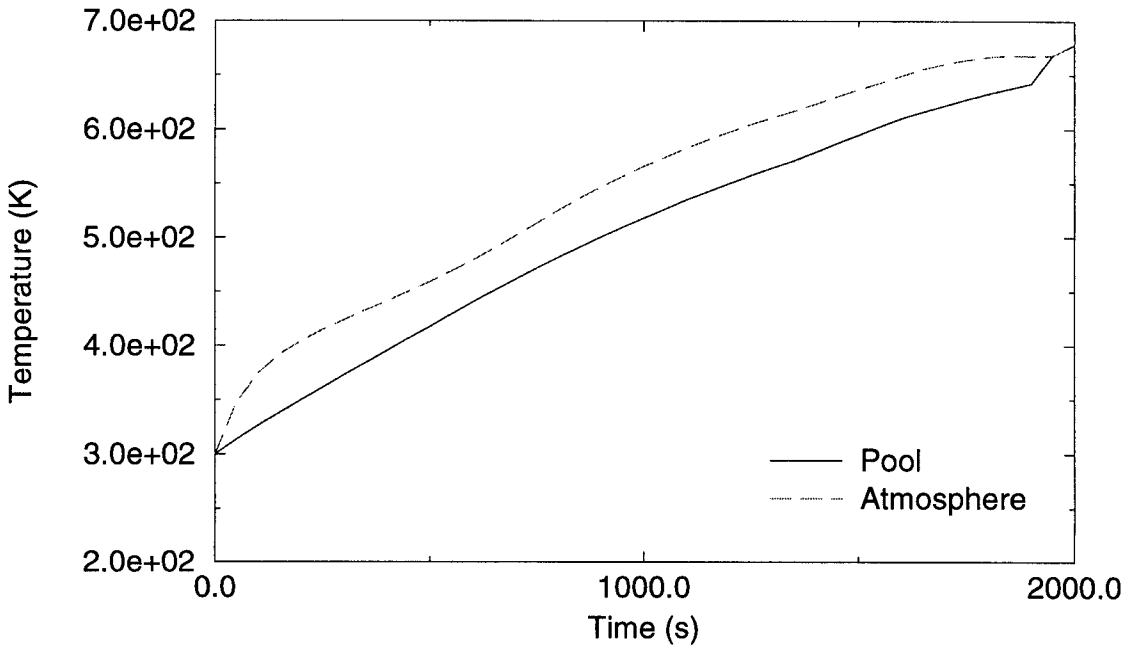

Figure 4. LPME Base Case - Volume Temperatures

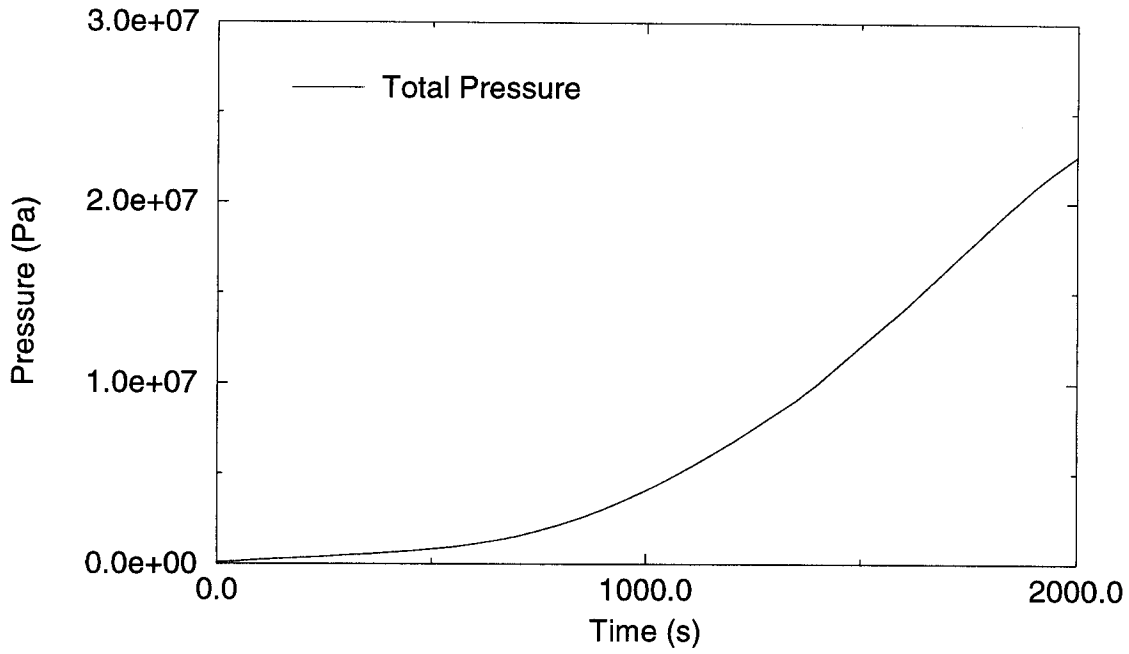

Figure 5. LPME Base Case - Volume Pressures

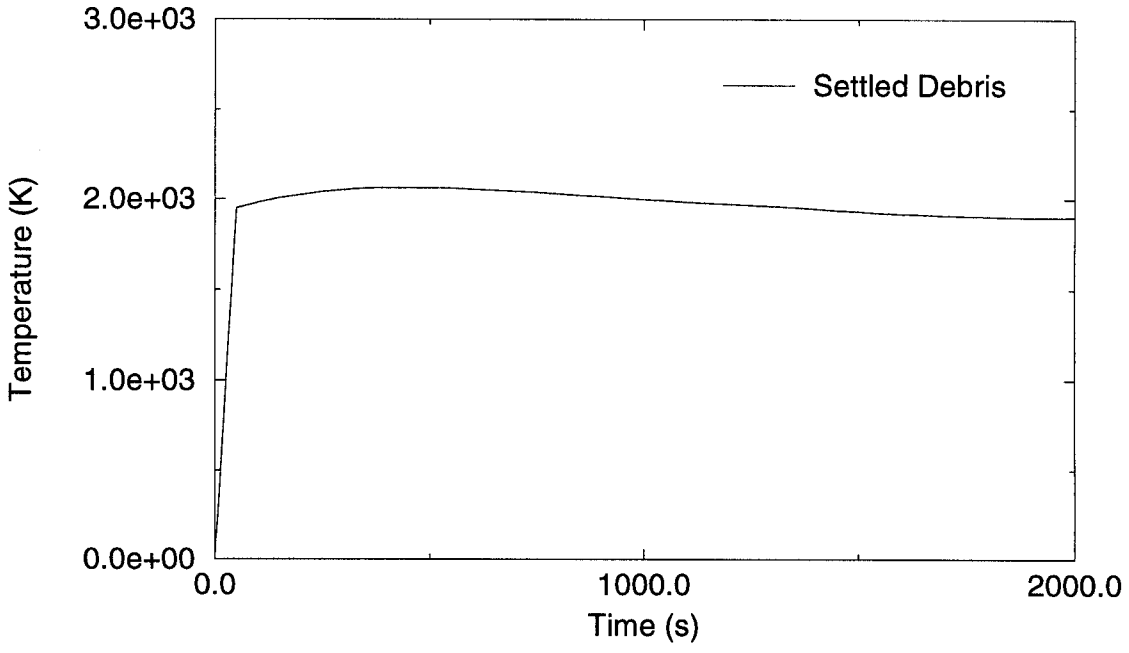

Figure 6. LPME Base Case - Debris Temperature

model. Future modifications may address this limitation if oxidation of fusion materials is a concern.

One can distinguish three distinct regions in the HPME output. The first region is where the debris boils the water into steam. This is marked by a slow increase in volume pressure and debris temperature. Once the cooling mechanism of the pool is gone, there is a sharper increase in pressure and temperature; however, the rate of oxidation is relatively unchanged. The final stage is when the steam is consumed and therefore oxidation ceases. This causes the temperatures and pressures to level off.

4.2. LPME Mass to a Heat Structure

The effect of diverting the debris mass to a heat structure as opposed to a cavity for the LPME case can be seen in Figures 11 – 14. Considering that no oxidation can occur in a LPME event and that a limited version of the HPME model was utilized to describe the heat transfer of the settled debris, one would expect that these results should compare favorably to a HPME scenario where all mass is transferred directly to a heat structure and no oxidation occurs. Such a scenario was run with the results appearing in Figures 15 – 18. As can be seen the results are in agreement. The higher pressures and temperatures seen in the LPME output are due to the additional effect of steam generation by the LPME fuel/coolant interaction. As with the earlier LPME base case, steam production is not primarily a function of the fuel/coolant interaction itself. Instead it is the effect the settled debris has upon the heat structure that causes the transition. As with the earlier LPME base case steam production is not primarily a function of the fuel/coolant interaction itself (Figure 19).

