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MELCOR/CONTAIN LMR Implementation Report – FY14 Progress

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Abstract

This report describes the preliminary implementation of the sodium thermophysical properties and the design documentation for the sodium models of CONTAIN-LMR to be implemented into MELCOR 2.1. In the past year, the implementation included two separate sodium properties from two different sources. The first source is based on the previous work done by Idaho National Laboratory by modifying MELCOR to include liquid lithium equation of state as a working fluid to model the nuclear fusion safety research. To minimize the impact to MELCOR, the implementation of the fusion safety database (FSD) was done by utilizing the detection of the data input file as a way to invoking the FSD. The FSD methodology has been adapted currently for this work, but it may subject modification as the project continues. The second source uses properties generated for the SIMMER code. Preliminary testing and results from this implementation of sodium properties are given. In this year, the design document for the CONTAIN-LMR sodium models, such as the two condensable option, sodium spray fire, and sodium pool fire is being developed. This design document is intended to serve as a guide for the MELCOR implementation. In addition, CONTAIN-LMR code used was based on the earlier version of CONTAIN code. Many physical models that were developed since this early version of CONTAIN may not be captured by the code. Although CONTAIN 2, which represents the latest development of CONTAIN, contains some sodium specific models, which are not complete, the utilizing CONTAIN 2 with all sodium models implemented from CONTAIN-LMR as a comparison code for MELCOR should be done. This implementation should be completed in early next year, while sodium models from CONTAIN-LMR are being integrated into MELCOR. For testing, CONTAIN decks have been developed for verification and validation use.

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NOMENCLATURE

BRISC	Burner Reactor Integrated Safety Code of Laboratory
BUR	Burn Package designator for MELCOR code
CAV	Cavity Package designator for MELCOR code
CVH	Control Volume Hydrodynamics Package designator for MELCOR Code
DOE	Department of Energy
EOS	Equation of state
FSD	Fusion Safety Database
FY	Fiscal Year
INL	Idaho National Laboratory
JAEA	Japan Atomic Energy Agency
LDRD	Laboratory Directed Research and Development
LMR	Liquid metal reactor
LWR	Light water reactor
NAM	NaModel Package (new) for MELCOR code
NRC	Nuclear Regulatory Commission
PNC	Power Reactor and Nuclear Fuel Development Corporation
SNL	Sandia National Laboratories
STD	Standard test deck

Symbol – Applicable only for Chapters 2 and 3

A_G	Fitted constants for Equation V-7
A_L	Fitted constants for Equation A-7
A_{SAT}	Fitted constants for Equation A-6
B_{SAT}	Fitted constants for Equation L-4
b_L	Fitted constants for Equation A-8
C_{SAT}	Heat capacity along the saturation curve
C_P	Heat capacity at constant pressure
C_V	Heat capacity at constant volume
C_{VG}	Specific heat at constant volume at dilute vapor
c_{SAT}	Fitted constants for Equation L-7
d_L	Fitted constants for Equation V-2
E_{coh}	Cohensive energy for Equation L-10
e	Specific internal energy
e_{liq}^{D}	Specific internal energy of infinitely dilute vapor
G_a	Fitted constants for Equation V-10
H	Enthalpy
h_p	Planck constant
k	Thermal conductivity
mw	Molecular weight
N	number of atoms, 2.62×10^{25}
n	Young's fitted value for sodium defined in Equation L-9

Q	Correction factor for sodium in Equation L-9
S	Entropy defined in Equation L-9
T	Temperature
u	Temperature ratio defined in Equation V-6
u_L	Specific internal energy ratio to molten state in Equation V-2
v	Specific volume
α_p	Volumetric thermal expansion coefficient
α_{SAT}	Thermal expansion coefficient along the saturation curve
β_S	Adiabatic compressibility
$\beta_{S,m}$	Adiabatic compressibility at the melting point
β_T	Isothermal compressibility
δ	Constant defined in Equation L-9
Δ	Change in quantity in Equation V-4
ϵ	Constant defined in Equation L-9
γ	Thermal pressure coefficient
γ_{SAT}	Thermal pressure coefficient along the saturation curve
γ_g^C	Constant defined in Equation V-10
κ	Boltzmann's constant
θ	Temperature ratio defined in Equation L-14
ψ'	Variable defined in Equation V-7
ρ	Density
τ	Temperature difference variable for Equation L-7
μ	Viscosity
σ	Surface tension
ν	Sonic velocity as given in Equation L-14
ξ_L	Specific internal energy ratio to critical state in Equation V-2

Subscript

AVG	Average
C	Critical state
g	Vapor
NA	Sodium
l	Liquid
liq	Molten solid state at 371 K
SAT	Saturation

Symbol – Applicable only for Chapters 4 and 5

c_l	Liquid specific heat
c_{vf}	Vapor specific heat at constant pressure
D_O	Diffusion constant
f_1	Fraction of total oxygen consumed, see Equation 5-12
f_2	Fraction of sensible heat from the reaction to the pool
f_3	Fraction of the Na_2O product that enters the pool as a solid
f_4	Fraction of Na_2O_2 product that enters the pool as a solid

h( )	Scratch array for reals or doubles
ih( )	Scratch array for integers
ah( )	Scratch array for characters
lh( )	Scratch array for logical
k_l	Conductivity of the liquid
k_{vf}	Conductivity of the vapor evaluated at the film temperature
P	Pressure
$\mathbf{P_p}$	Pool pressure
q(reaction)	Specific reaction energy per unit mass of reaction product
q_{bot}	Heat flux through the bottom of pool at the onset of film boiling
q_{chf}	Critical heat flux
$q_{chf,s}$	Critical heat flux for a subcooled pool
T_{bot}	Layer temperature below the pool layer
T_{chf}	Critical heat flux temperature
T_{film}	Film temperature
T_{pool}	Pool layer temperature
T_{sat}	Saturation temperature
λ	Heat of vaporization of sodium at T_{sat}
λ'	Coefficient defined in Equation 5-8
ρ_l	Liquid density
ρ_v	Density of the vapor
ρ_{vf}	Density of the vapor evaluated at the film temperature
μ_{vf}	Viscosity of the vapor evaluated at the film temperature
σ	Sodium liquid surface tension at T_{sat}
Ψ	Coefficient defined in Equation 5-6

1 INTRODUCTION

A sodium coolant accident analysis code is necessary to provide reactor designers and regulators with a means to perform severe accident analyses for future liquid metal reactor (LMR) application, such as sodium fast reactors (SFRs). A gap analysis of the ability for computer codes and models in the U.S. to support the licensing of SFRs identified a gap in the current ability to model source terms and accidents involving the containment [Schmidt 2011]. This gap was identified as a high priority gap, which requires a near term action as determined as, a subsequent review of gaps involving sodium technology, accident sequences and initiators, source terms, codes and models, and fuels and materials [Denman et al., 2012].

MELCOR and CONTAIN, which are currently employed by the U.S. Nuclear Regulatory Commission (NRC) for light water reactor (LWR) licensing, have been traditionally used for level 2 and level 3 probabilistic risk analyses as well as for the containment design basis accident analysis. Recent endeavors, in part due to increases in containment-reactor pressure vessel coupling through the use of passive safety systems, MELCOR has been employed for the containment design basis accident analysis as well [Tills 2008, Tills 2009 and Tills 2010].

To meet future design basis analysis needs [Schmidt 2011], new models will be added to the MELCOR code for simulation of LMR designs. Existing models developed for separate effects codes will be integrated into the MELCOR architecture. In particular, many LMR models were added to the CONTAIN code (version 1.11) as part of CONTAIN-LMR code released in the 1990s [Murata 1993,Scholtyssek 1994]. This work will integrate those CONTAIN code capabilities that feasibly fit within the code architecture. Among the LMR code capabilities to be considered are models for:

- sodium pool and spray fires,
- treating two condensable (sodium and water) simultaneously,
- sodium atmosphere and pool chemistry,
- sodium condensation on aerosols,
- heat transfer from oxide core-debris beds (lower priority due to the current focus on metallic fuel) and to sodium pools, and
- sodium-concrete interactions.

Implementation of such models for the sodium reactor simulation into an actively maintained, full-featured integrated severe accident code fills a significant gap in the capability for providing the necessary analysis tools. This project will close this gap by implementing, improving, and verifying model development efforts into the MELCOR source code. The current scope will focus on the following implementation goals:

Phase 1 (FY13): Implement sodium Equations of State (EOS) as a working fluid for a MELCOR calculation from:

- The fusion safety database (FY13)
- The SIMMER-III Code (FY13)
- The SAS4a Code

Phase 2 (FY14): Examine and test changes to the CONTAIN-LMR Implemented by Japan Atomic Energy Agency (JAEA), specifically:

- Aerosol Condensation
- Implementation of the capability for simultaneous sodium and water condensation modeling

Phase 3 (FY15): Implementation and Validation of CONTAIN physics models [Jeppson 1986]

- Sodium Spray Fires (including new test data)
- Sodium Pool Modeling
- Sodium Pool Fires

Phase 4 (FY16): Implementation and Validation of CONTAIN chemistry models

- Debris Bed/Concrete Cavity Interactions
- Sodium Pool Chemistry
- Atmospheric Chemistry

Note that beginning with MELCOR 2.0, the code architecture and input formats are significant different than its predecessor, MELCOR 1.8.6. MELCOR 2.0 utilizes many features of FORTRAN 95 such as dynamic memory management and user defined types, which allows for future changes in compilers and hardware. With MELCOR, the working fluid field is modeled as water. Thus the equation of state is strictly applicable for water and steam. Because a single fluid field is allowed in a given problem, the use of a different fluid model requires that the property model for the new fluid must be defined to replace that of the water. Once this has been accomplished, MELCOR should be extended to include sodium specific models as described in this chapter.

This report summarizes what was completed in FY13 as well as in FY14. In FY13, the implementation and testing of sodium properties into MELOCR 2.1 was completed. Some minor issues related to the property implementation were identified, and would be addressed by the end of the 2014. Thus, Chapter 2 and Chapter 3 document the tasks completed in FY13. In FY14, the design documentation of the sodium physics models from CONTAIN-LMR have been developed. The sodium physics models focused in this design document are mainly the models to be implemented in FY15, which include two-condensable option (the implementation has been started in FY14), sodium spray fire, sodium pool physics, and sodium pool fire. The sodium concrete interaction and the sodium chemistry – atmospheric chemistry, and pool chemistry will be addressed in FY16. Therefore, Chapter 4 discusses the upgrade/modification done to CONTAIN-LMR and CONTAIN 2 which allow them to run within the MELCOR code development environment. Chapter 5 describes the design documentation for the FY15 implementation to MELCOR. Finally, Appendix B provides the testing of the CONTAIN 2 and CONTAIN-LMR codes. For CONTAIN-LMR, a number of preliminary code verifications and validations were performed. Thus a list of the CONTAIN input decks is provided.

2 LIQUID METAL PHYSICAL PROPERTIES

To accommodate sodium as the working fluid field in MELCOR, the sodium thermophysical properties, such as enthalpy, heat capacity, heat of fusion, vapor pressure, heat of vaporization, density, thermal conductivity, thermal diffusivity, viscosity and thermal expansion must be provided to replace those currently used for water. The equation of state (EOS) for water is based on the polynomials in a tabular format. These polynomials relate pressure, specific internal energy, specific entropy and heat capacity to temperature and density, and are expressed analytically in terms of the Helmholtz free energy. In MELCOR, additional thermodynamic properties are derived from the thermodynamic relationships involving Helmholtz free energy, such as fluid internal energy, enthalpy, entropy, specific heat, and derivatives of pressure with respect to temperature and density. The resulting EOS is valid for temperature ≥ 273.15 K and for pressure ≤ 100 MPa. Water surface tension is calculated in Subroutine tHS_HSBOIL. Additional thermodynamic properties of water can be found in Module M_H2O. This module also contains the single phase EOS for water, which is modeled in Subroutine tH2O_H2O1PH. The mixed-phase (or 2-phase) EOS for water is modeled in subroutine tH2O_H2O2PH. The binary diffusion coefficient for water vapor in a gas mixture is defined in Module M_NCG.

There are a number of data sources for sodium properties that can be considered for implementing into MELCOR. For supporting fusion safety research, Idaho National Laboratory (INL) modified MELCOR 1.8.5 to include lithium and other metallic fluid [Merrill 2000]. This database is called herein the Fusion Safety Database (FSD). The second database (SIMMER) from the SIMMER-III data was considered in the Burner Reactor Integrated Safety Code of Laboratory (BRISC) Laboratory Directed Research and Development (LDRD) at Sandia National Laboratories (SNL). This work was leveraged in SNL's FY13 efforts. Subsequent work will also include the EOS from SAS4a, but this work does cannot leverage an historical effort like the FSD and SIMMER EOSs.

2.1 Fusion Safety Database (FSD)

Implementation of non-water fluids into MELCOR have been explored in the past. Earlier work performed at INL allowed the modeling of lithium fires with MELCOR 1.8.5. This modification permitted MELCOR to access properties from the fusion safety data set, which was originally designed for the ATHENA code and is an extension of the RELAP5 environmental library [Merrill 2000]. It includes 13 fluids: water, hydrogen, lithium, potassium, helium, nitrogen, sodium, sodium-potassium, lithium-lead, etc. Code modifications were made to allow evaluation of the equation of state for an array of potential materials. These models were updated to FORTRAN 95 and tested within the code. Also, several interpolation routines used in the MELCOR 1.8.5 implementation, were proprietary and new ones have been used. This is our first approach for implementation of liquid metal properties and has already been started, as many of the 1.8.5 models have been ported to the MELCOR 2.1 code as part of this project and shows great promise.

FSD_EOS module contains property interpolation and correlations for processing the input data file as described in NaLibrary program. In this FSD_EOS module, surface tension, thermal conductivity, viscosity, and critical heat flux correlations are also given for various fluids as

described above. Examples of the transport property for the liquid sodium modeled in FSD_EOS are given as:

Viscosity, Pa-s [Gierszewski 1980]:

$$\mu = \frac{3.24\times10^{-3}e^{508/T}}{T^{0.4925}} \qquad [2\text{-}1]$$

Thermal Conductivity, W/m-K [Gierszewski 1980]

$$k = 110 - 0.0645 \cdot T + 1.173 \times 10^{-5}T^2 \qquad [2\text{-}2]$$

Surface Tension, N/m (curve fitted)

$$\sigma = 0.235115 - 1 \times 10^{-4}T \qquad [2\text{-}3]$$

Note that the development of the FSD set requires the user to provide a property input file in order to utilize the FSD_EOS and other program files for this database. The required input file must be named such that it matches the desired fluid to be simulated. Section 3.2 describes more details of the filename requirement. The required unformatted input file contains the thermodynamic properties of simulated fluid. The input file is generated by running the NaLibrary Program. A brief description is given below:

NaLibrary

For the FSD data set, the input data file for sodium is required. A FORTRAN program written by J.E. Tolli of EG&G Idaho, Inc. in September 1991 can be used to produce this input data file. This program requires the user to provide an input containing temperatures and pressures in metric units.