4.3. Fusion Materials

The initial conditions for this set of simulations is the same as mentioned earlier with the exception of the input streams to the FDI package. Instead of LWR fuel materials the new fusion materials are used. The flow rates for debris entering the FDI volume are 27 kg/s of Ga, 4.56 kg/s of Pb and 16.76 kg/s of Li-Pb.

The impact of using these new materials can be seen in Figures 20 – 23. The total steam generated by the FDI package is about 800 kg. The apparently slow conversion of water and steam is due to the relatively poor thermophysical properties of lead and Li-Pb (conductivity and specific heat).

5. Conclusion

In summary, this work accomplished three tasks:

1. three liquid metal materials were added to the MELCOR database
2. these materials are accessible by the FDI package
3. the LPME model in the FDI package is now 'stand alone'.

These tasks were accomplished in four new versions of MELCOR. Version UA incorporates the ability of the LPME model in the FDI package to deposit mass to a heat structure as opposed to a

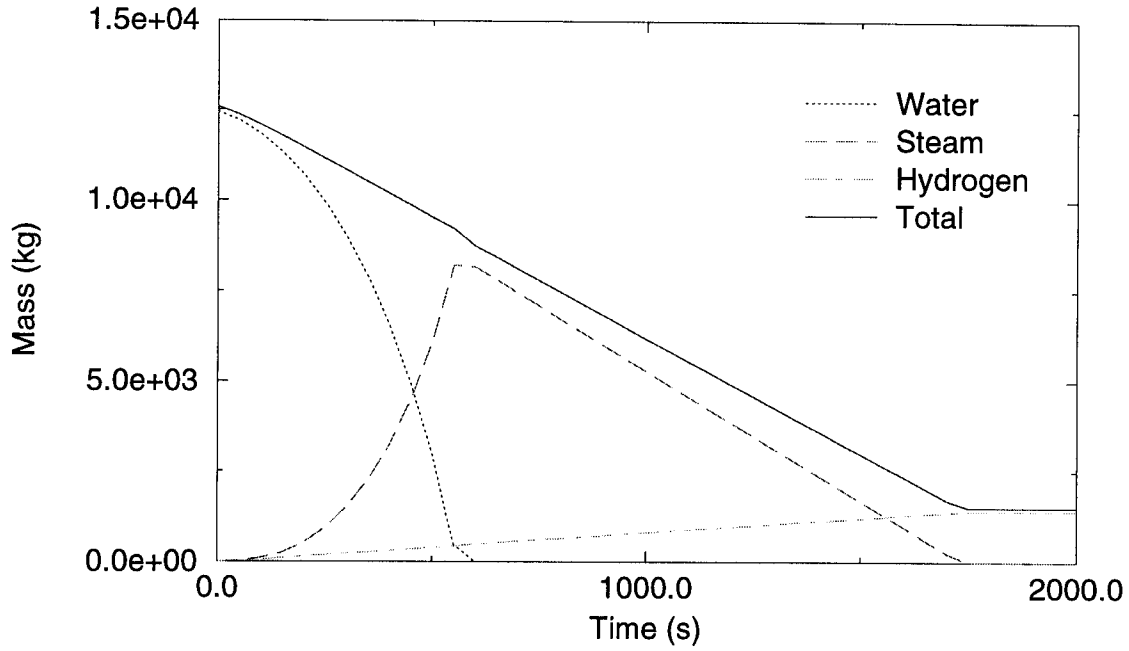

Figure 7. HPME Base Case - Volume Masses

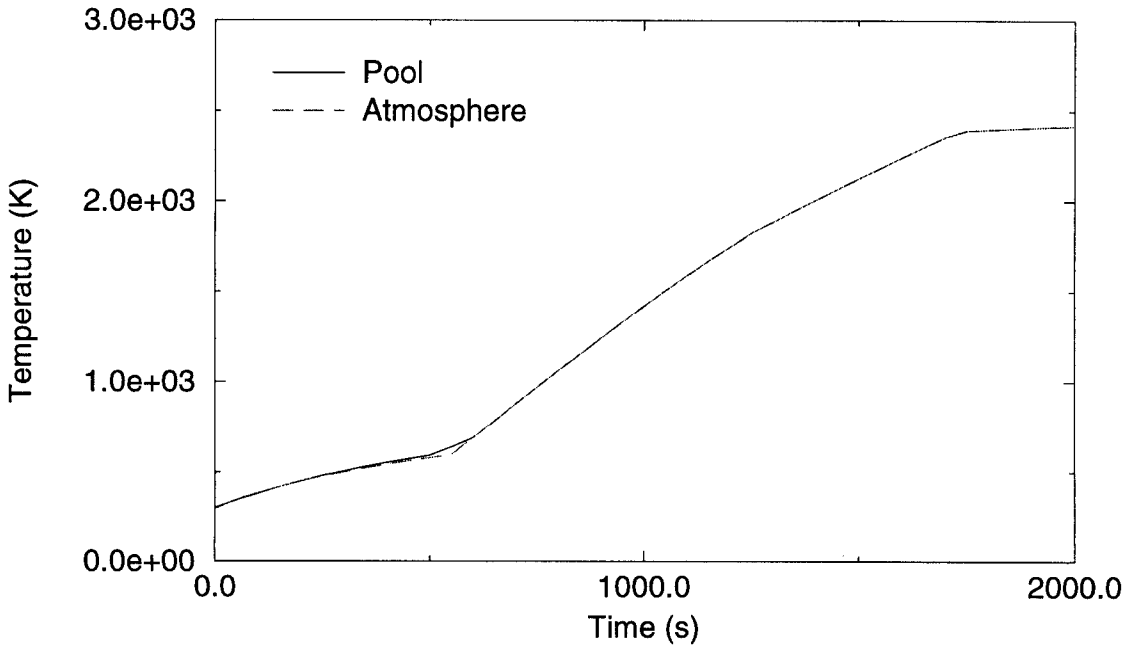

Figure 8. HPME Base Case - Volume Temperatures

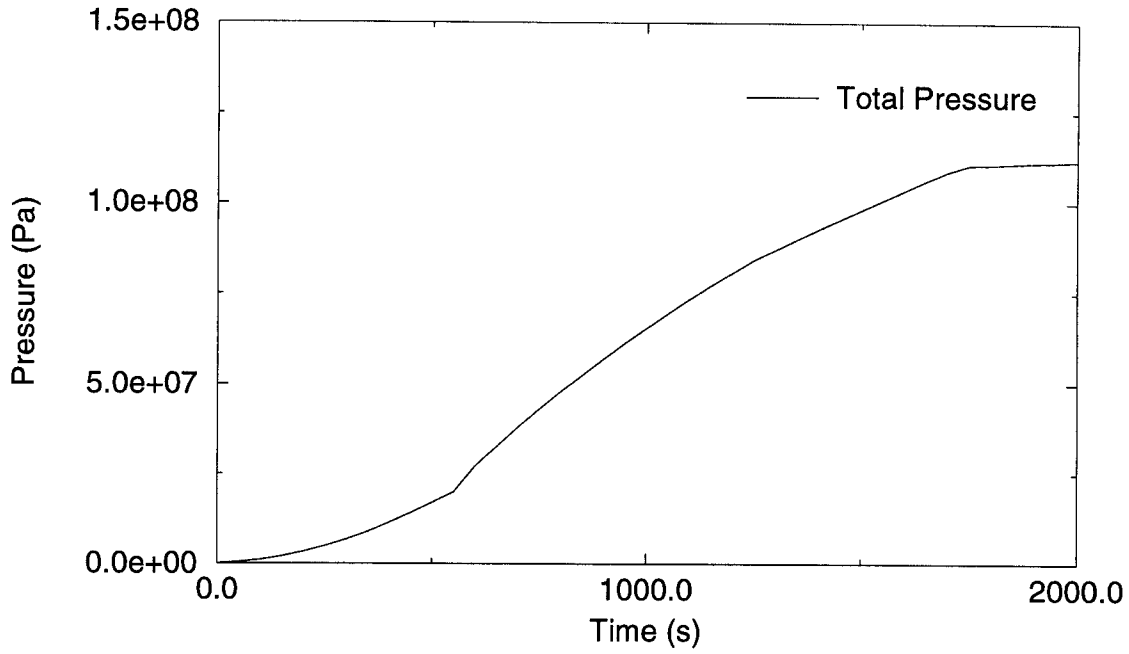

Figure 9. HPME Base Case - Volume Pressures

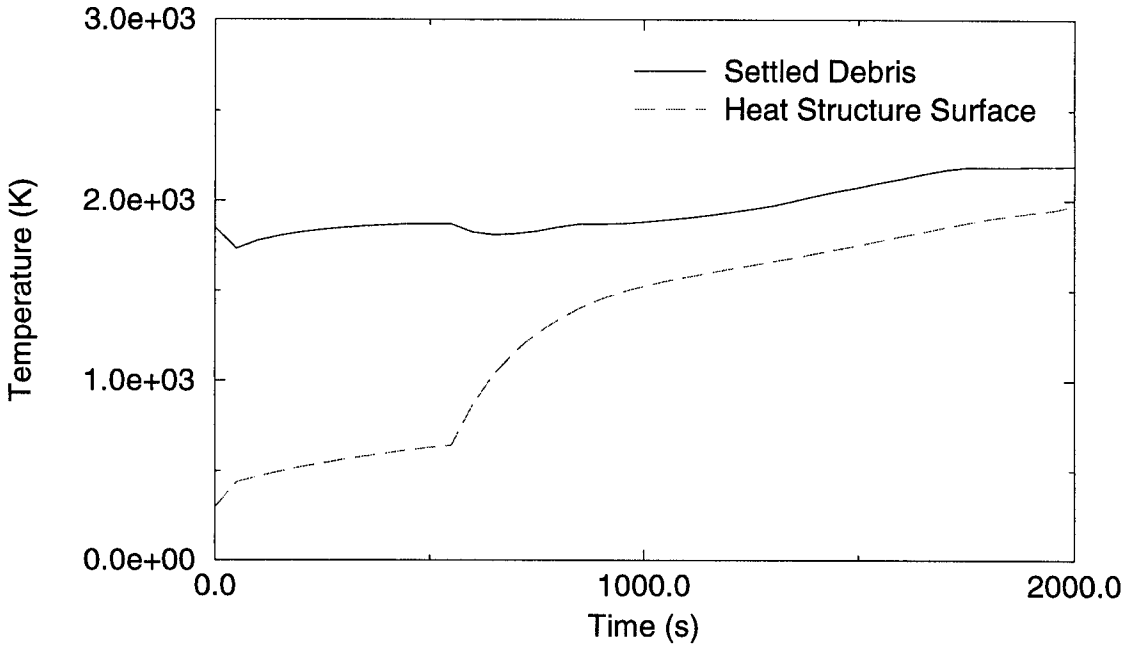

Figure 10. HPME Base Case - Debris Temperature

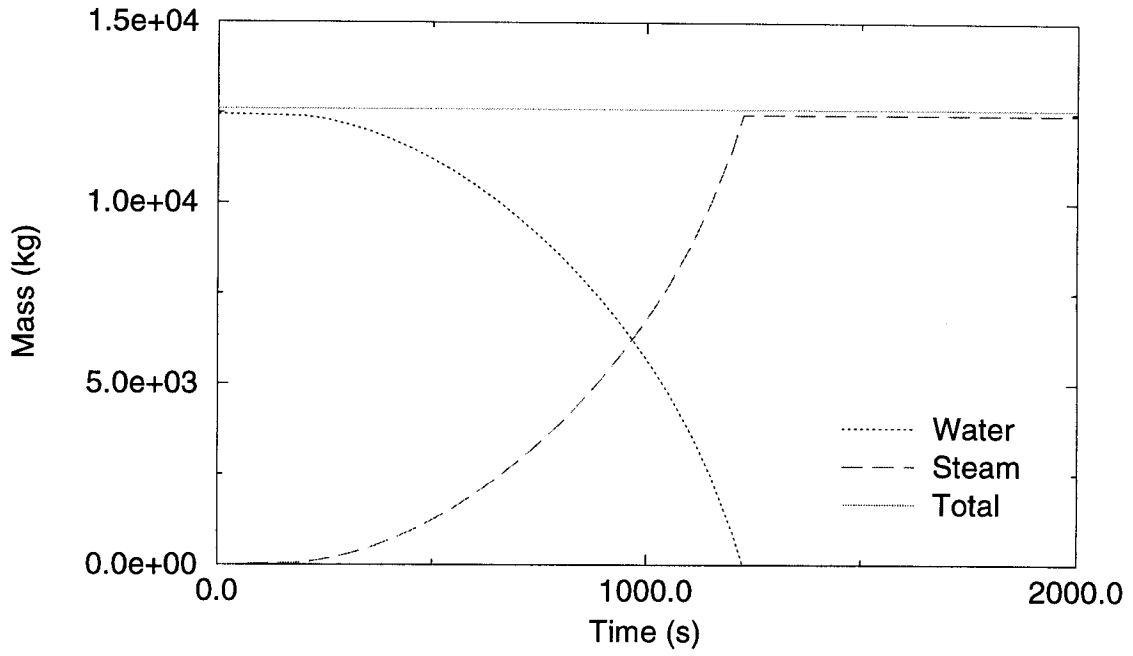

Figure 11. LPME Mass to HS - Volume Masses

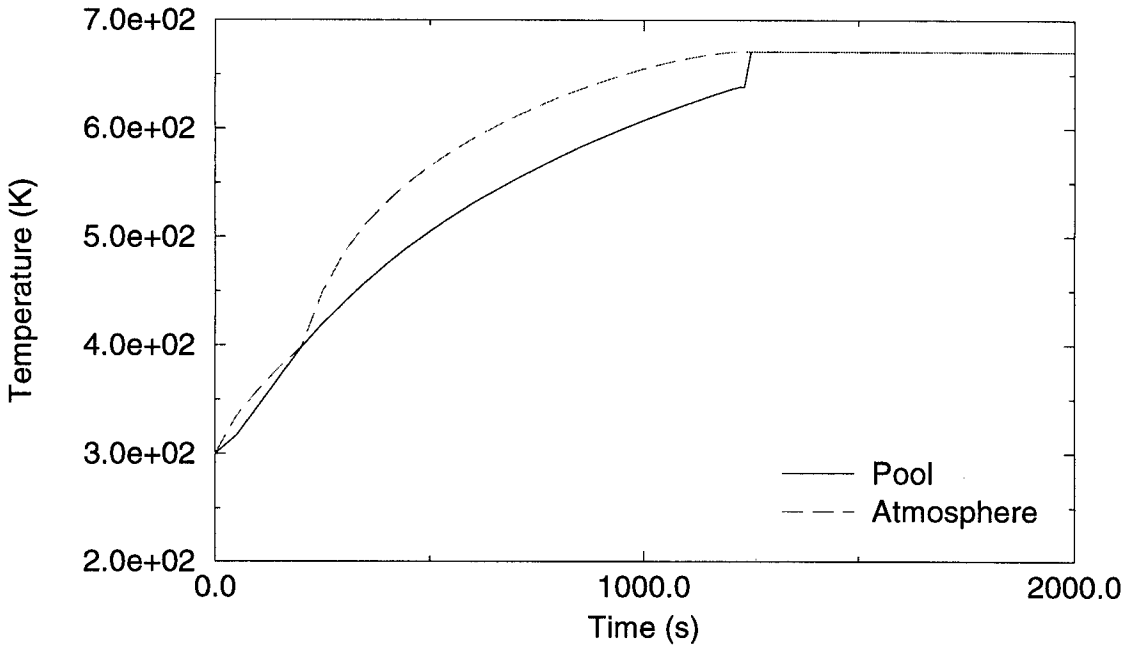

Figure 12. LPME Mass to HS - Volume Temperatures

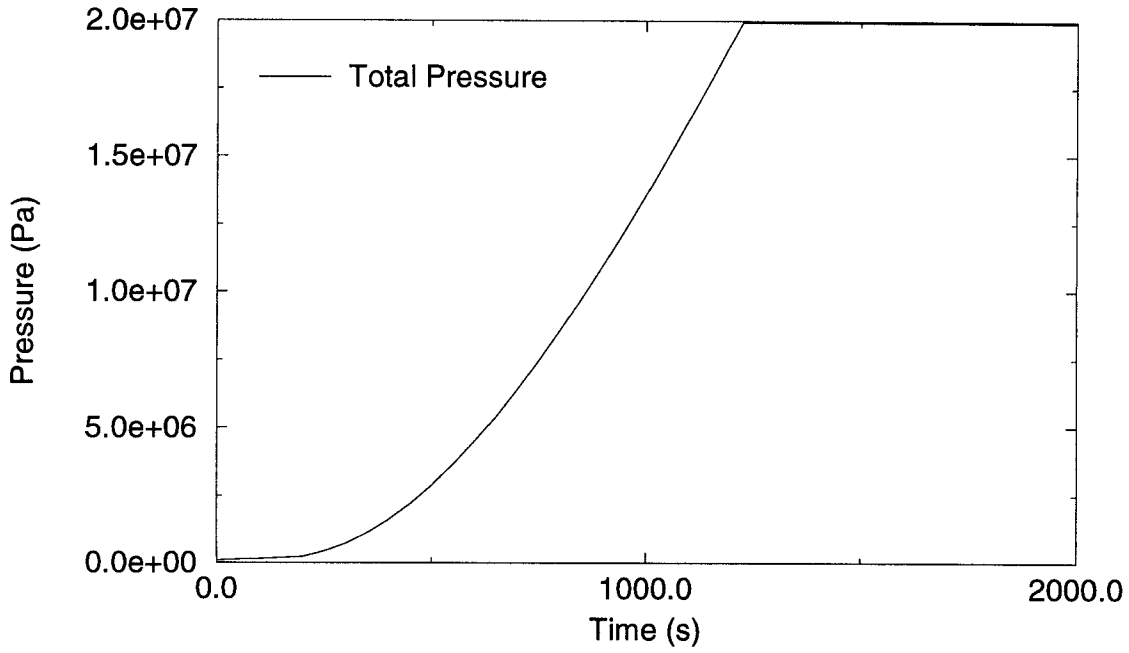

Figure 13. LPME Mass to HS - Volume Pressures