The program generates tables of selected thermodynamic properties as functions of temperature and pressure for both saturation and single phase conditions, liquid and/or vapor states for sodium using the soft-sphere model free energy equation [Young 1977, Blink 1982]. The output of this program provides the triple and critical temperatures, pressures and volumes; saturation properties (temperature versus pressure) tables of temperature, pressure, specific volume, internal energy, thermal expansion, isothermal compressibility, specific heat and entropy all the input range of temperature and pressure; saturation properties (pressure versus temperature) tables of the same property parameters as listed before. It is followed by the thermodynamic properties tables for specific volume, internal energy, thermal expansion, isothermal compressibility, specific heat and entropy. To limit the file size, this program generates the output file in binary form. This output file is input to the multi-fluid MELCOR code. As previously described, MELCOR determines the fluid type by the name of the property data filename. (See Appendix A for the list of the tables input/outputs by this program.)

2.2 SIMMER Database

Our second approach builds off the BRISC LDRD performed at SNL. The BRISC approach took sodium coolant properties and directly implemented them a branch version of the MELCOR 1.8.6 code. Due to the limited scope, the implementation was performed as a proof of concept which restricted to the complete implementation, validation, verification, full test case development, etc. The property model was based on an analytic EOS model developed for the SIMMER-III code. Many of the code modifications that are required for this modeling approach are identical or extensions to those modifications developed for the previously described FSD approach. As part of this project, the code changes made to the 1.8.6 code were ported to MELCOR 2.1. Debugging is in progress.

Some of the properties and EOS as described by Fink and Leibowitz for the inclusion of the sodium in SAS4A, a severe accident code for liquid metal analyses [Cahalan 1994, Dunn 2012], were also implemented as SIMMER database. For the liquid sodium, much of the thermodynamic and transport properties are derived from saturated condition. Table 2-1 shows the property equations/correlations modeled in MELCOR. For the vapor sodium, examples of the thermodynamic and transport properties are given in Table 2-2. Additional properties and values used in the property determination are given in Table 2-3. Most of the correlations shown in these tables were originated mainly from the SIMMER data set. However, the entropy correlations are obtained from the soft-sphere model as described in the NaLibrary Program.

Table 2-1 Liquid Sodium Thermophysical Properties Modeled*

Property [reference]	Equation	Range	Equation #
Melting temperature (K), Eq.(L-1) [Fink 1979]	$T_{liq} = 370.98$		L-1
Melting density (kg/m^3), Eq.(L-2)	$\rho_{liq} = 927.63$		L-2
Molten specific internal energy (J/kg)	$e_{liq} = 2.06494 \times 10^5$		L-3
Density (kg/m^3) [Morita 1998a]	$\rho_l = \rho_{liq} \cdot \left[1 + \sum_{i=1}^{3} B_{SAT,i}(T - T_{liq})^i\right]$ $\rho_l = \rho_C \cdot \left[1 + B_{SAT,5} \cdot \tau^{0.5} + B_{SAT,6} \cdot \tau^2\right]$ $\rho_l = \rho_C$ where $B_{SAT,i}$ = fitted constants, where i is from 1 to 6 $\tau = T_C - T$	$T_{liq} < T \leq B_{SAT,4} T_C$ $B_{SAT,4} \cdot T_C < T \leq T_C$ $T > T_C$	L-4a L-4b L-4c
Specific heat at constant pressure (J/kg-K) [Fink 1979]	$C_P = C_{SAT} \cdot T \cdot \alpha_P \cdot \gamma_{SAT}/\rho_l$ where $\gamma_{SAT} = \left(\frac{dP}{dT}\right)_{SAT}$. Note this derivative is taken as $\left(\frac{dP}{dT}\right)_{SAT} = p_v \cdot \left(b_{L,2} - \frac{b_{L,3}}{T^2} + \frac{b_{L,4}}{T}\right)$ where $b_{L,i}$ is given by p_g		L-5
Specific heat at constant volume (J/kg-K) [Fink 2979]	$C_V = C_P \cdot \beta_S/\beta_T$		L-6
Specific internal energy (J/kg) [Morita 1998a]	$e_l = e_{liq} \cdot \left[\sum_{i=1}^{3} C_{SAT,i}(T - T_{liq})^i\right]$ $e_l = e_C \cdot \left[1 - C_{SAT,5} \cdot \tau^{0.5} + CB_{SAT,6} \cdot \tau^2\right]$ where	$T_{liq} < T \leq C_{SAT,4} T_C$ $C_{SAT,4} \cdot T_C < T \leq T_C$	L-7a L-7b

Property [reference]	Equation	Range	Equation #
	$C_{SAT,i}$ = fitted constants, where i is from 1 to 6 $\tau = T_C - T$		
Enthalpy (kJ/kg) [Fink 1995]	$H_l = -365.77 + 1.6582 \cdot T - 4.2375 \times 10^{-4} T^2 + 1.4847 \times 10^{-7} T^3 + 2992.6/T$ $H_l = 2128.4 + 0.86496 \cdot T$	$T_{liq} \leq T < 2000K$ $2000K \leq T \leq T_C$	L-8a L-8b
Entropy (J/K) [Young 1977, Blink 1982]	$S = \frac{dH_z}{dT} = \frac{E - A}{T}$ $= N\kappa \left[\frac{3}{2} + \ln \left(\frac{\frac{e}{\left(N \cdot \left(h_p \sqrt{N/(2\pi\kappa)}\right)^3\right)} T^{1.5}}{\rho_l} \right) + \frac{1}{3}(n+4) Q \cdot (\rho_l \delta)^{n/9} \left(\frac{\epsilon}{\kappa T}\right)^{1/3} \right]$ where N = number of atoms, 2.62×10^{25} κ = Boltzmann's constant, 1.3806×10^{-23} J/K h_p = Planck constant, 6.62618×10^{-34} J s $\delta = 7.12349 \times 10^{-30}$ Q = correction factor, 0.95 for sodium $\epsilon = 6.21332 \times 10^{-19}$ J/atom for sodium $n = 8$ for sodium $E = N\kappa T \left[\frac{3}{2} + c_n \rho_l^{n/3} \left(\frac{\epsilon}{\kappa T}\right) + \frac{1}{6}(n+4) Q \rho_l^{n/9} \left(\frac{\epsilon}{\kappa T}\right)^{1/3} - \rho_l^m \left(\frac{\epsilon}{\kappa T}\right) \right] + E_{coh}$ $A = N\kappa T \left[-\ln\left(\frac{Ve}{n\lambda^3}\right) + c_n \rho_l^{n/3} \left(\frac{\epsilon}{\kappa T}\right) + \frac{1}{2}(n+4) Q \rho_l^{n/9} \left(\frac{\epsilon}{\kappa T}\right)^{1/3} - \rho_l^m \left(\frac{\epsilon}{\kappa T}\right) \right] + E_{coh}$ where E_{coh} = cohensive energy Note the first term in Eq.(L-10b) can be reduced when determining the right hand side of Eq.(L-9)	$4 \leq n \leq 12$	L-9 L-10a L-10b

Property [reference]	Equation	Range	Equation #
Derivative of Partial pressure [Morita 1998a]	$\frac{dP}{d\rho_l} = \frac{R \cdot T}{(1-\rho_l)^2} - \frac{a(T)\left(\frac{2}{\rho_l} + a_{G,3}\right)}{\left(\frac{1}{\rho_l} + a_{G,3}\right)^2}$ where $a(T) = a_{G,2}\left(\frac{T}{T_C}\right)^{a_{G,4}}$ $a(T) = a_{G,2}\left[1 + a_{G,4}\left(\frac{T}{T_C} - 1\right)\right]$	 $T < T_C$ $T \geq T_C$	L-11a
	$\frac{dP}{dT} = \frac{C_P - C_V}{T}\left(\frac{dP}{d\rho_l}\right)^{0.5} \rho_l$		L-11b
Volumetric thermal expansion coefficient (K^{-1}) [Fink 1979]	$\alpha_p = \alpha_{SAT} + \beta_T \cdot \gamma_{SAT}$ where $\alpha_{SAT} = -\left(\frac{d\rho_l}{dT}\right)_{SAT} / \rho_l$ Note that $\left(\frac{d\rho_l}{dT}\right)_{SAT}$ is calculated by taking the derivative of ρ_l equation above.		L-12
Isothermal compressibility (1/Pa) [Fink 1979]	$\beta_T = \frac{\beta_S C_{SAT} + \frac{T}{\rho_l}\alpha_{SAT}(\alpha_{SAT} + \beta_S \gamma_{SAT})}{C_{SAT} - \frac{T}{\rho_l}\gamma_{SAT}(\alpha_{SAT} + \beta_S \gamma_{SAT})}$ where $C_{SAT} = \left(\frac{dH_l}{dT}\right)_{SAT} - \frac{\gamma_{SAT}}{\rho_l}$ $\left(\frac{dH_l}{dT}\right)_{SAT} =$ $35.206 - 2 \cdot 7.0513 \times 10^{-3}T + 3 \cdot 2.5711 \times 10^{-6}T^2 + 12480/T^2$ $18.525 + 0.5 \cdot 43.402 \cdot 0.32227 \cdot (1 - T/T_C)^{0.32227-1}$ 18.525	 $T < 1644K$ $1644K \leq T \leq T_C$ $T > T_C$	L-13
Adiabatic compressibility (1/Pa) [Fink 1979]	$\beta_S = 1/(\rho_l v^2)$ where $v = 2660.7 - 0.3766\,T - 9.0356 \times 10^{-5}T^2$ $\beta_S = \beta_{S,m}\left(1 + \frac{\theta}{b}\right)/(1-\theta)$ Where	371K ≤ T ≤1700K 1700K <T < T_C	L-14a L-14b

Property [reference]	Equation	Range	Equation #
	$\beta_{S,m}$= adiabatic compressibility at the melting point, 1.717×10^{-4} MPa^{-1} $\theta = \frac{T - T_{liq}}{T_C - T_{liq}}$		

*See Table 4 of [Morita 1998b] for the values of the fitted constants and other numerical values provided. Note that ρ_{liq} is calculated from v_{liq} in this reference.

Table 2-2 Vapor Sodium Thermophysical Properties Modeled

Property [reference]	Equation	Range	Equation #
Density (kg/m^3) [Morita 1998a]	$\rho_g = \rho_C / \exp\left[\sum_{i=1}^{6} B_{G,i}(1-\tau)^{n_{G,i}}\right]$ where $B_{G,i}$ = fitting constants as a function of i $n_{G,i}$ = fitting exponents as a function of i $\tau = T/T_C$		V-1
Specific liquid volume (m^3/kg) [Morita 1998a]	$v_l = v_{liq}\left[1 + \sum_{i=1}^{3} d_{L,i}(u_L - 1)^i\right]$ $v_l = v_C\left[1 + d_{L,5}(1-\xi_L)^{0.5} d_{L,6}(1-\xi_L)^2\right]$ where $u_L = e/e_{liq}$ $\xi_L = e/e_C$ $d_{L,i}$ = fitted constants, i = 1 to 6	$e_{liq} < e \le d_{L,4}e_{liq}$ $d_{L,4}e_{liq} < e \le e_C$	V-2a V-2b
Specific internal energy (J/kg) [Morita 1998a]	$e_{vg} = C_{VG}(T - T_{liq}) + e_{liq}^D + \frac{y_B R \cdot T}{1 + y_B}\left(1 - \frac{d_{G,2}}{T}\right) - \frac{A_{G,2}(1 - A_{G,4})\psi}{A_{G,3}} \ln(1 + A_{G,3}\rho_v)$ where $y_B = \frac{1 + 2x_G - \sqrt{1 + 8x_G}}{2(x_G - 1)}$ $x_G = \frac{\rho_g \cdot k_G R \cdot T}{1 - A_{G,1}\rho_g}$		V-3

Property [reference]	Equation	Range	Equation #
	$k_G = \exp\left(d_{G,1} + \frac{d_{G,2}}{T}\right)$ $\psi = \left(\frac{T}{T_C}\right)^{A_{G,4}}$ $\psi = 1$	 $T < T_C$ $T \geq T_C$	
Specific enthalpy (kJ/kg) [Fink 1995]	$H_g = H_l + \Delta H_g$ $H_g = H_{AVG} + 0.5\,\Delta H_g$ where $\Delta H_g = 393.37\left(1 - \frac{T}{T_C}\right) + 4398.6\left(1 - \frac{T}{T_C}\right)^{0.29302}$ $H_{AVG} = 2128.4 + 0.86496 \cdot T$	$T < 2000K$ $T \geq 2000K$	V-4a V-4b
Entropy (J/kg-K) [Young 1977, Blink 1982]	$\frac{dH_z}{dT} = \frac{E - A}{T} = Nk\left[\frac{3}{2} + \ln\left(\frac{\frac{e}{N \cdot \left(h_p\sqrt{N/(2\pi k)}\right)^3} T^{1.5}}{\rho_v}\right) + \frac{1}{3}(n+4)Q \cdot (\rho_v \delta)^{n/9}\left(\frac{\epsilon}{kT}\right)^{1/3}\left(\frac{\epsilon}{kT}\right)^{1/3}\right]$ See Eq.(L-10) for the definitions of the variables, except replacing ρ_l with ρ_g.		V-5
Derivative of specific energy (J/kg-K) [Fink 1979]	$\left(\frac{de_g}{dT}\right)_{SAT} = \left(\frac{dH_g}{dT} + \frac{dH_v}{dT}\right)/mw_{Na}$ $\left(\frac{de_g}{dT}\right)_{SAT} = \frac{18.525 - 6.9936 \cdot (1-u)^{-0.6777}}{mw_{Na}}$ Where $\frac{dH_g}{dT} = 35.206 - 2 \cdot 7.0513 \times 10^{-3}T + 3 \cdot 2.5711 \times 10^{-6}T^2 + \frac{124280}{T^2}$	$T < 1644K$ $1644K \leq T \leq T_C$	V-6a V-6b V-6c