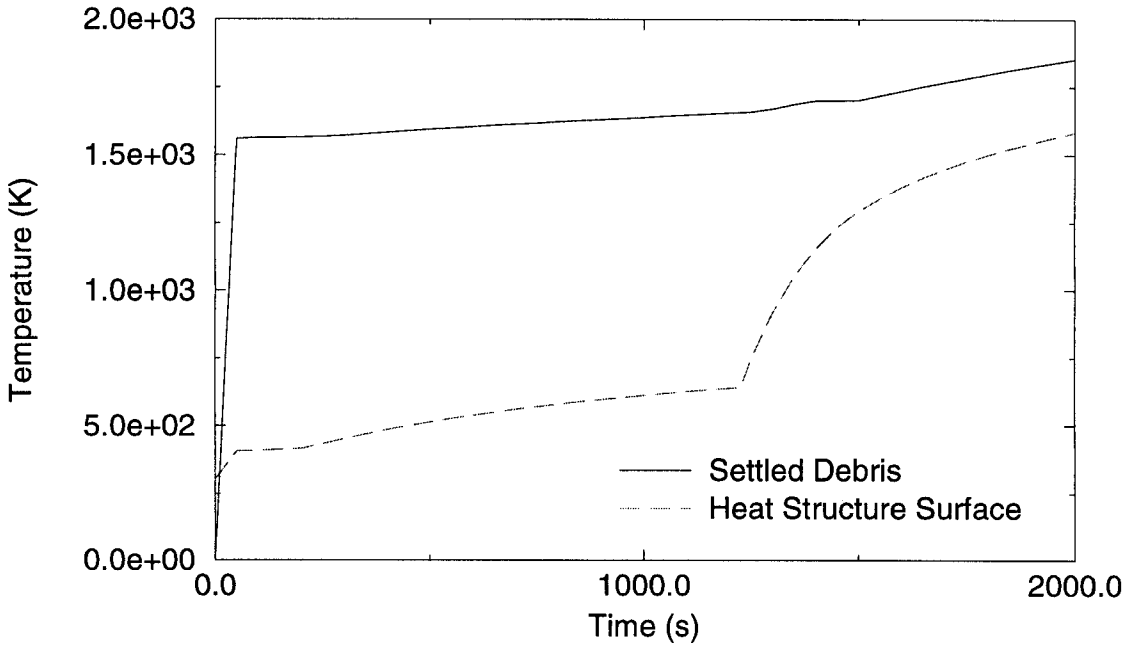

Figure 14. LPME Mass to HS - Debris Temperature

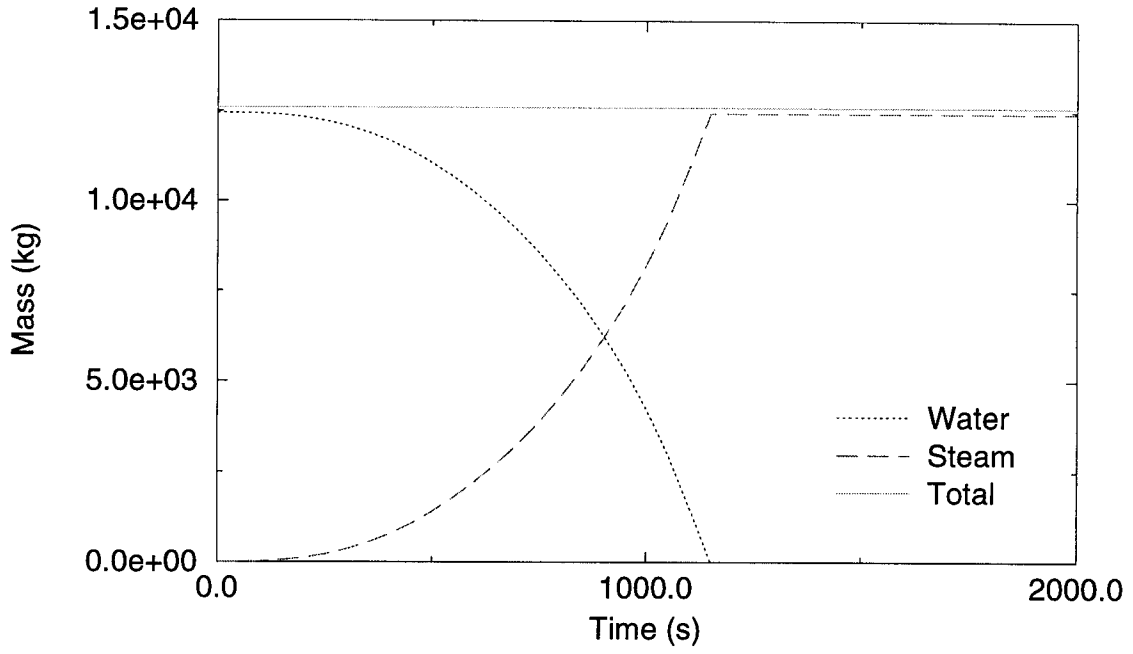

Figure 15. HPME No Oxidation - Volume Masses

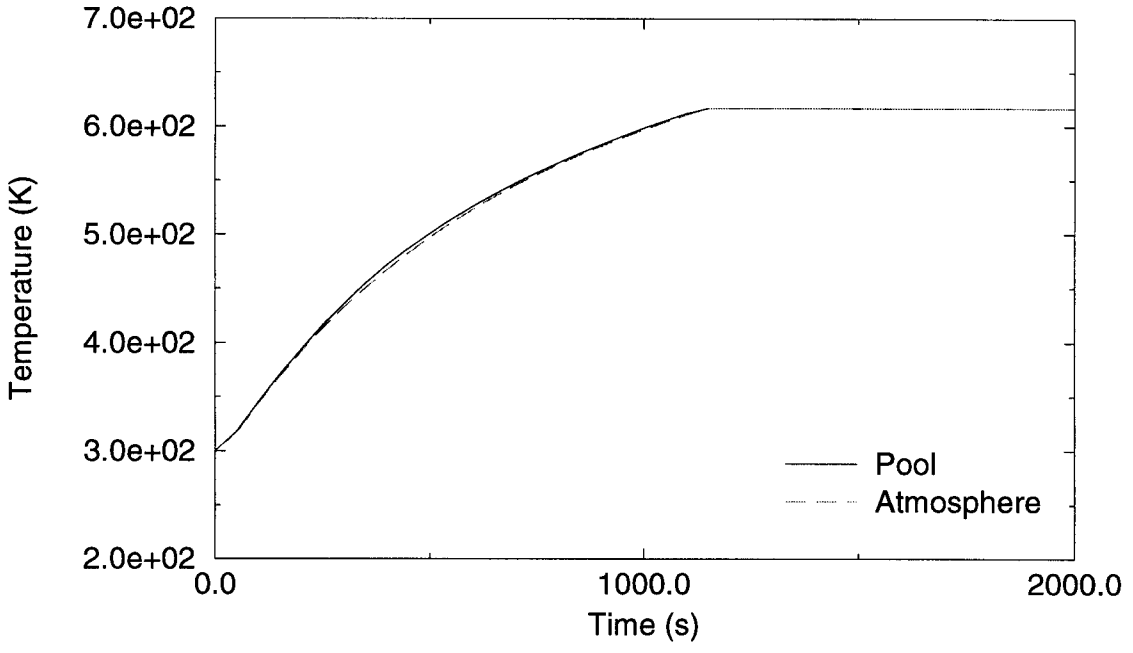

Figure 16. HPME No Oxidation - Volume Temperatures

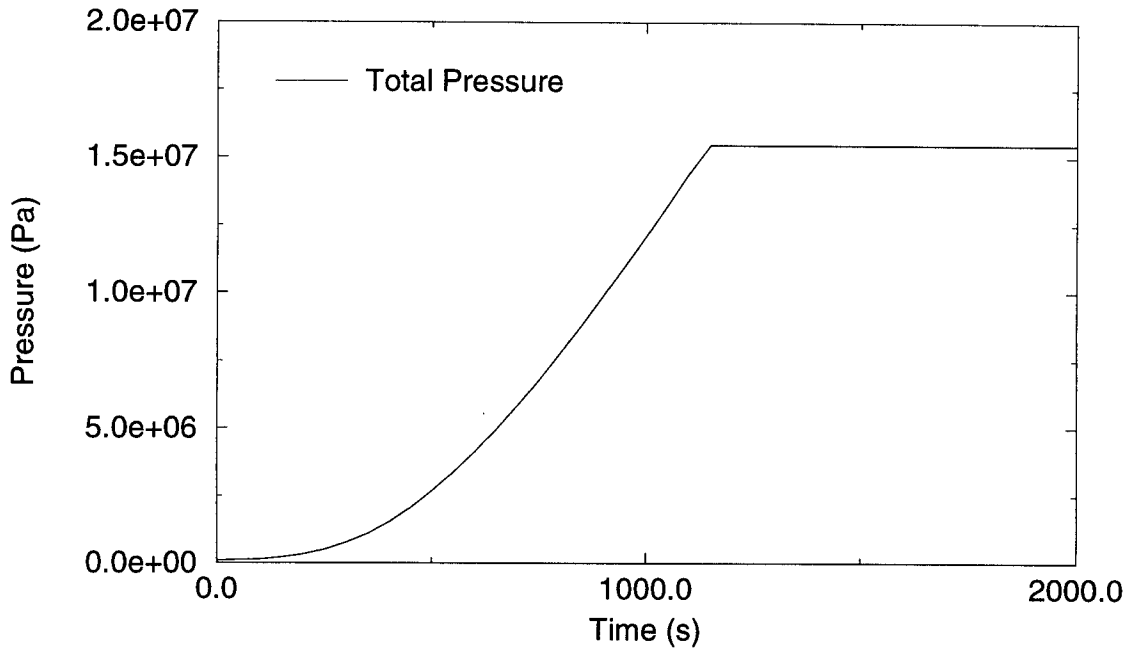

Figure 17. HPME No Oxidation - Volume Pressures

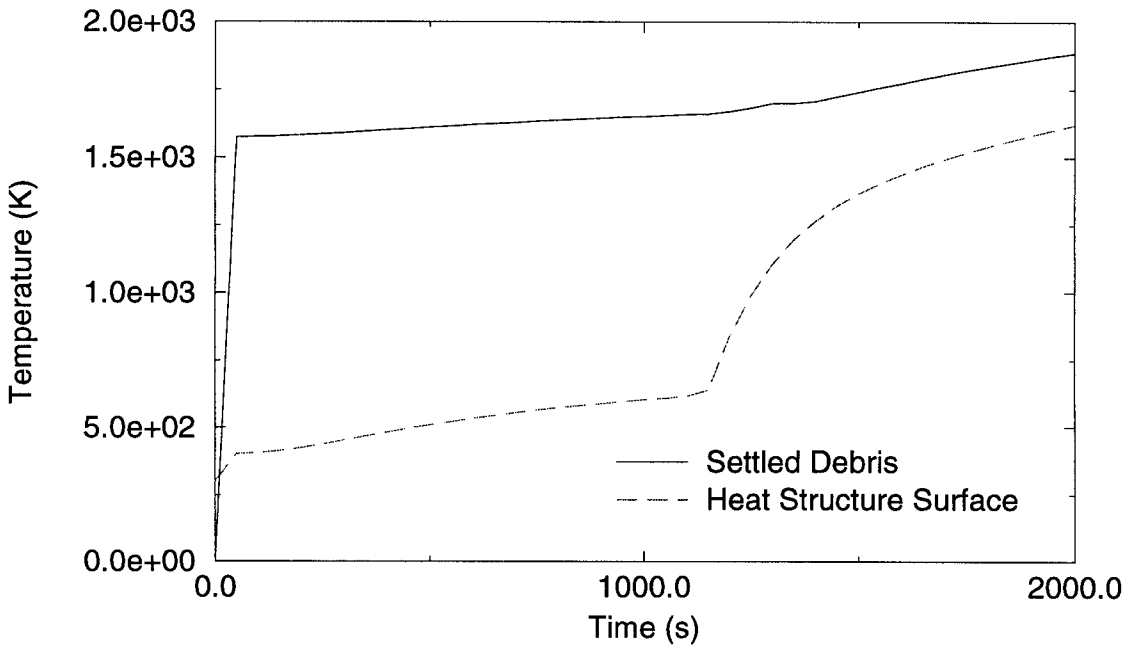

Figure 18. HPME No Oxidation - Debris Temperature

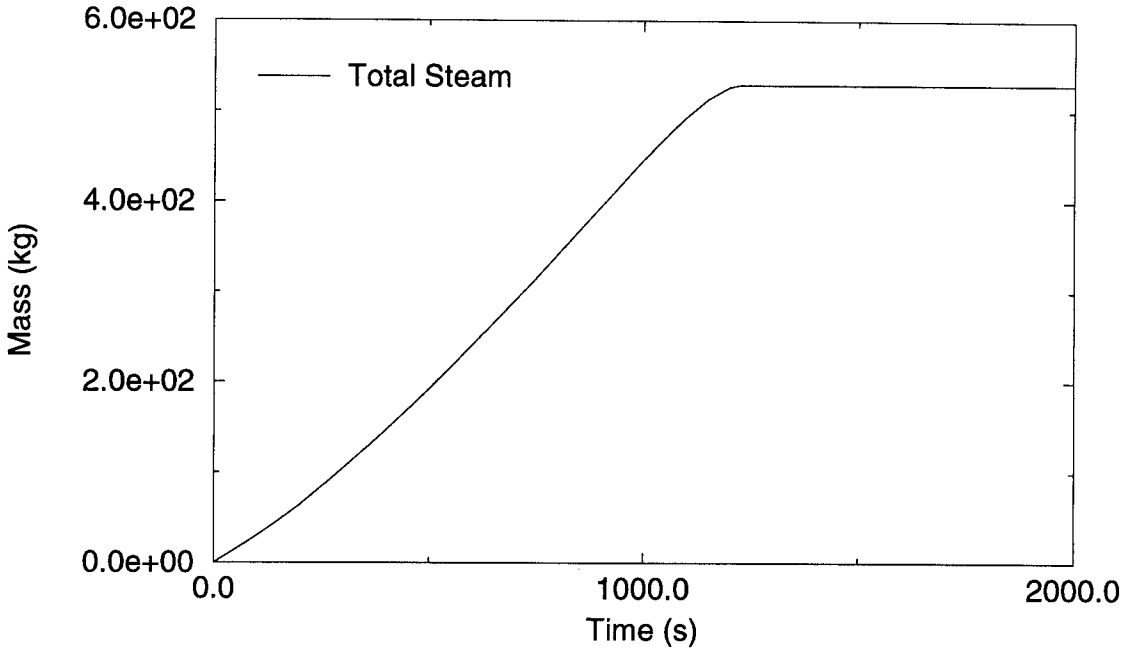

Figure 19. LPME Mass to HS - Steam Generation

of the changes made in this last version appear in the primary output file so that the FDI model edits are more informative. The combination of these modifications allows MELCOR to study a wider variety of phenomena related to the ITER project.

The executables and source can be found on *isambard.inel.gov*. The `/home/gracy/melcor/bin` directory contains the UD version executable. The `/home/gracy/melcor/transfer` directory contains the PRL files that the MELCOR utilities use to generate updated source code. Changes that were made to the source are all in lowercase and have the author's name in a comment statement nearby. Example input files and the data files for the plots used in this report can be found in `/home/gracy/melcor/work`.

Future work in this area could include:

- oxidation in the LPME model. There is no reason why oxidation can't occur in the LPME model and would be easy to incorporate by including the appropriate code from the subroutine FDIHI into FDIHIL.
- addition of more fusion related materials such as beryllium, lithium or copper.

Acknowledgment

Support for this work has been provided by the U.S. Department of Energy.