Property [reference]	Equation	Range	Equation #
	$\frac{dH_g}{dt} = \frac{4186}{T_C}(5.557012 - 0.4 \cdot 31.25992 \cdot u^{-0.6})$ $u = 1 - T/T_C$ mw_{Na} = molecular weight of sodium		V-6d
Specific heat at constant volume (J/kg-K) [Morita 1998a]	$C_V = C_{VG} - \frac{A_{G,2}(1 - A_{G,4})\psi'}{A_{G,3}} \ln(1 + A_{G,3}\rho_g) + \frac{y_B R}{1 + y_B}\left\{1 + \frac{1 - y_B}{1 + 3y_B}\left(1 - \frac{d_{G,2}}{T}\right)\right\}$ where $\psi' = \frac{A_{G,4}}{T_C}\left(\frac{T}{T_C}\right)^{A_{G,4}-1}$ $\psi' = 0$	 $T < T_C$ $T \geq T_C$	V-7
Specific heat at constant pressure (J/kg-K)	$C_P = C_V + \frac{T \cdot {\alpha_P}^2}{\rho_{gv}\beta_T}$		V-8
Volumetric thermal expansion coefficient (K^{-1}) [Fink 1979]	$\alpha_p = \alpha_{SAT}(1 - \gamma_{SAT}/\gamma_g)^{-1}$ where $\alpha_{SAT} = \left(\frac{d\rho_g}{dT}\right)_{SAT} / \rho_g$ $\gamma_{SAT} = \left(\frac{dP}{dT}\right)_{SAT}$		V-9
Thermal-pressure coefficient (MPa/K) [Fink 1995]	$\gamma_g = \left(-\frac{G_{a,1}}{T^2} + \frac{G_{a,3}}{T} + G_{a,4} - 2 \cdot e \cdot T\right) EXP\left(G_{a,1} + \frac{G_{a,2}}{T} + G_{a,3}\ln(T) + G_{a,4} \cdot T + G_{a,5} \cdot T^2\right)$ where $G_{a,1} = 8.35307, G_{a,2} = -12905.6, G_{a,3} = -0.45824, G_{a,4} = 2.0949 \times 10^{-3},$ $and\ G_{a,5} = -5.0786 \times 10^{-7}$	T < 1600K	V-10a
	$\gamma_g = \gamma_g^C - 2.5696 \times 10^{-3}\left(1 - \frac{T}{T_C}\right)^{0.5} + 3.5628 \times 10^{-5}\left(1 - \frac{T}{T_C}\right)$	T > 1600K	V-10b

Property [reference]	Equation	Range	Equation #
	Where $\gamma_g^C = 0.046893$		
Isothermal compressibility (1/Pa) [Fink 1979]	$\beta_T = \alpha_p/\gamma_g$		V-11

Table 2-3 Additional EOS Properties Modeled

Property [reference]	Equation	Range	Equation #
Critical temperature (K) [Fink 1979]	$T_C = 2509.46$		A-1
Critical density (kg/m^3) [Fink 1979]	$\rho_C = 214.1\ \mathrm{kg/m^3}$		A-2
Critical specific internal energy (J/kg)	$e_C = 4.13028 \times 10^6$		A-3
Critical temperature (K) [Fink 1979]	$T_C = 2509.46$		A-4
Specific internal energy of infinitely dilute vapor (J/kg)	$e_{liq}^{D} = 4.67732 \times 10^6$		A-5
Specific heat at constant volume for dilute vapor (J/kg-K)	$C_{VG} = 399.177$		A-6
Saturation temperature (K) as a function pressure[Morita 1998a]	$T_{SAT} = \dfrac{1}{A_{SAT,1} + \sum_{i=2}^{4} A_{SAT,i}\left(\ln(P)\right)^{i-1}}$ where $A_{SAT,i}$ = fitted constants, i = 1 to 4		A-7
Saturation temperature (K) as a function specific internal energy [Morita 1998a]	$T_{SAT} = T_{liq}\left[1 + \sum_{i=1}^{3} A_{L,i} \cdot u^i\right]$ $T_{SAT} = T_C \cdot \left[1 - A_{L,5}w^2 - A_{L,6}w^3\right]$ where $u = \left(e/e_{liq} - 1\right)$ $w = (1 - e/e_C)$ $A_{L,i}$ = fitted constants, i = 1 to 6	$e_{liq} < e \le A_{L,4}e_{liq}$ $A_{L,4}e_{liq} < e \le e_C$	A-8a A-8b
Saturation vapor pressure (Pa) [Morita 1998a]	$p_g = \exp\left[b_{L,1} + b_{L,2}T + \dfrac{b_{L,3}}{T} + b_{L,4}\ln\left(\dfrac{T}{T_C}\right)\right]$ where $b_{L,i}$ = fitted constants, i = 1 to 4 T = liquid temperature	$T \ge T_{liq}$	A-9

3 MELCOR CODE MODIFICATION AND TESTING

3.1 Code Modification

MELCOR 2.1 is modified (as Revision 5311) to add liquid metal fluid properties and EOS. A separate MELCOR branch has been created for this modification (Revision 5311).

Following the same general code modification performed by INL for the lithium fluid replacement in MELCOR [Merrill 2000], the water EOS and other property function and table lookup in MELCOR must be re-directed to the appropriate routines or tabular look-up for the sodium properties. Significant effort was made to structure the supporting code changes and input requirements for the SIMMER database and FSD database so that they were as similar as possible to simplify code maintenance requirements and user input. To activate the liquid metal capability, an unformatted file must be present in order to activate a particular fluid's equation of state for the simulation. An array of 20 (NATNAM_Eos(20)) is set up for the fluid type and an array (FILNAM(20)) is set up for each of the corresponding file name for the fluid type. The corresponding fluid type and file name are presented in Table 3-1. As shown in this table, there are unfilled slots in the array for future expansion. Without any matching filename in the working directory where the MELGEN and MELCOR input files located, the default MELCOR fluid, water will be used. Fluid 1, water as shown in Table 3-1 is for the water properties provided by the FSD data set. Fluid 20, sodium, is for the SIMMER data set. Unlike the FSD data set, there is no need to input property data files for the SIMMER data set, though a dummy file is required to designate the use of the SIMMER model in a manner consistent to the FSD formulation.

Table 3-1 Corresponding Input Filename to Fluid Identifier

Fluid Material [#]	File Name	Fluid Material	File Name	Fluid Material	File Name
H2O [1]	TPFH2O	H2 [2]	TPFH2	Li [3]	TPFLI
K [4]	TPFK	He [5]	TPFHE	N2 [6]	TPFN2
Na [7]	TPFNA[1]	NaK [8]	TPFNAK	LiPb [9]	TPFLIPB
FLIBE [10]	TPFFI	Na [20]	SIMMER[2]		

[1]Refer to FSD data set
[2]Refer to SIMMER data set

In order for MELCOR to model a fluid other than water, new subroutines for calculating the equations of state must be added. Table 3-2 shows the list of the files required to be modified to include both the FSD and SIMMER sodium data sets. In this table, a brief description is provided to include what is being changed and added to the source code. As shown in Table 3-2, the majority of the files modified resided in the EOS package of the MELCOR source. The major change were in module M_H2O, where the transport property routines of the FSD data and initialization of the working fluid, other than the standard MELCOR water is done.

A number of new files are included in MELCOR, as shown in Table 3-3. As shown in this table, the new files are color coded to identify which database these files belong to. For the FSD data

set, the module FSD_EOS contains many routines and functions that account for the property data, in addition to those thermodynamic data that are provided in the input data file (see Section 2.1 for the details of the NaLibrary program). For the SIMMER data set, both NALIQUID and NAVAPOR modules contain the majority of the property correlations (see Section 2.2).

Table 3-2 MELCOR Files Modified

Package/File Name	Description
COR/COR_CORABS [s]	Call TH2O_VAPOREMISS for the vapor emissivity of the fluid
CVH/CVH_GenerateDB [s]	Add use statement of M_MFLDATA and M_MFLBLS in various subroutines to allow diagnostic messages, redefine saturation temperature of the fluid by adding 100 to triple point of the fluid
CVH/CVH_CVHDBE [s]	Provide fluid name to outputs
CVH/THYDR_FLCOK[s]	Add multi-fluid model, and define Henery-Fauske Subcooled pool routine (GCSUB) for the FSD property model.
CVH/THYDR_FLCOK_NEWMODEL [s]	Add multi-fluid model, and define Henery-Fauske Subcooled pool routine (GCSUB) for the FSD property model.
EOS/THYDR_CVTHRM[s]	Add RHOL values for different fluids – multi-fluid model
EOS/EOS_CVTNEQ[s]	Add variable H2OPHX, and other variables for multi-fluid capability
EOS/EOS_CVTNQE[m]	Add variable H2OPHX, and other variables for multi-fluid capability
EOS/CVH_CVTSAT[m]	Redefine PMAX1,PMIN1,TMIN for multi-fluid properties
EOS/TEOS_CVTSVE[s]	Add variable H2OPH as passing variable, and other variables for multi-fluid capability
EOS/CVH_CVTWGE[m]	Add variable H2OPHX, and other variables for multi-fluid capability
EOS/H2O_H2ODBE[s]	Minor change to H2O package call summary to output
EOS/TH2O_H2OEPT[s]	Add multi-fluid capability to allow single phase properties return, in addition to water
EOS/TH2O_H2OEST[s]	Add multi-fluid capability to allow the determination of the thermodynamic state of the fluid
EOS/TH2O_H2OESU[s]	Redefine RU variable for fluid other than water
EOS/TH2O_H2OSAT[s]	Add multi-fluid capability to allow the determination of the saturation properties of fluid, in addition to water
ESF/TCND_CVTWGE[s]	Add variable H2OPHX, and other variables for multi-fluid capability
EXEC/MEG_RW	Add call to INIT_MFLUIDS[s] for the multi-fluid capability to PREPARETOINPUT[s], and add multi-fluid capability in other routines in this file.
EXEC/EXEC_MXXPBD[s]	Add call to INIT_MFLUIDS[s] for the multi-fluid capability
FP/FP_PLOTMANAGER[s]	Add plotting variables for multi-fluid for the FP Package
HS/THS_HSBOIL[s]	Add the call to TH2O_SURFTENSION[f] for the multi-fluid capability
HS/THS_HSCNDS[s]	Add the call to TH2O_SURFTENSION[f] for the multi-fluid capability
HS/THS_HSDMTC[s]	Add pass variable DIFFUS for the mass transfer coefficient calculations – multi-fluid, in addition to water
HS/THS_HSLHX[s]	Add call to TH2O_SURFTENSION[f] for multi-fluid capability
HS/THS_HSTRAN[s]	Add multi-fluid option key, use M_MFLBLS[m], FSD parameters, mass transfer calculations for other fluids other than water.
M_ARGUMENTS[m]	Add USENQE = 0 from M_H2O[m] for the multi-fluid capability
M_CONST[m]	Modified variable constants (mainly for critical conditions) for the multi-fluid capability
M_EXECRTN[m]	Modified the use statement for M_ARGUMENT[m] usage
M_H2O [m]	Add multi-fluid option key, and add use statement for M_MFLDATA, M_MFTBLS. Modifications to a number subroutines/functions in the module to add functionality of the multi-fluid capability: TH2O_H2O1PH[s], TH2O_H2O1PH[s], TH2O_SPECIFICVOL[f], TH2O_WATERHEATCONDUCT[f], TH2O_WATERVISC[f], TH2O_SURFTENSION[f], tH2O_WATERSATTEMP[f], TH2O_VAPOREMISS[f], TH2O_VAPORCOMPRESS[f], TH2O_VAPORCP[f], TH2O_VAPORHEAT[f], TEOS_H2O2PL[s], INIT_MFLUIDS[s] and FLUIDEOS[s]. INIT_MFLUID allows the selection of the fluid data set (nfluid=0, standard MELCOR fluid is used; nfluid=20, use SIMMER sodium data set; and else use FSD data set that could be more than sodium). FLUIDEOS is only used for the FSD data set.
M_H2OD1[m], M_H2OD2 [m], M_H2OD3[m],	Replace minor Fortran directive

M_H2OD4[m]	
M_H2O_VARS[m]	A module contains water data moved from original M_H2O module.
M_NCG[m]	Add multi-fluid check and related changes, including M_MFTBLS and M_MFLDATA use statements. Add "use FSD_EOS" statement and other calls to tNCG_GetHeatConduct[f], tNCG_GetVisc[f], and tNCG_DefProps[f],
RN1_ENTRAINMENT[s]	Add multi-fluid model, replacing surface tension correlation with a call to tH2O_SurfTension[f]
RN1_RN1HYG[s]	Add multi-fluid model, replacing surface tension correlation with a call to tH2O_SurfTension[f]
RN2_RN2DFP[s]	Add multi-fluid model, replacing surface tension correlation with a call to tH2O_SurfTension[f]

Table 3-3 New MELCOR Files

File Name*	Description
M_H2O_VARS[m]	A module that contains data sets from the original M_H2O module. It utilizes M_MFLDATA [m] and M_MFTLS[m], and re-do minor FORTRAN directories.
M_MFLDATA [m]	A module to deal with multiply fluid properties. Define MATNAM_Eos array to hold the name of the fluid, and the corresponding FILNAM array for each fluid defined. A number of empty slots can be filled for future development.
M_MFTBLS[m]	Set up the multi-fluid variables and identify the number of fluids, and data size for mainly the INL data usage.
M_Na[m]	A module to deal with sodium properties from BRISC: NA1PH[s], NA2PD[s], NA_INITTABLES[s], and NA2PL[s].
M_STCOM [m]	Replace common block STCOM that FSD_EOS shared
M_STD2XC [m]	Replace common block STD2XC that FSD_EOS shared
M_STH2XC[m]	Replace common block STH2XC that FSD_EOS shared
NA1[m]	A module for thermodynamic properties of sodium: P_VAPOR[f], DPDR_VAPOR[f], PV_NA[f], DPRHO[f], DPTEMP[f], EVAPFUN[f], CVVAPFUN[f], TEMPDENSATL[f], CUBIC[s], DTDP[f], DVDP[f], DRHOVDT_SAT[f], DRHOLDT[f], and DPDVL[f].
NAEOS[m]	A module that deals with critical, saturation and other thermal related properties for sodium. This module contains a number of functions: PSATFUN[f], DPDTSATL[f], GAMMA_SAT[f], TSAT33[f] and TSATP[f]. It is used by NALIQUID and NAVAPOR modules.
NALIQUID[m]	A module describes densities, heat capacity and other thermodynamic properties for liquid sodium. This module contains a number of functions that are function of temperature: DENL[f], CV_LIQ[f], ALPHA_LIQ[f], CP_LIQ[f], ALPHA_SAT[f], DRHOLDT_SAT_ANALYTIC[f], ENTHL[f], ENTHLOLD[f], ENTHLNEW[f], ENTHLINV[f], DENTH_LIQUID[f], CSAT_L[f], SLIQUID[f], DELDT_SAT_ARGONNE[f], BETA_T[f], BETA_S[f], DPR_LIQ[f] and DPT_LIQ[f].
NAVAPOR[m]	A module describes densities, heat capacity and other thermodynamic properties for vapor sodium. This module contains a number of functions that are function of temperature: CV_VAP[f], DENV[f], ENTHV[f], ALPHA_SATV[f], DVGDT_SAT2[f], DRGDT_SAT[f], BETA_T_VAP[f], ALPHAP[f], GAMMA_V[f], GAMMA_V_1600[f], SVAPOR[f], VS[f], DP_VAPOR_DT[f], DP_VAPOR_DV[f], DEVDT_SAT_ARGONNE[f], DH_NA_V[f], H_NA_L[f], HVAP_NA[f], H_NA_AVG[f], H_NA_V[f], CSAT_V[f], DP_VAPOR_DR[f], CP_VAP[f] and DPT_VAP[f].
FSD_EOS [m]	A main module for the INL data set. It contains a number of routines and functions that are used for the multi-fluid capability. ICMPNX [s] provides access through input data file. ICMPNXSIMMER [s] provides access few data in the routine. STREAD routine reads and initializes the data tables. Water property routines include STH2XL, STH2X3, STH2X4, STRTP, STRSAT, STRPX and STRX. Non-water property routines include STUPX4 and STRPX. Other specified routines are: SURFTN-surface tension, THCOND-thermal conductivity, VISCOS-dynamic viscosity, and GCSUB-critical mass flux for a given fluid.