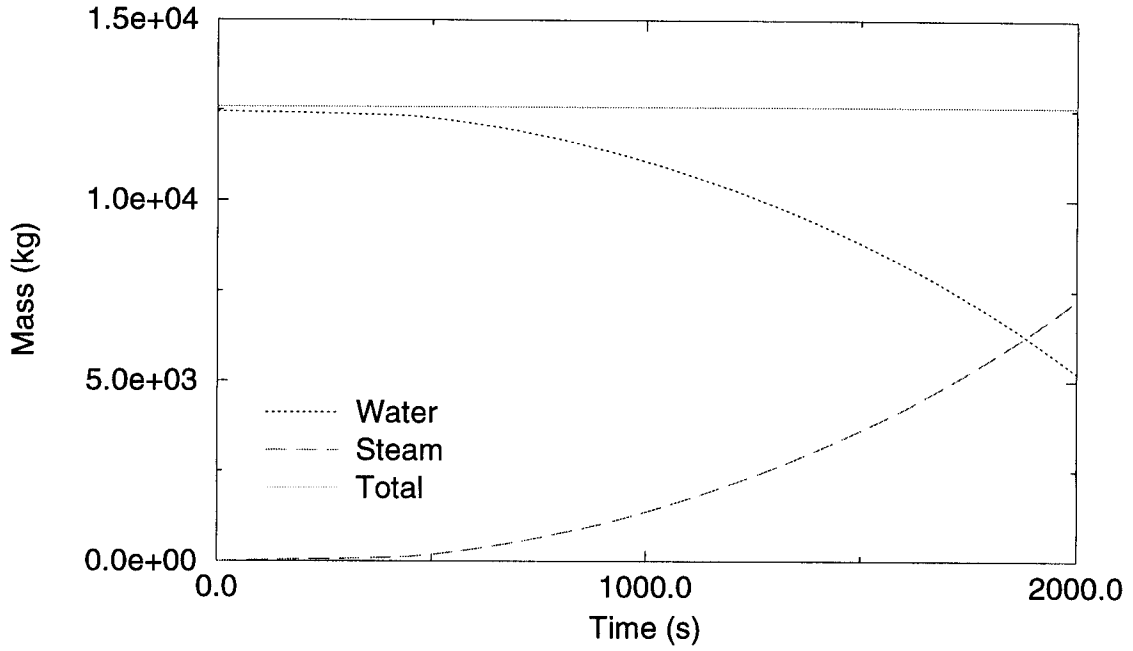

Figure 20. LPME Fusion Materials - Volume Masses

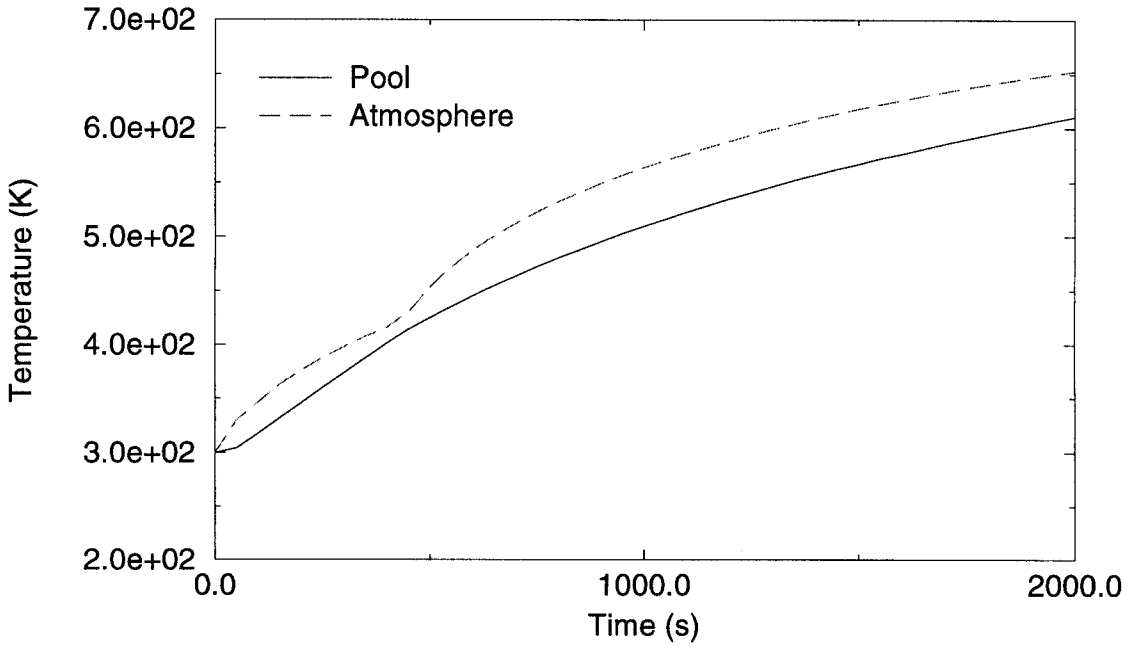

Figure 21. LPME Fusion Materials - Volume Temperatures

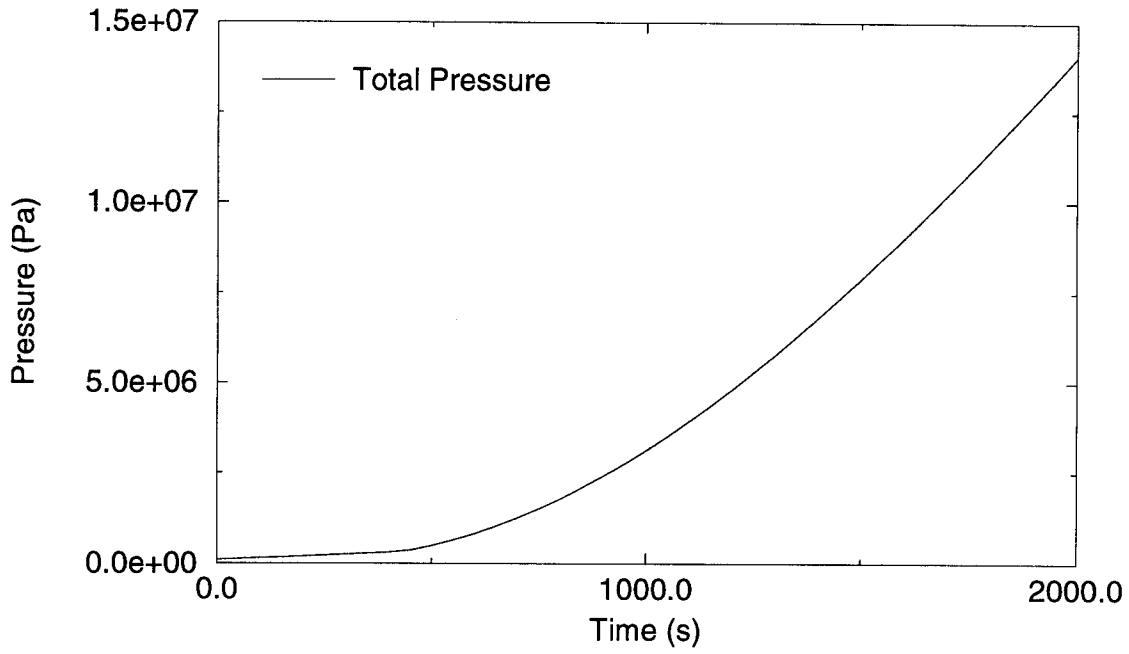

Figure 22. LPME Fusion Materials - Volume Pressures

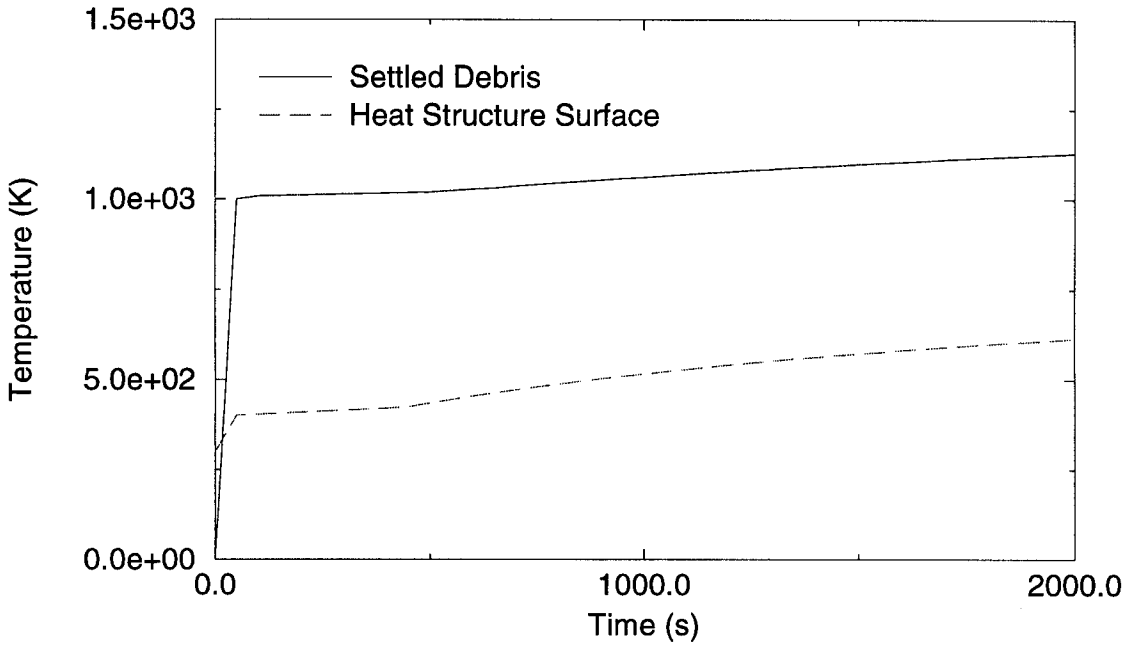

Figure 23. LPME Fusion Materials - Debris Temperature

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[6] M.W. Chase, **JANAF Thermochemical Tables**, 3rd Edition, American Institute of Physics for the National Bureau of Standards, New York, NY (1986).