*The bracket next to each file indicates: m = module, s = subroutine and f = function
**Red colored file is for FSD data set and Blue colored file is for SIMMER data set.

Table 3-4 New Control Functions Defined for the Working Fluid

Control Function Parameter	Description
CVH-CVP(NameCV)	Specific heat at constant volume for liquid in control volume NameCV (units = J/kg/K)
CVH-CPP(NameCV)	Specific heat at constant pressure for liquid in control volume NameCV (units = J/kg/K)
CVH-CVA(NameCV)	Specific heat at constant volume for vapor in control volume NameCV (units = J/kg/K)
CVH-CPA(NameCV)	Specific heat at constant pressure for vapor in control volume NameCV (units = J/kg/K)
CVH-BETATP(NameCV)	Isothermal compressibility for liquid in control volume NameCV (units = 1/Pa)
CVH-BETATA(NameCV)	Isothermal compressibility for vapor in control volume NameCV (units = 1/Pa)
CVH-SP(NameCV)	Specific entropy for liquid in control volume NameCV (units= J/kg)
CVH-SA(NameCV)	Specific entropy for vapor in control volume NameCV (units = J/kg)
CVH-ALPHAA(NameCV)	Volumetric thermal expansion for vapor in control volume NameCV (units = 1/K)
CVH-ALPHAP(NameCV)	Volumetric thermal expansion for liquid in control volume NameCV (units = 1/K)
CVH-THCP(NameCV)	Thermal conductivity for liquid in control volume NameCV (units = W/m-K)
CVH-THCA(NameCV)	Thermal conductivity for vapor in control volume NameCV (units = W/m-K)
CVH-VISCP(NameCV)	Viscosity for liquid in control volume NameCV (units = Pa-s)
CVH-VISCA(NameCV)	Viscosity for vapor in control volume NameCV (units = Pa-s)

3.2 Preliminary Testing and Results

To support the developmental phase of the liquid metal property implementation, a set of three simple test problems were created. Each test was selected to test the model implemented, except the first test which is to ensure the water property has not be altered for the LWR application:

(a) Water test to demonstrate that liquid metal properties implemented would not affect the current water properties modeled when liquid metal is not invoked
(b) Sodium SIMMER (BRISC) test – Testing the sodium properties in SIMMER and SAS4A database.
(c) Sodium FSD test – testing the sodium properties in FSD database. Note that much of the thermodynamic properties are generated using the NaLibrary program.

Except the first test, the comparison to the second and third tests is done by using tabular data and correlations from various sources and codes.

A simple test problem which contains a single test volume with a working fluid (water or sodium) in a closed system is subjected to external enthalpy sources. This test is particularly challenging because it covers a very broad range of test conditions extending from very low pressure near freezing point to near critical pressures. Although the test problem did not run to completion for all three cases due to small time steps, the resulting plots from these runs demonstrate that the addition of working fluid other than water is possible for MELCOR. Note that this test problem was created to test the extreme conditions of the fluid properties. In the future, a refinement of the test problem will be done to represent the physical conditions encountered in severe accident situations.

3.2.1 Water Test Case

A test problem was created to ensure that the default water properties have not been modified. This test problem was terminated by MELCOR at about 1.7×10^4 seconds due to a very small subcycle timestep due to the reach of the supercritical conditions for water. Despite this issue, the results of this water test problem are presented in the plots given below. As indicated before, the thermodynamic condition of the test problem is at saturation. Figure 3-1 shows the water mass as a function of time. As the control volume heats up, the liquid mass decreases while the vapor mass increases. Figure 3-2 plots the pool and atmosphere entropies. Figure 3-3 plots the pressure versus temperature for the problem. As indicated in this figure, MELCOR predicts the saturation temperature up to the point near the supercritical temperature before the code was terminated. Thus this problem is to test the extreme conditions of the coolant properties.

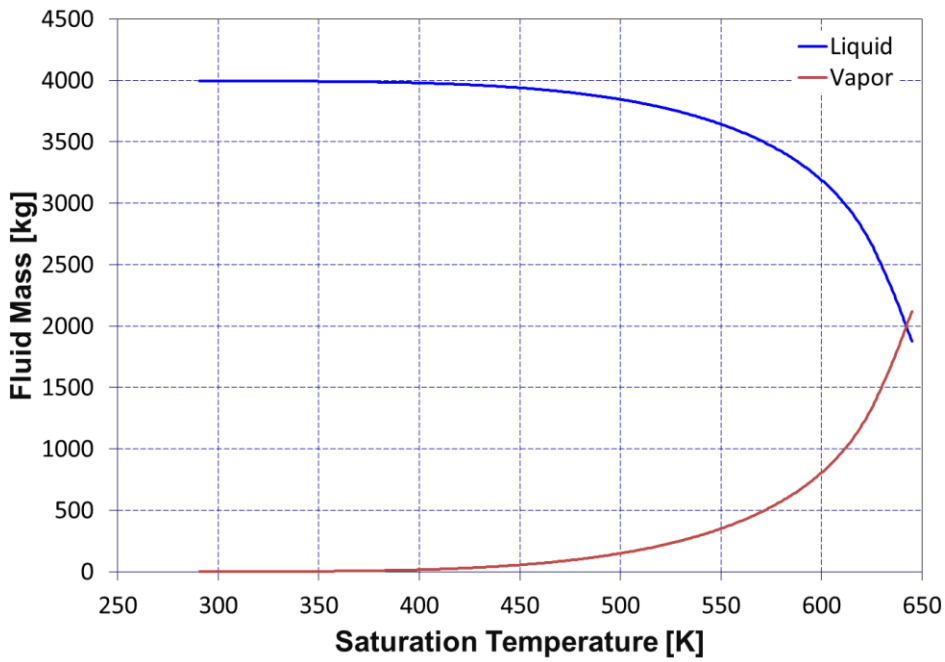

Figure 3-1 Calculated Water Mass in Problem

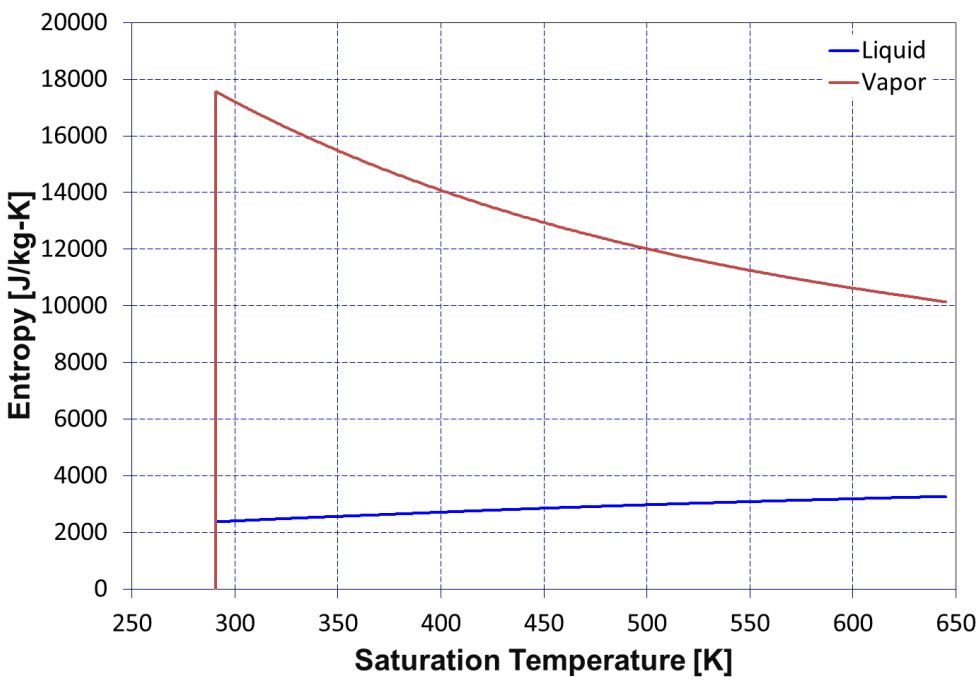

Figure 3-2 Entropy versus Saturation Temperatures

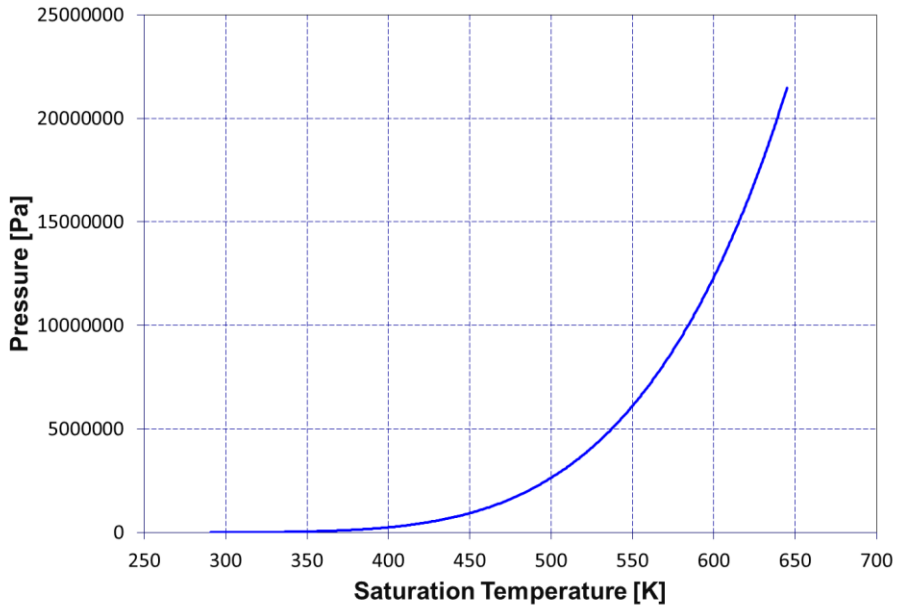

Figure 3-3 Pressure versus Temperature

3.2.2 Sodium

The implementation of the EOS and other thermophysical properties of sodium for the SIMMER/SAS4A and FSD data sets were tested with the previously described test problem. Note that original SIMMER/SAS4A input was aborted ungracefully at about 3×10^4 seconds. It was thought that the rate of enthalpy sources introduced was too large. So, it was scaled down from 4×10^5 J/kg to 1×10^5 J/kg at a specific time interval. The following figures show the results of the revised input for the SIMMER/SAS4A dataset as indicated as SIMMER, although the run was continued beyond 3.8×10^4 seconds, but at a very small timestep of 10^{-7} second. Figure 3-4 shows the sodium mass versus saturation temperatures. As the temperature increases, the sodium liquid vaporizes as shown in this figure. The corresponding entropies for the liquid and vapor sodium are shown in Figure 3-5. The pressure-temperature plot is given in Figure 3-6. The third test was conducted for the FSD data set. Figure 3-7 shows the sodium mass versus saturation temperature for this data set. This test was stopped much earlier than the test problem for the SIMMER/SAS4A data set. Figure 3-8 shows the entropy versus temperature for the FSD data set while Figure 3-9 plots the pressure as a function of the saturation temperature.

To benchmark the implemented sodium properties for both the SIMMER/SAS4A and FSD data sets, comparisons to the existing tabular data available from various SIMMER/SAS4A sources [Fink 1979 and Fink 1995] and FSD sources from equations given in this report and those correlations documented in the NaLibrary Program. The rest of the plots shown in this section contain comparison data from various references, denoted as symbols with MELCOR calculated values, denoted as line curves. Figure 3-10 plots the saturation temperature-pressure curves with the comparison of the available data from various references. As shown in this figure, calculated values for both data sets match closely with the references. As indicated earlier, both FSD and SIMMER/SAS4A runs were stopped before the end of the problem. For the FSD test case, it

stops at a saturation temperature of about 1500 K and 1×10^6 Pa pressure as shown in this figure. On the other hand, the SIMMER test case runs to about 2500 K saturation temperature and 2.2×10^7 Pa pressure. Figure 3-11 presents the density versus temperatures. As shown in this figure, the calculated densities for both liquid and vapor follow similarly with the reference values; however, the liquid density calculated for the SIMMER data set contains more oscillations at low temperatures than that of FSD data set, and suddenly drops from 800 K to 1000 K. These oscillations and sudden drops need to be reviewed, as a potential issue in MELCOR. Figure 3-12 shows the same plots as in Figure 3-11, except the SIMMER data was generated using the original SIMMER input with higher enthalpy sources (4×10^5 J/kg, instead of 1×10^5 J/kg). As indicated in Figure 3-12, there is no sudden drop from 800 K to 1000K as seen in Figure 3-11 for the SIMMER data set. This illustrates that there is still a lot of refinement of the property routines developed for this data set, particularly relating to the liquid density. In terms of the liquid specific heat, both Figure 3-13 and Figure 3-14 plot this property at constant pressure and volume, respectively. These variables are particularly important in determining the stability of transient conditions. As shown in these figures, the calculated SIMMER data set closely matches to the reference values. Both Figure 3-15 and Figure 3-16 show the vapor specific heat at constant pressure and volume, respectively. As shown in these figures, the calculated SIMMER data matches closely at lower temperatures. At high temperatures, MELCOR underestimates these properties for the SIMMER/SAS4A data set. The calculated MELCOR FSD data do not match to the SIMMER reference at all. The primary reason for this is because of the soft-sphere model for the FSD vapor specific heat correlation where the differentiation of the Helmholz free energy [Young 1977, Blink 1979] may not be suitable for low pressure and temperature conditions.

In terms of transport properties, Figure 3-17 and Figure 3-18 show the viscosity and thermal conductivity curves, respectively. As shown in these figures, MELCOR calculated values are closely matched to the references.

For further analysis of the implemented SIMMER/SAS4A data set in MELCOR, the next three plots (Figure 3-19, Figure 3-20 and Figure 3-21) for isothermal compressibility, volumetric thermal expansion, and heat of vaporization, respectively. As shown in Figure 3-19, MELCOR predicts closely with the reference values. Similarly MELCOR predicts closely for the volumetric thermal expansion, except at lower temperatures. For the heat of vaporization, MELCOR calculated values are closely matched at lower temperatures, but slightly underestimate the values at higher temperatures.

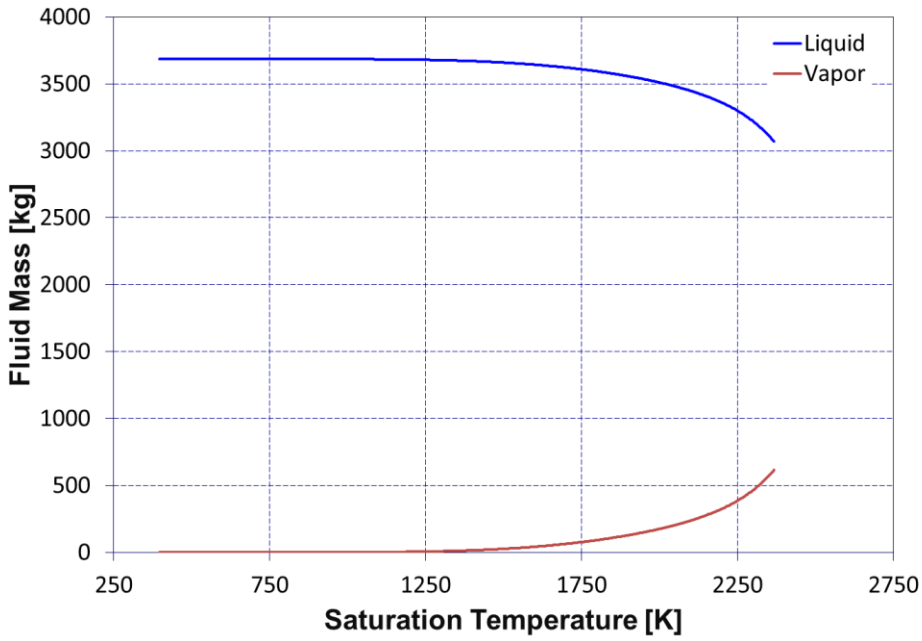

Figure 3-4 Fluid Mass versus Temperature for the SIMMER/SAS4A Database

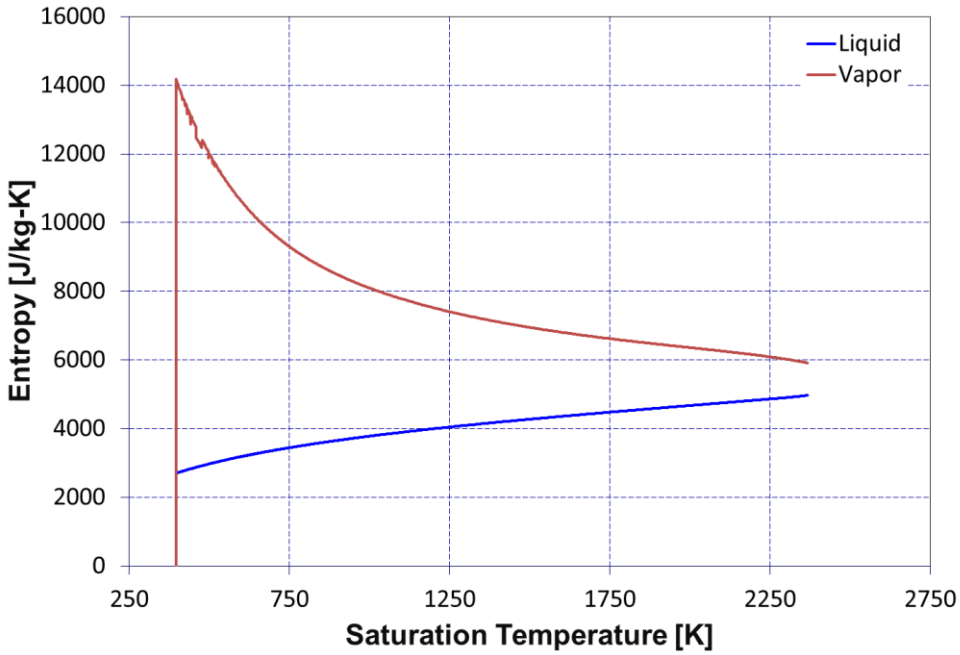

Figure 3-5 Entropy versus Temperature for the SIMMER/SAS4A Database

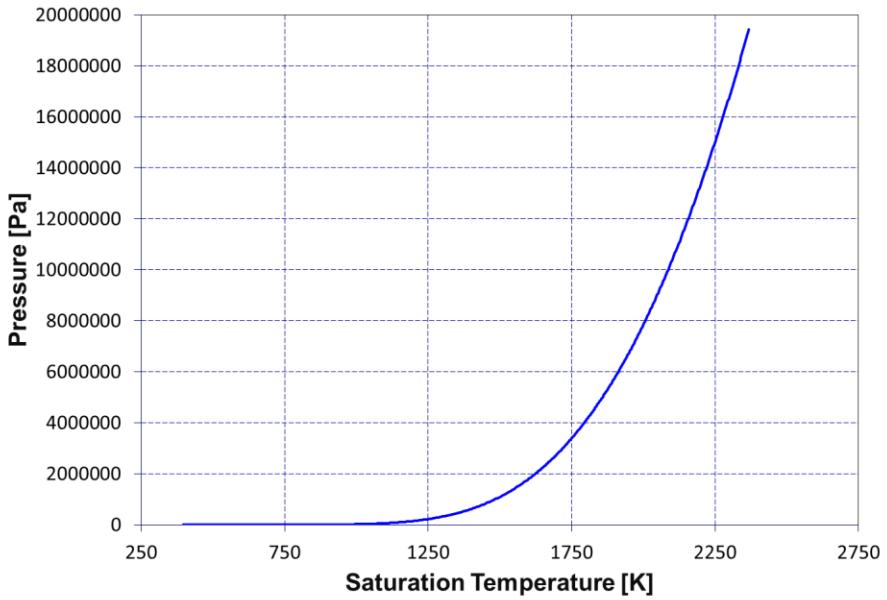

Figure 3-6 Pressure versus Temperature for the SIMMER/SAS4A Database

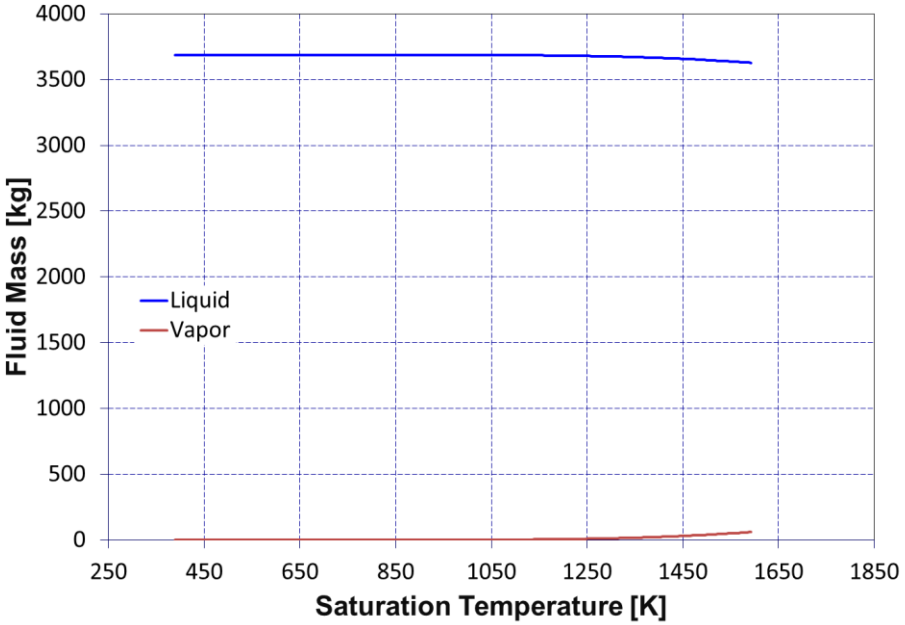

Figure 3-7 Fluid Mass versus Temperature for the FSD Database

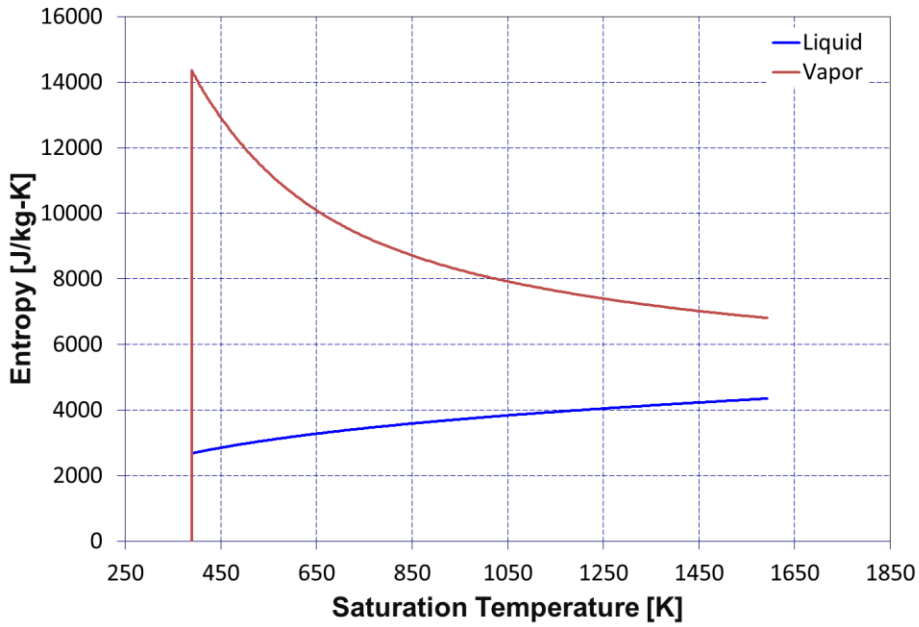

Figure 3-8 Entropy versus Temperature for the FSD Database

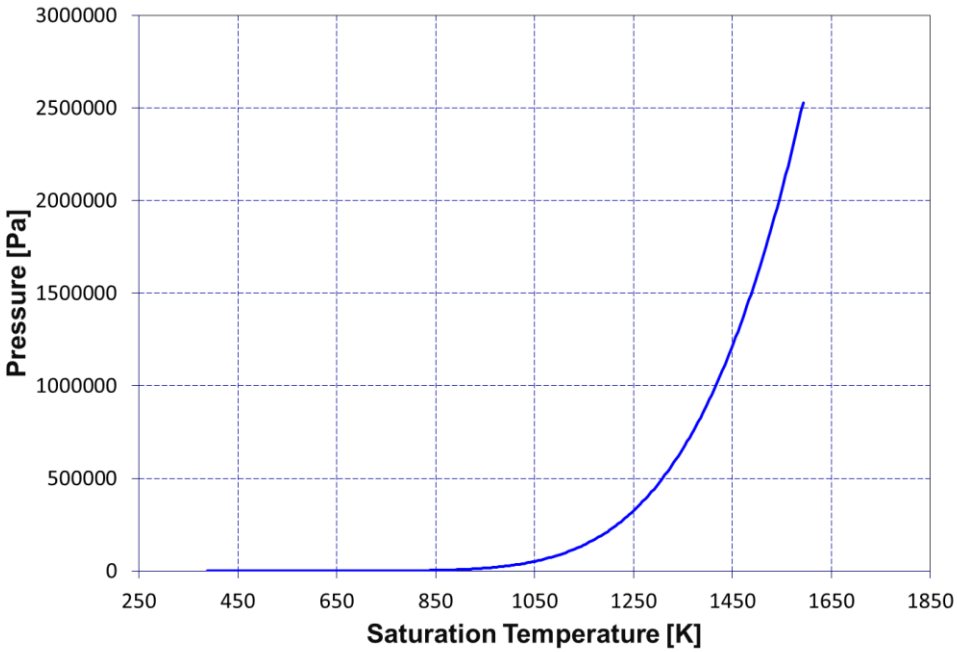

Figure 3-9 Pressure versus Temperature for the FSD Database

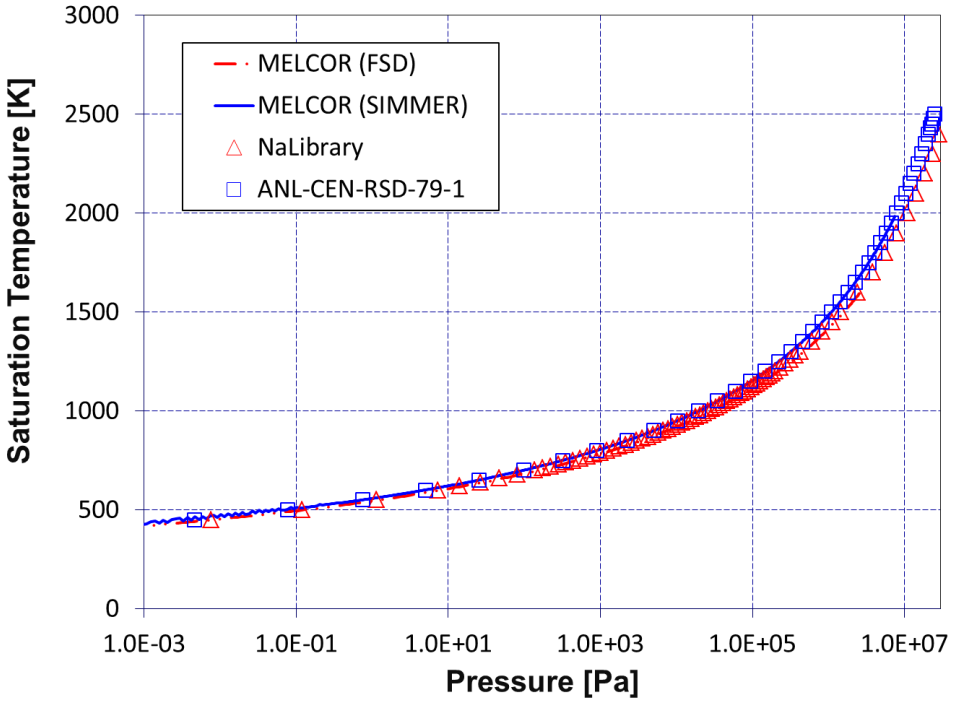

Figure 3-10 Saturation Temperature versus Pressure

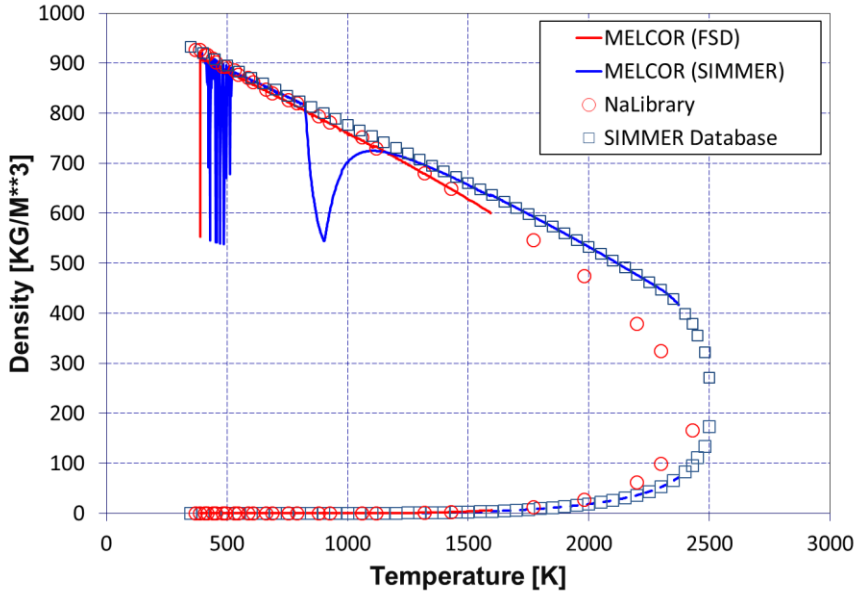

Figure 3-11 Density versus Temperature

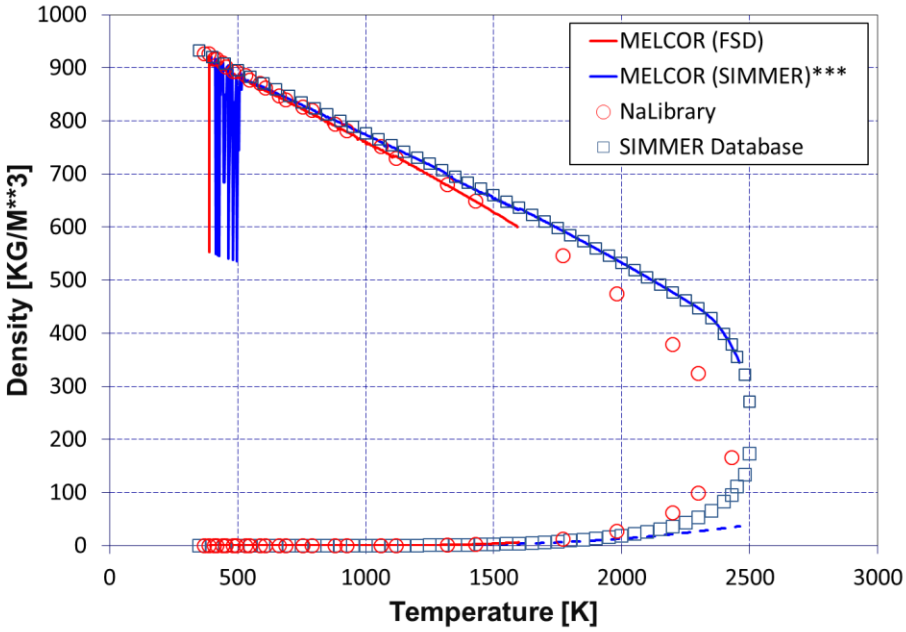

Figure 3-12 Density versus Temperature ***Input with a higher enthalpy source for the SIMMER/SAS4A case.