[7] **CRC Handbook of Chemistry and Physics**, 71st Edition, CRC Press, Inc., Boca Raton, FL (1990).

A Material Properties

This section identifies the default thermophysical property tabular values of gallium, lead and lithium lead as defined in MELCOR. Any or all of these values may be overridden by using Tabular Function input as described in the Material Properties Package Users' Guide. Property units and references are given with each table. The Temperature vs. Specific Enthalpy tables are simply the invert of the Specific Enthalpy as a function of Temperature tables and are therefore not listed below.

A1. Gallium

A1.1. Ga Specific Enthalpy as a Function of Temperature

Temperature (K)	Specific Enthalpy (J/kg)	Reference
298.0	0.0	Ref. [2]
300.0	688.464	Ref. [2]
302.92	1821.561	Ref. [2]
302.93	81984.59	Ref. [2]
400.0	120595.9	Ref. [2]
500.0	159264.7	Ref. [2]
600.0	197531.8	Ref. [2]
700.0	235698.5	Ref. [2]
800.0	273807.9	Ref. [2]
900.0	311917.2	Ref. [2]
1000.0	350026.6	Ref. [2]
1100.0	388121.6	Ref. [2]
1200.0	426230.9	Ref. [2]
1300.0	464340.3	Ref. [2]
1400.0	502449.6	Ref. [2]
1500.0	540559.0	Ref. [2]
1600.0	578668.3	Ref. [2]
1700.0	616763.3	Ref. [2]
1800.0	654872.7	Ref. [2]
1900.0	692982.0	Ref. [2]
2000.0	731091.4	Ref. [2]
2100.0	769200.7	Ref. [2]
2200.0	807310.1	Ref. [2]
2300.0	845405.1	Ref. [2]
2400.0	883514.5	Ref. [2]
2478.0	913247.5	Ref. [2]

A1.2. Ga Specific Heat Capacity as a Function of Temperature

Temperature (K)	Specific Heat (J/kg-K)	Reference
298.0	375.7866	Ref. [2]
300.0	375.7866	Ref. [2]
302.92	375.7866	Ref. [2]
302.93	408.0584	Ref. [2]
400.0	390.7033	Ref. [2]
500.0	383.9621	Ref. [2]
600.0	381.8107	Ref. [2]
700.0	381.8107	Ref. [2]
700.01	381.0935	Ref. [2]
800.0	381.0935	Ref. [2]
900.0	381.0935	Ref. [2]
1000.0	381.0935	Ref. [2]
1100.0	381.0935	Ref. [2]
1200.0	381.0935	Ref. [2]
1300.0	381.0935	Ref. [2]
1400.0	381.0935	Ref. [2]
1500.0	381.0935	Ref. [2]
1600.0	381.0935	Ref. [2]
1700.0	381.0935	Ref. [2]
1800.0	381.0935	Ref. [2]
1900.0	381.0935	Ref. [2]
2000.0	381.0935	Ref. [2]
2100.0	381.0935	Ref. [2]
2200.0	381.0935	Ref. [2]
2300.0	381.0935	Ref. [2]
2400.0	381.0935	Ref. [2]
2478.0	381.0935	Ref. [2]

A1.3. Ga Thermal Conductivity as a Function of Temperature

Temperature (K)	Conductivity (W/m-K)	Reference
303.0	28.1	Ref. [5]
400.0	37.8	Ref. [5]
500.0	48.2	Ref. [5]
600.0	58.6	Ref. [5]

A1.4. Ga Density as a Function of Temperature

Temperature (K)	Density (kg/m^3)	Reference
303.0	6200.0	Ref. [5]
350.0	6150.0	Ref. [5]
400.0	6100.0	Ref. [5]
500.0	6010.0	Ref. [5]
600.0	5920.0	Ref. [5]

A1.5. Ga Constant Properties

Property	Value	Units	Reference
Melting Temperature	302.92	K	Ref. [6]
Latent Heat of Fusion	80177.85	J/kg	Ref. [6]
Density	6095.0	kg/m^3	Ref. [7]

A2. Lead

A2.1. Pb Specific Enthalpy as a Function of Temperature

Temperature (K)	Specific Enthalpy (J/kg)	Reference
298.0	0.0	Ref. [2]
300.0	236.51	Ref. [2]
400.0	13398.92	Ref. [2]
500.0	26981.25	Ref. [2]
600.0	40983.51	Ref. [2]
600.6	41128.31	Ref. [2]
600.61	64291.64	Ref. [2]
700.0	78858.62	Ref. [2]
800.0	93401.47	Ref. [2]
900.0	107780.2	Ref. [2]
1000.0	122009.3	Ref. [2]
1100.0	136108.1	Ref. [2]
1200.0	150100.7	Ref. [2]
1300.0	164011.3	Ref. [2]
1400.0	177873.5	Ref. [2]
1500.0	191711.7	Ref. [2]
1600.0	205559.5	Ref. [2]
1700.0	219441.1	Ref. [2]
1800.0	233395.1	Ref. [2]
1900.0	247440.8	Ref. [2]
2000.0	261616.8	Ref. [2]
2020.0	264469.4	Ref. [2]

A2.2. Pb Specific Heat Capacity as a Function of Temperature

Temperature (K)	Specific Heat (J/kg-K)	Reference
298.0	129.4521	Ref. [2]
300.0	129.5004	Ref. [2]
400.0	133.7479	Ref. [2]
500.0	137.9471	Ref. [2]
600.0	142.1463	Ref. [2]
600.6	142.1946	Ref. [2]
600.61	147.9384	Ref. [2]
700.0	146.2973	Ref. [2]
800.0	144.6079	Ref. [2]
900.0	143.0151	Ref. [2]
1000.0	141.5671	Ref. [2]
1100.0	140.4087	Ref. [2]
1200.0	139.4916	Ref. [2]
1300.0	138.8159	Ref. [2]
1400.0	138.478	Ref. [2]
1500.0	138.3815	Ref. [2]
1600.0	138.6228	Ref. [2]
1700.0	139.1055	Ref. [2]
1800.0	139.926	Ref. [2]
1900.0	141.0844	Ref. [2]
2000.0	142.4842	Ref. [2]
2020.0	142.8221	Ref. [2]

A2.3. Pb Thermal Conductivity as a Function of Temperature

Temperature (K)	Conductivity (W/m-K)	Reference
100.0	39.6	Ref. [3]
200.0	36.6	Ref. [3]
300.0	35.2	Ref. [3]
400.0	33.8	Ref. [3]
500.0	32.5	Ref. [3]
600.0	31.2	Ref. [3]
600.6	31.2	Ref. [3]
600.61	15.5	Ref. [3]
700.0	17.4	Ref. [3]
800.0	19.0	Ref. [3]
900.0	20.3	Ref. [3]
1000.0	21.5	Ref. [3]

A2.4. Pb Density as a Function of Temperature

Temperature (K)	Density (kg/m^3)	Reference
298.15	11350.0	Ref. [4]
600.6	11000.0	Ref. [4]
600.61	10670.0	Ref. [4]

A2.5. Pb Constant Properties

Property	Value	Units	Reference
Melting Temperature	600.6	K	Ref. [6]
Latent Heat of Fusion	23023.46	J/kg	Ref. [6]
Density	10670.0	kg/m^3	Ref. [7]

A3. Lithium Lead ($Li_{17}Pb_{83}$)

A3.1. Li-Pb Specific Enthalpy as a Function of Temperature

Temperature (K)	Specific Enthalpy (J/kg)	Reference
298.0	0.00	Ref. [5] (calculated from c_p)
300.0	384.55	Ref. [5] (calculated from c_p)
400.0	19565.49	Ref. [5] (calculated from c_p)
500.0	38655.27	Ref. [5] (calculated from c_p)
508.0	40178.51	Ref. [5] (calculated from c_p)
508.01	74078.51	Ref. [5] (calculated from c_p)
523.0	77026.11	Ref. [5] (calculated from c_p)
600.0	93326.42	Ref. [5] (calculated from c_p)
623.0	98588.28	Ref. [5] (calculated from c_p)
700.0	117569.23	Ref. [5] (calculated from c_p)
798.0	144848.45	Ref. [5] (calculated from c_p)