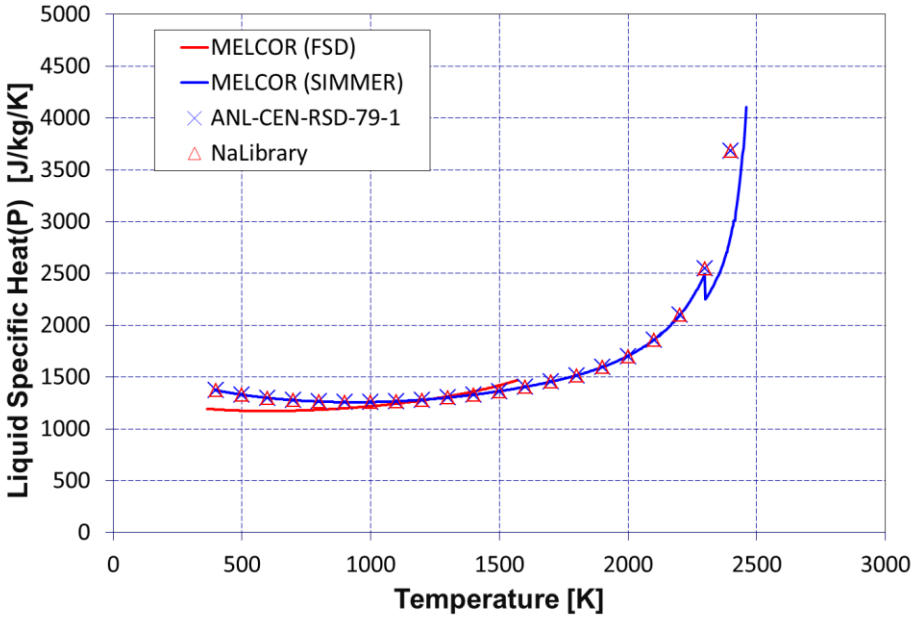

Figure 3-13 Liquid Specific Heat at Constant Pressure

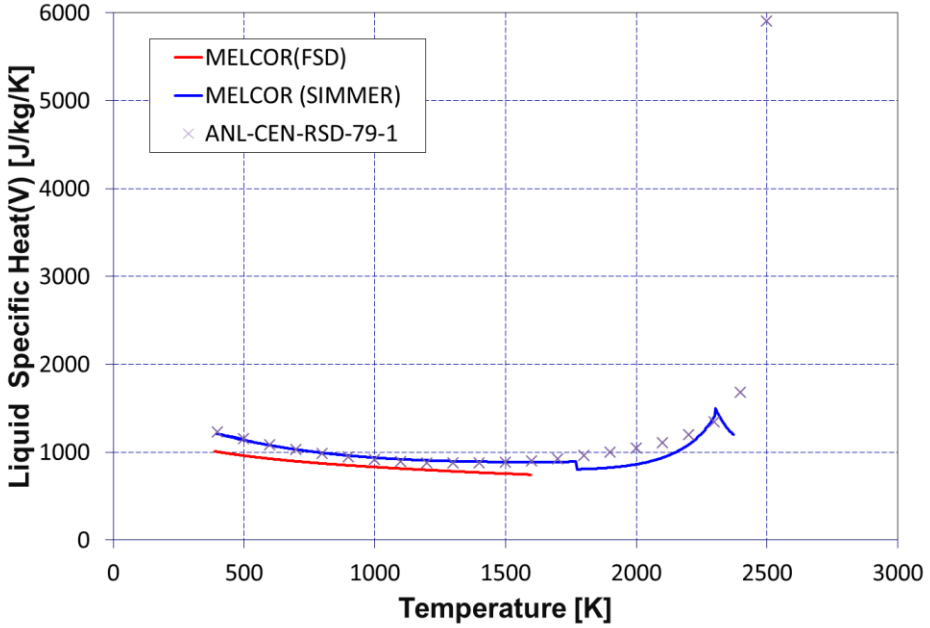

Figure 3-14 Liquid Specific Heat at Constant Volume

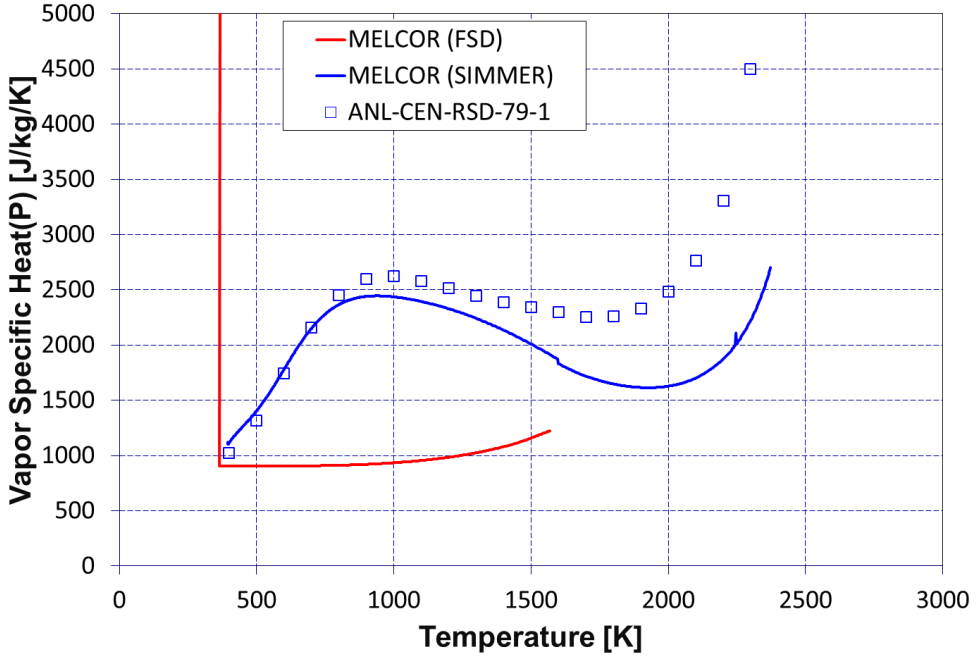

Figure 3-15 Vapor Specific Heat at Constant Pressure

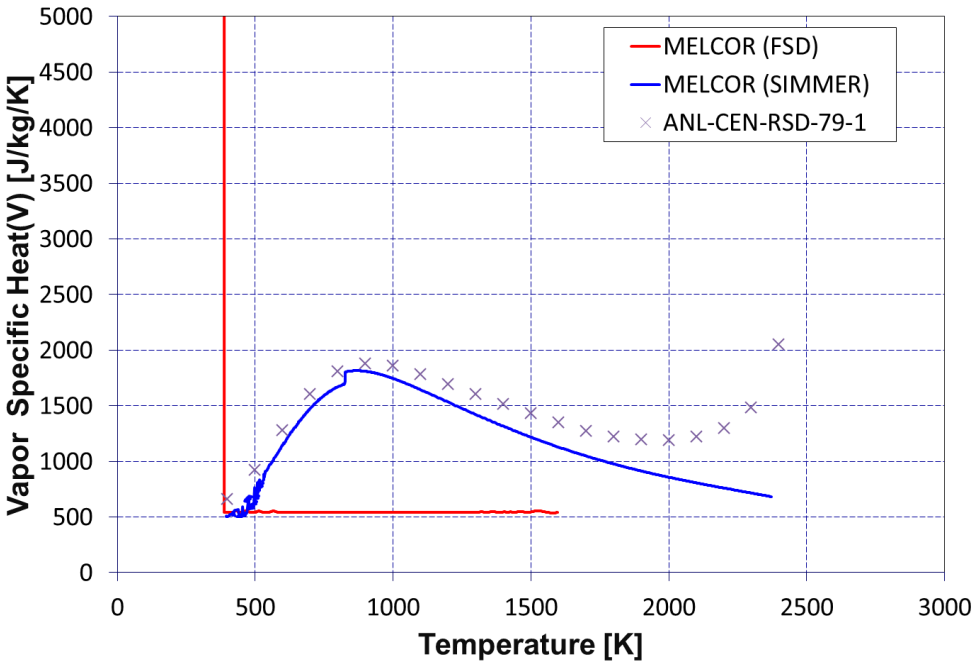

Figure 3-16 Vapor Specific Heat at Constant Volume

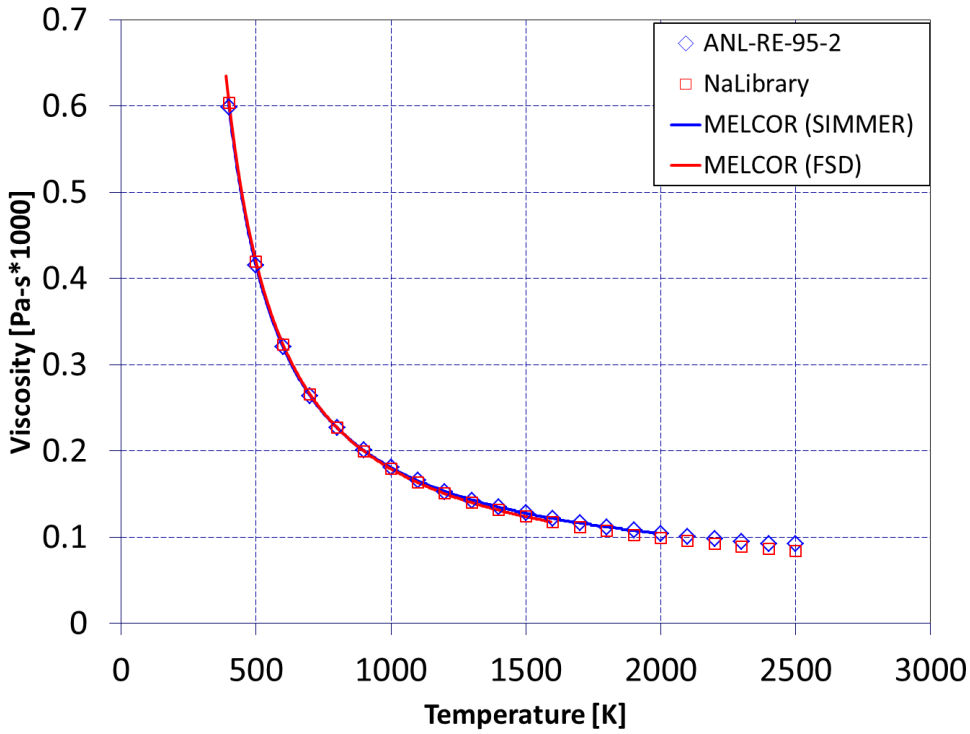

Figure 3-17 Viscosity

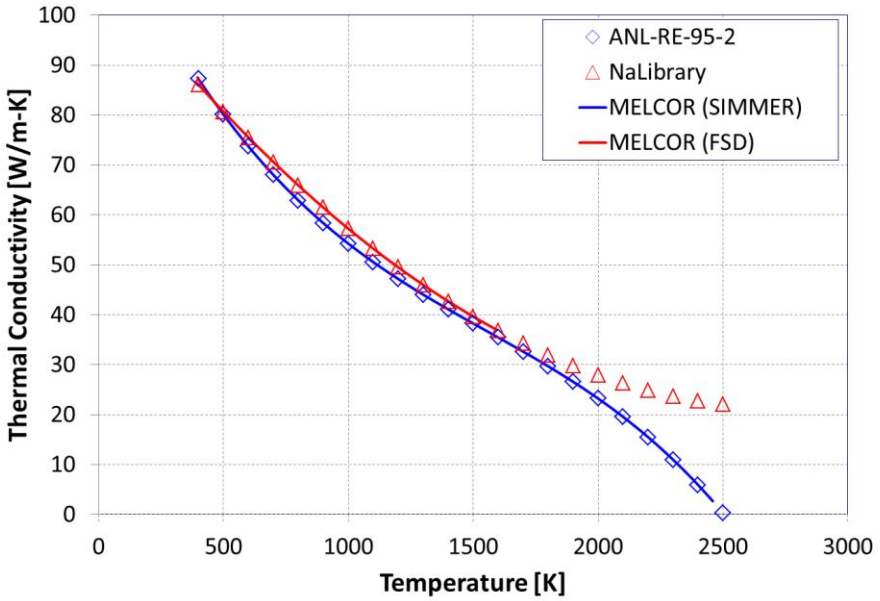

Figure 3-18 Thermal Conductivity

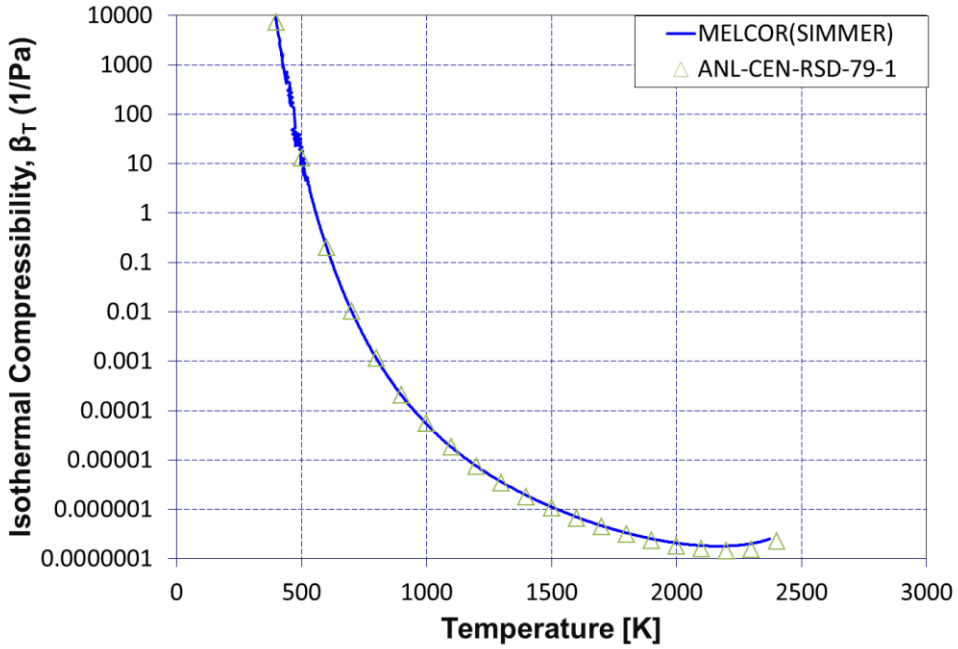

Figure 3-19 Isothermal Compressibility

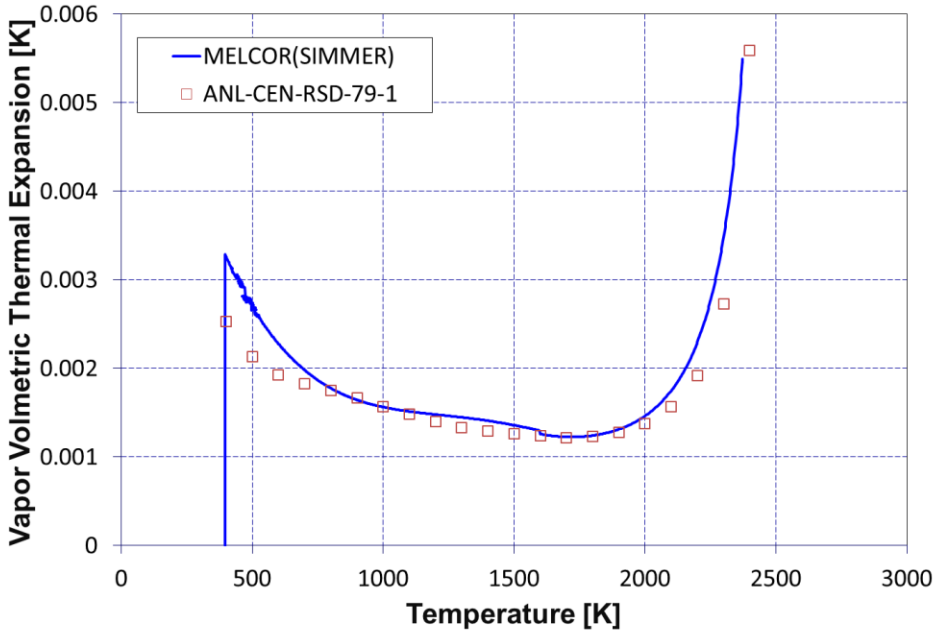

Figure 3-20 Volumetric Thermal Expansion

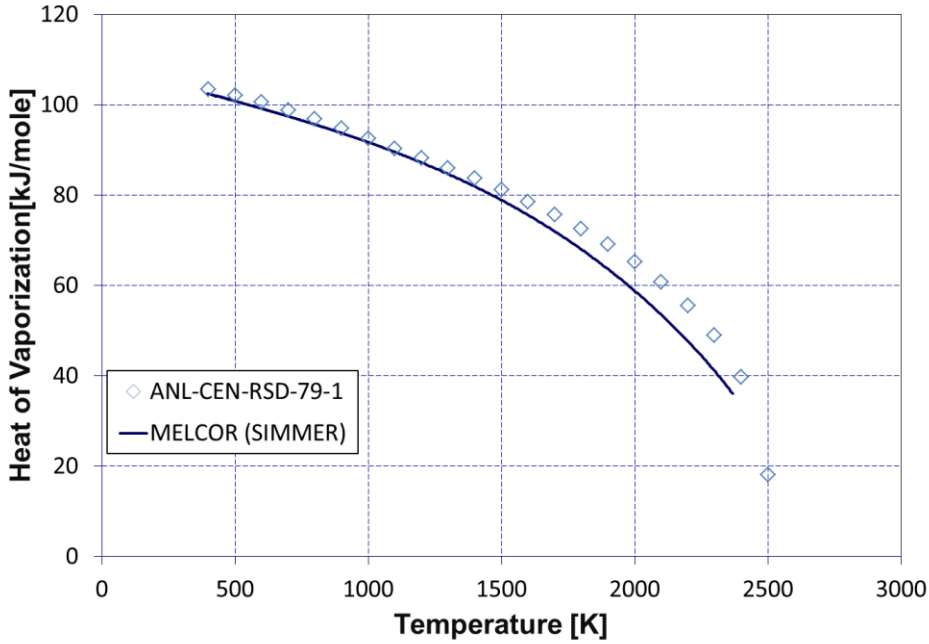

Figure 3-21 Calculated Heat of Vaporization

3.2.3 Discussion

The results of these tests, as described in more detail in the previous section, demonstrate that these models are able to reproduce the thermophysical properties upon which they are based over a wide range of conditions. However, there are still improvements that must be made to improve code numeric at both high and low saturation pressures. Also, currently the SIMMER models appear to perform better at high pressure whereas the FSD models perform better at low pressure.

The test results also indicate that additional refinements will be necessary to ensure that the properties MELCOR calculated for either data sets (FSD or SIMMER/SAS4A) are numerically stable over the full range of liquid states, particularly when iterations are required. As mentioned before test cases presented here did not run to completion. In one case when a higher enthalpy source was used, MELCOR aborted ungracefully. The small time step in the order of 10^{-7} s is also unacceptable. Therefore, further evaluations of the correlations selected as shown in Chapter 2 (see Table 2-1 to Table 2-3) are necessary for the SIMMER/SAS4A data set. Also it is necessary to ensure that the variables passed (mainly the temperature) are correctly used as intended for the property functions. The range of the correlations implemented requires a close examination of out-of-range issue, which may yield unrealistic results. Error trapping is required to ensure that extrapolation outside the valid range includes error messages or remediation. The current iteration scheme used for the water properties may be examined to ensure that it is valid for evaluating fluid other than water.

Additional test problems may be required to test out each of the implemented property correlations, particularly for different packages of the MELCOR code, for example, condensation and vaporization on heat structures (HS Package) and aerosols (RN Package).

As a part of follow-on activity, a comparison of the FSD and SIMMER/SAS4A data set should be performed to identify any difference between the two data sets. For example, to explain the difference in the vapor specific heat calculation, Figure 3-15 and Figure 3-16 are provided.

4 CONTAIN UPGRADE

This chapter documents the code changes and upgrades that are necessary to bring CONTAIN 2 [Murata 1997] and CONTAIN-LMR [Murata 1993] codes to modern Software Quality Assurance practices as used in MELCOR code development environment currently employed. Both CONTAIN codes were developed in FORTRAN 77 or early versions of the compilers with the designation of older computer platforms, such as CRAY, CDC, and UNIX. Much of the system interfaces to these older computer platforms must be altered to adapt the current development environment.

CONTAIN 2 is the latest version of CONTAIN that was developed before the development work was completely stopped. Although CONTAIN 2 is designed for the LWR applications, it does contain many of the sodium models as described in Chapter 5, such as sodium pool fire model, atmospheric chemistry model and sodium spray fire model. To enhance CONTAIN 2 to include all models in CONTAIN-LMR, several routines and interfaces must be built.

The CONTAIN-LMR source code used for this work was originated from Power Reactor and Nuclear Fuel Development Corporation (PNC) of Japan. It is believed that this version of code was the first version the PNC received from SNL, and might have been modified by PNC. However, many of the sodium models are similarly found in SAND91-1490 [Murata 1993]. In addition, this first version of CONTAIN-LMR may not have many latest physics models introduced in comparison to CONTAIN 2, which was the last version of the CONTAIN to be developed. The source code was received as a single file, which was difficult to debug and modify. File splitting was used to separate individual files into a file for a subroutine, function or small set into individual files. Figure 4-1shows the top calling sequence of CONTAIN-LMR, where many of the sodium models were identified. As shown in this figure, the sodium models identified include those in the atmosphere calling routines as well as for the lower cell calling routines.

Figure 4-1. Top Level Call Sequence of CONTAIN-LMR.

```
Program main
{
        call input

        call contrl
}

subroutine input
{
        call setma [define the particular machine]
        call timdat [call system time and date]
        call gloset [initialize global common blocks]
        call redef [call restart and redefine parameters through inputs]
        call cpusnd [call cpu time and time]

        call iglobl [read global variable inputs]

        call celset [cell level setup]
        call icell [read cell level variable inputs]
}

subroutine contrl
{
        call output
        call cpusnd
```

```
        call chozdt [first step is determined]
        call glrest [set global parameters]
             call zero to zero out all arrays

        call clcntr [cell level main controls]
        call glcntr [global level main controls]

        call output
}

subroutine clcntr [it is looping over all cells]
{
        call nxtcel [next cell information]
        call setgas [reset gas properties]
        call celldt [choose time step]
        call clrest [reset atmosphere quantities and deposition cals]

        call rhcntr [control routine for radiative HT]
        call rbcntr [lower cell controls] - since this routine does not pass ncell, so it must be
                                            explicit declared
             call phydt [allocate timestep for lower-cell physics]
             call atmlcr [heat transfer from lower-cell to atmosphere/structure]
             call laysrc [lower cell explicit source]
             call bctset [set B.C. for lower cells]
             call concrm [SLAM model and other CORCON models] - this routine calls:
             {
                       call slinpt [initialize boundary layer, SLAM chemistry data, concrete
                                       regions] - this routine calls:
                       {
                              call slchem [read chemical reaction data]
                              call concpt [detemines concrete array pointers]
                              call slcoor [initialize SLAM coordine system]
                              call tranb [store concrete storage array, ch()]
                       }
                       call trana [loads storage array for the concrete calculations]
                       call stime [determine timestep for this model]
                       call slam [physics of the sodium-concrete interactions] - this routine
                                                   calls:
                       {
                                       call coneqs [estimate water release and HT calculations for
                                                   the interactions]
                                       call natcon [calculates SLAM physics]
                                       call wtrrls [calculates water release]

                       }
                       call tranb [loads concrete storage array, ch()]
                       call tranc [transports mass and energy of SLAM]
                  }
             call pfire [sodium pool fire model]
             call pmhxfr [computer heat/mass transfer between pool and atmosphere]
             call htset [interlayer heat transfer coefficients]
             call fpheat [compute fission product heating to layers]
             call tabhet [load volumetric heat source arrays]
             call hxlow [compute conduction and heat transfer among lower cell layers]
             call concre [load physics of concrete layers]
             call interm [load physics of interm layers]
             call pool [load physics of pool]
             call atmosp [load physics of atmosphere layers] -currently there is no coding in
                                                             this routine
             once the layers are done
                  call cvtoat [process cavity physics]
                  call bctset [set B.C. for lower cell for radiation HT]

        call ccntrl [atmospheric control routine] - this routine calls following:
        {
                 call soratm [atmospheric external source]
                 call engctl [call engineered systems]
                 call soratm [fission product atmospheric source]
                 call fpsurf [calculate HT for FPs to/from structures]
                 call chemrx [sodium atmosphere chemistry models]
                      *** reaction: na + h2o => naoh + 0.5 h2
```

```
                    call chmrep [aerosol or within aerosol deposit and condensable film]
                    *** reaction: 2*na + h2o => na2o + h2
                    call chmgas [reaction with gases]
                    call chmaer [reaction of aerosols and gases -h2o]
                    call chmaer [reaction of aerosols and gases -sodium]
                    call chmdep [reaction of deposits and film with gases]
                    *** reaction: 2*na + (1-0.5x)*o2 => x*na2o + (1-0.5x)*na2o2
                    call chmgas [reaction with gases]
                    call chmaer [reaction of aerosols and gases]
                    call chmdep [reaction of deposits and film with gases]
                    *** reaction: na2o2 + 2*na => 2*na2o
                    call chmrep
                    call chmaer
                    call chmdep
                    *** reaction: na2o + h2o => 2*naoh
                    call chmrep
                    call chmaer
                    call chmdep
                    *** reaction: na2o2 + h2o => 2*naoh + 0.5*o2
                    call chmrep
                    call chmaer
                    call chmdep
                call hburn [burn models]
                call qxlos [calculate heat structure temperatures]
                call spray [sodium spray model]
                    call sorspr [sodium spray external sources]
                    call velt [calculate terminal velocity of spray droplets]
        }

        call sor [sources]
        call hotemp [set host temperature in atmosphere]
        call savcel [store cell information]
}

subroutine glcntr
{
        call acntrl [aerosol control] - this routine calls the following:
        {
                call aersl [aerosol physic calculation]
        }
        call dchbin [process DCH bins]
        call trpflw [calculates gas and debris velocities]
        call webdrp [calulcates the mass distribution for debris drop]
        call rpv [main routine for RPV DCH models]
        call entfra [user defined fraction for debris dispersion]
        call entrat [entranment rate models for debris]
        call gsourc [convert and consolidate sources]
        call decay [estimate decay of FPs]
        call fpmove [redistribute FPs]
        call flow [atmosphere flow model]
        call hmpwr [calculate host decay power]
}

subroutine prcell
{
    call pratm [print atmosphere information]
    call rbout [print lower-cell information, including sodium pool fire]
    call praero [print simple aerosol output]
    call praero [print detailed aerosol output]
    call htmout [print heat structure information, including degassing]
    call prspry [print sodium spray fire information]
}
```

Currently the MELCOR code development environment is using Microsoft Visual Studio ® 2008 with INTEL Visual FORTAN Compiler ® XE 2011. To enable both CONTAIN 2 and CONTAIN-LMR codes to run in these environments, the following code modifications were made:

- All passing arrays through subroutine calls, such as (*) and (1) were converted to the explicit size of the arrays in order to compile without errors.
- Scratch arrays such as h(…), ih(…), ah(…) and lh(…) had been increased in sizes in order to function correctly.
- Other bugfixes were also performed, such as “divide by zero”, syntax errors, and uninitialized variables.
- To be consistent with CONTAIN 2 structures, CONTAIN-LMR source code was converted from the upper cases to lower cases.
- Fortran 77 data and programming structures were untouched to minimize the effort.
- Because of the large common blocks used without converting them into modules, implicit none feature was not implemented.