A3.2. Li-Pb Specific Heat Capacity as a Function of Temperature

Temperature (K)	Specific Heat (J/kg-K)	Reference
298.0	148.479	Ref. [5]
300.0	148.518	Ref. [5]
400.0	163.547	Ref. [5]
500.0	191.597	Ref. [5]
508.0	194.115	Ref. [5]
508.01	190.369	Ref. [5]
523.0	190.232	Ref. [5]
600.0	189.530	Ref. [5]
623.0	189.321	Ref. [5]
700.0	188.619	Ref. [5]
798.0	187.725	Ref. [5]

A3.3. Li-Pb Thermal Conductivity as a Function of Temperature

Temperature (K)	Conductivity (W/m-K)	Reference
298.0	25.559	Ref. [5]
300.0	25.616	Ref. [5]
400.0	28.454	Ref. [5]
500.0	31.293	Ref. [5]
508.0	31.520	Ref. [5]
508.01	11.955	Ref. [5]
523.0	12.250	Ref. [5]
600.0	13.767	Ref. [5]
623.0	14.220	Ref. [5]
700.0	15.737	Ref. [5]
798.0	17.667	Ref. [5]
800.0	17.706	Ref. [5]
900.0	19.676	Ref. [5]
973.0	21.113	Ref. [5]

A3.4. Li-Pb Density as a Function of Temperature

Temperature (K)	Density (kg/m^3)	Reference
298.0	10210.0	Ref. [5]
300.0	10210.0	Ref. [5]
400.0	10080.0	Ref. [5]
500.0	9950.0	Ref. [5]
508.0	9940.0	Ref. [5]
508.01	9940.0	Ref. [5]
523.0	9920.0	Ref. [5]
600.0	9820.0	Ref. [5]
623.0	9790.0	Ref. [5]

A3.5. Li-Pb Constant Properties

Property	Value	Units	Reference
Melting Temperature	508.0	K	Ref. [6]
Latent Heat of Fusion	33900.0	J/kg	Ref. [6]
Density	9940.0	kg/m^3	Ref. [7]

B Material Property Addition Checklist

The following list summarizes the changes necessary when adding new materials to the Material Properties package in MELCOR.

1. Find properties for materials you wish to add in a tabular format. Generally the properties needed are enthalpy, density, thermal conductivity, and specific heat all as a function of temperature. Also needed are the melting temperature, the latent heat of fusion and a constant density value. For appropriate units, see page MP-RM-8 of the Material Properties Reference Manual.

2. Modify the necessary include blocks that are included in the MP package. Follow the notes for modifying common blocks found in the file `/home/gracy/melcor/misc/notes_modifying.txt` on *isambard.inel.gov.*

Common Block		Modification
MPMATS	-	increase NMPPNT by number of new materials.
	-	add variables to MPMATS common block. Make sure variables are not already in use.
MPCOM	-	increase NDMATL by number of new materials.
MPTBNM	-	increase NDTABL by number of new tables describing new materials. Generally this is 5 times the number of new materials.

3. Include the common block modifications to other code packages that utilize these common blocks. The modules that require recompilation include: COR, ESF, FDI, HS, RN1, RN2, SPR. Also BH only if the ORNL version is used (it isn't by default). Of course the MP package would also have to be updated.

4. Modify code (data statements) to include new material properties.

Subroutine		Modification
MPPBD	-	add table pointers to MPTABD. It is fairly evident on how to do this by looking at the other definitions.
	-	add constant properties to XMPCOD data statements. Look at first definitions to see where to put what properties.
	-	add material names to MATRLD.
	-	add table names to TABNMD.

Subroutine	Modification
MPDFVL	- add to parameter list NPNT___. ___ is the table number of the pointers you specified in MPPBD. It is fairly evident on how to do this by looking at the other definitions. - add to parameter list IBEG___. It is fairly evident on how to do this by looking at the other definitions. - increase dimension of TABLE array. Use the highest IBEG___ parameter where appropriate. - add to IBEG array with the IBEG___ parameters. It is fairly evident on how to do this by looking at the other definitions. - add new data to TABLE array. It is fairly evident on how to do this by looking at the other definitions. - define extrapolation types in IENDFG for each table 0 - constant 1 - linear extrapolation 2 - out of range, return error.

5. Recompile MP package and link together all newly generated libraries made in Step 3.

C Sample MELCOR Input

The following is the input used for the LPME scenario where mass is diverted to a heat structure. Other input files are available in `/home/gracy/melcor/work` on *isambard.inel.gov*.

```
************************************************************************
*EOR* MELGEN
*
TITLE 'FDI LPME HS - 125 m3 volume w/ 0.5 m of H2O in CV'
*
DIAGFILE    'fdi.dia1'
OUTPUTFILE  'fdi.out1'
RESTARTFILE 'fdi.rst'
*
TSTART 0.0
*
*CRTOUT
*DTTIME 0.5
JOBID LPMEHS
*RUNONLY PN
*
NCG001   N2   04                    * In Atmosphere
NCG002   H2   05                    * part of FDI
NCG003   CO   06                    * part of FDI
NCG004   O2   07                    * In Atmosphere
*
EDF00100  'EDF2FDI DATA'  15  READ  * Internal name, # channels, IO type
EDF00101  'edflpme.dat'             * Filename
EDF00102  '(8E9.3)'                 * Date format
EDF00103  0.0                       * Time offset
*
TPIN10100  5  9                     * # of masses and thermo values
TPIN10101  READ  001                * EDF input
TPOT10200  5  101  DEF.1            * # masses, TPIN #, translation matrix
*
TPIN20100  5  9                     * # of masses and thermo values
TPOT20200  5  201  DEF.1            * # masses, TPIN #, translation matrix
*
FDI0100  300  20001  -1  102          * CV#, CAV#, EDF, TP #
FDI0101  'FDI TEST'                 * Internal name
FDI0102  0.0  5.0                   * Z bot, Z top
*
MPMAT00600  'STEEL'                 * part of FDI
MPMAT00699  1.0  0.0  0.0  0.0      * 100 % Fe
*
CV30000 'FDI/CAV volume'  2  2  1   * int. name, non.equil, vert. flow, CV type
CV30001  0  0                       * pool - fog allowed, active
CV30002  0.0  0.0                   * vel. of atm, vel. of pool
CV300A0  3                          * separate pool/atm. input
```

```
CV300A1  PVOL 101350.0                  * volume pressure
CV300A2  RHUM 0.50                      * relative humidity
CV300A3  TATM 300.0                     * atmos. temperature
CV300A4  MLFR.4 0.8                     * mole fraction gas in atmos. N2
CV300A5  ZPOL  0.5
CV300A6  TPOL  300.0
CV300A7  MLFR.7 0.2
CV300B0  0.0  0.0                       * Z, Vol
CV300B1  5.0  125.0                     * Z, Vol
*
HS20001000  2  1  0                     * # nodes, geom, stead. state flag
HS20001001 'Bottom FDI CVH'             * Internal name
HS20001002  -0.1  -1.E-7                 * angle of HS, horizontal LHS on top
HS20001003  1.0                         * multiplicity
HS20001004  0  0                        * flued temp. options
HS20001100  -1  1  0.0                  * temp. node data, T-n, x(0)
HS20001101  0.1  2                      * location, node
HS20001201  'STAINLESS-STEEL-304'  1     * material, mesh
HS20001300  0                           * no internal power
HS20001400  1  300  EXT  1.0  0.0       * LHS - conv. BC, CV#, type of flow, ?, ?
HS20001500  25.0  5.0  5.0              *       BC area, char len, axial length
HS20001600  0                           * RHS - symetry
.
*****************************************************************************
*EOR* MELCOR
*
TITLE 'FDI LPME HS - 125 m3 volume w/ 0.5 m of H2O in CV'
*
DIAGFILE     'fdi.dia2'
MESSAGEFILE  'fdi.mes'
PLOTFILE     'fdi.plt'
OUTPUTFILE   'fdi.out2'
RESTARTFILE  'fdi.rst'
STATUSFILE   'fdi.stat'
STOPFILE     'fdi.stop'
*
*       start  max    min      edit    plot  restart
TIME1   0.0    1.0    0.00001  200.0   50.0  1000.0
TEND 2000.0
*
*COMTC 20
CPULEFT 20.0
CPULIM 20000.0
*CRTOUT
CYMESF 100 1
*DTINCR 1.5848932
*DTSUMMARY
*DTTIME
```

```
*EDITCF .FALSE.
*EXACTTIME1 3600.0
*FORCEPLOT 0.2 20
JOBID LPMEHS
NOCOPY
*PLOTCF .FALSE.
*RESTART -1
*RESTART TIME 3600.0
*RESTARTCF .FALSE.
*RFMOD
*RUNONLY PN
*SOFTDTMIN 1.0 0
WARNINGLEVEL 2 2 -1
.
```