To ensure proper working conditions, both CONTAIN codes were tested with a number of test inputs on hand. For CONTAIN 2, a series of the standard test decks (STDs) were used, since CONTAIN 2 is designed for the LWR applications. On the other hand, CONTAIN-LMR code is only used for fast reactor applications. The discussion of the CONTAIN testing is provided in Appendix B of this document.

In the coming year, it is planned to develop additional validation testing for these CONTAIN models, if any experiments exist. This validation is used to verify CONTAIN models before they are implemented into MELCOR. This validation will include porting the existing sodium models from CONTAIN-LMR that have not been included in CONTAIN 2 to CONTAIN 2 code. This step is necessary to ensure that the latest code development of the CONTAIN is used, which is CONTAIN 2. This code upgrade to CONTAIN 2 will be used as a tool for the code-to-code comparison when the sodium models have also been implemented in MELCOR 2.1. At the same time, this validation is also used after the models have been incorporated in MELCOR to ensure consistent results. The validation testing for the sodium models is discussed in Chapter 5 of the document.

5 SODIUM MODEL IMPLEMENTATION PLAN

This chapter describes the design documentation of the sodium specific models that will be adapted from CONTAIN-LMR to MELCOR for this year and FY15. Note that this implementation plan including the description of how MELCOR will be modified is preliminary. When performing actual code modification, this design document will be updated to reflect the actual changes that are required.

This chapter describes the sodium models in SAND91-1490 and those FORTRAN source codes in the CONTAIN-LMR code that was obtained from PNC. In SAND91-1490, it describes a number of models (see Table 5-1). As shown in this table, the types of the models are identified, including the implementation time frame. In terms of the model implementation as shown in Table 5-1, only the first four models will be implemented completely in FY15. The remaining models will be addressed in FY16. Note that it is not certain that the models in the CONTAIN-LMR code are similar to those models described in SAND91-1490. However, CONTAIN 2, which is developed at SNL, contains coding for many sodium models which may be included in SAND91-1490 (see Table 5-1). In this document, attempts are made to identify the sodium models listed from Table 5-1 and the sodium models identified from the source codes of CONTAIN-LMR and CONTAIN 2 as shown in Table 5-2. All sodium models from the CONTAIN-LMR coding would be imported to MELCOR. All MELCOR code modification will be done in MELCOR 2.1. Note that because the sodium models involve the calling of the CVH package routines for handling sensible energy from and to the reaction energy associated with sodium fire and reactions, calling of the NCG package routines for oxygen and hydrogen depletion and generation, respectively, and calling of the RN package routines for aerosol generations, the creation of an independent package, namely NaModel for handling all sodium models may be required. NaModel (NAM) should be created similarly as the BURN (BUR) package and the CAVITY (CAV) package, which should be included in the calling sequence within the RUNSTEP subroutine. Note that NAM would be invoked when sodium fluid and fast reactor are selected. In addition, the preliminary MELCOR code modification described in this chapter is tentative, and subject to change when the actual implementation takes place.

Table 5-1 CONTAIN-LMR Sodium Models for MELCOR

No	Model	Physical(P)/ Chemical(C) Type	Description
1	Two-Condensable Option/Condensate Removal (FY14/FY15)	P	This option allows the modeling of the condensation, evaporation and boiling of both sodium and water within a single calculation. This model allows removal of condensate from the atmosphere. This model may have been addressed in MELCOR already.
2	Sodium Spray Fires (FY15)	P/C	This model allows the treatment of the combustion of sodium spray resulting from an energetic event that causes droplets of sodium spraying out of the reactor system
3	Sodium Pool Modeling (FY15)	P	This model allows boiling of sodium pool. It also models the heat transfer between the pool and the debris layers such as CORCON layers. The pool chemistry is addressed in the Sodium Pool Chemistry model
4	Sodium Pool Fires (FY15)	P/C	This model simulates the chemical reaction between sodium located in a pool and the oxygen in the atmosphere above the pool.
5	Debris Bed/Concrete Cavity Interaction (FY16)	P/C	This model allows the modeling of the debris bed in the cavity where sodium pool can be present. The physical interaction of the sodium pool and the debris bed can be challenged, such as the heat transfer aspects

			of the interaction. In addition, the chemical aspect of the interaction can also be occurred. In terms of sodium-concrete interactions, SLAM model from CONTAIN will be implemented
6	Sodium Pool Chemistry (FY16)	C	As a part of the pool chemistry, only eight major chemical reactions are considered in this model. The constituents considered including those species from the sodium-concrete interaction, and those sodium with water content in the concrete.
7	Atmospheric Chemistry (FY16)	C	This model allows atmospheric constituents to interact chemically to form stable compound. The chemical reactions consider including those for sodium.

Table 5-2 Sodium Model Coding in CONTAIN Codes

No	Code Description	
	CONTAIN-LMR*	**CONTAIN2**
1	ACNTRL routine formulates a flag, ICONDN, which designates the condensing component, such as water or sodium (see Two Condensable Option Section for more details).	This model is not available.
2	It contains SPRAY routine to allow the simulation of sodium spray fire.	It also contains SPRAY routine to allow the simulation of sodium spray fire, which is similar to that of CONTAIN-LMR.
3	PMHXFR routine contains heat transfer equations for evaporation and condensation of the coolant in the pool. It also models sodium coolant. BOILER routine contains a number of boiling/film boiling equations, and critical heat flux equations for sodium.	Although both PMHXFR and BOILER routines exist in this version, no sodium correlation is included.
4	PFIRE routine calculates sodium pool fire, which is based on SOFIRE-II code. Limited the burned sodium to ½ of the initial mass at a given timestep. In tracking, it distributes the mass and energies between the atmosphere and the pool. It includes Na2O, Na2O2, Na and O2. IPFIRE routine is the input processing for the sodium pool fire.	Similarly PFIRE routine as described in CONTAIN-LMR calculates the sodium pool fire.
5	SLAM routine contains the physics of the sodium-concrete interactions	Although SLAM routine exists, but there is no coding in the file.
6	NFPCHM is a flag to designate a pool chemistry model call to PCHEM routine. However, this routine does not exist. According to SAND91-1490, six of the eight chemical reactions in the pool have been modeled in the SLAM model. In fact, SLCHEM routine shows the coefficients for the reactions for the SLAM model. The actual reaction calculation routine is REACSL, which takes these coefficients to perform reactions. See SAND91-1490, Equation 8-20 to identify the reactions modeled.	Similar to CONTAIN-LMR code, these calls are there, but there is no PCHEM routine.
7	CHEMRX routine models the sodium atmosphere chemistry. It references HEDL-TC-730. It also contains more sets of heat of reaction equations for different reactants. Account for reactions with gases (CHMGAS routine), and with aerosols and gases (CHMAER routine), consider contact reactions within one aerosol particles or within an aerosol deposit or condensable film (CHMREP routine), react deposits or film with gas (CHMDEP).	CHEMRE routine models the sodium atmosphere chemistry. It references HEDL-TC-730. It does not have the heat of reactions equations as described in CONTAIN-LMR. In this routine, it calculates the gas reactions and call AERREA routine for aerosol related reactions.

*See Figure 4-1 for the calling sequence and top tree level of the code.

In each section of this chapter, the model is described first, followed by a discussion of the CONTAIN-LMR coding of the model. Finally, the implementation approach to migrate this CONTAIN-LMR model into MELCOR is given.

5.1 Two Condensable Option

In most system codes (e.g., CONTAIN and MELCOR), only a single coolant is permitted at one time. The original CONTAIN code, such as CONTAIN 1.1 only permitted a single coolant to be present at a given time. The introduction of sodium for the coolant in CONTAIN-LMR will posed issues relating condensation processes of both sodium and water simultaneously. To address the problem of modeling of the condensation, evaporation and boiling of both sodium and water within a single calculation, the two-condensable option was implemented in CONTAIN-LMR. In fact, the CONTAIN code architecture prevents a completely general treatment of two condensables in the calculation. To permit two condensables, such as water and sodium, only atmosphere thermodynamics and flow, and aerosol condensation are allowed.

Two-condensable option in CONTAIN-LMR is intended to treat both sodium and water simultaneously [Murata 1993]. The treatment of this option for the atmosphere thermodynamics and flow is available for either thermal or fast reactor (which includes the LMRs). This general treatment includes modeling of the condensate dynamics within the aerosol model.
Since the code limitation only permits a single condensable in the atmosphere, the other condensable, if present, is treated as an ideal gas. This designation is required in order for the model to work. The two-condensable option permits condensation onto aerosols and deposition on surfaces. Within a cell (or control volume in MELCOR), the specified cell-level condensable is allowed to condense on surfaces, and the other condensable is treated as an ideal gas requiring its atmosphere properties (such as viscosity and conductivity). In addition, if both chemical reactions and aerosol condensation for the other condensable is modeled, the ideal gas assumption should be adequate. In CONTAIN, cell-level models are restricted with respect to the condensable used. These models are not extended to the two-condensable option, which includes (a) SPARC pool scrubbing model for aerosols, spray, ice condenser and fan cooler engineered systems. Allowing the presence of other condensable and other materials in liquid pools is treated in CONTAIN-LMR; however, it is assumed that this would not affect the transfer rate of the cell-level condensable and transfer through flow between pools.

As pointed out later on for the chemical reactions, CONTAIN LMR assumes that chemical reactions take place among repositories associated with the atmosphere. In this model, there is a limitation on the reaction rates, which impose at most ½ of any gaseous reactant or atmosphere condensable to be allowed to react per system timestep. If any sodium is sufficiently cold to preclude significant vapor-phase transport and is not settling out rapidly on surfaces, the reaction rate may be controlled by the evaporation rate of the water films (a slow process). Also chemical reactions between atmosphere and surface films or deposits that depend on the gas transport or condensables from the atmosphere to the surface in general are assumed to occur instantaneously. However, the reactions of sodium in the atmosphere and surface water are not included in the model due to the low sodium pressure. By default, the reactions between sodium in the atmosphere and surface water require the transport of water vapor from the surface through evaporation, which controls the rate of the reaction. Thus the evaporate rate is important. Note that this can only occur, if water is the cell-level condensate.

Aerosol condensation within this condensable option is relying on the condensation model used. The old method relies on the fixed grid method to estimate the water condensation, which is used to calculate the aerosol population change in the aerosol size classes due to condensation, but did not consider hygroscopic effects. The second method, adapted from CONTAIN 1.1 is the moving grid method, which allows to models hygroscopic or Kelvin effects. This second method should minimize the numerical diffusion instability. In terms of input requirement, keyword SOLAER is an option for AEROSOL global block to deal when both water and sodium are declared as condensable. Two possible cases if SOLAER option is invoked: a) water uses fixed grid, and b) sodium is not active; or c) water uses moving grid and sodium uses fixed grid. Later case allows the modeling of both water and sodium in a single problem. In CONTAIN-LMR, when the cell is used to model environment or any volume that is not active for aerosol flow will not be allowed to model aerosol physics. For the new moving grid method for aerosol condensation, aerosol nucleation is permitted.

5.1.1 CONTAIN Coding

In CONTAIN-LMR, subroutine ACNTRL provides a control for aerosol modeling. A flag, ICONDN is used to identify the condensation phenomena (see Table 5-3). This routine contains logics according the value of ICONDN as described in Table 5-3. It calls AERSL routing, which is a driver routine for the multicomponent aerosol module. Within this routine is the model of the moving grid formulation. Note that the moving grid method is only applicable for water used. Sodium is still using the fixed grid method. In the moving grid formulation, the subroutine CONDEN is called. CONDEN routine controls the condensation calculation for aerosol.

Table 5-3 ICONDN Flag Description

ICONDN Value	Description
1	Only water is a condensing component
2	Only sodium is a condensing component
3	Sodium is the only condensing component in the present cell (control volume in MELCOR) although water can condense in others
4	Both water and sodium are condensing components. Note that this requires the moving grid method be available for water

5.1.2 MELCOR Code Modification

In MELCOR, the current LWR version of the code only treats water as only condensable material. The suspended water droplets in the atmosphere are referred as fog. The atmosphere also includes water vapor and noncondensible gases. In pool, it includes liquid water and water vapor bubbles.

In RN package, ICOND is an index for condensation calculations in aerosol dynamics. ICOND index is defined in M_RN1 module. Currently an index of 0 refers to condensation onto all existing aerosols, and 1 refers as condensation onto water aerosols. Implementation of the ICONDN from CONTAIN-LMR may be possible using this ICOND index. In RN2_RN2RN2 routine, a number of aerosol masses are calculated, which includes aerosol masses in gas phase,

aerosol masses in liquid phase, vapor masses in gas phase, vapor masses in liquid phases, including those masses are radioactive. Output of this routine is the update of these masses. Thus the treatment of sodium and water onto aerosols can be done in this routine. This routine may need to incorporate the moving grid method or an equivalent method from the AERSL routine of CONTAIN-LMR, and the necessary interface between the CONDEN routine in CONTAIN-LMR. Note that MELCOR does not have moving grid for aerosol physics. Thus much of the SOLAER model may not be implemented into MELCOR.

5.2 Sodium Spray Fire

Of the two basic types of sodium fires postulated in sodium cooled fast reactors, spray and pool sodium fires, spray fires are generally considered to be more energetic. This is due to the fact that a sodium spray always burns at a higher rate than a sodium pool containing the identical amount of sodium because of the large surface area of the droplet versus the pool surface area. Pipe breaks are often postulated for developing sodium spray fire. The sodium released through the break is usually assumed to eject upward and impinge on the ceiling of the room, where a sodium liquid is formed and then break up to form droplets [Tsai 1980]. These droplets form a sodium spray. The interaction of the sodium spray with oxygen and available moisture in the atmosphere of the room creates the sodium spray fire phenomena.

The model for the sodium spray fire is based on the phenomenological model used in NACOM, a code developed and tested at Brookhaven National Laboratory [Tsai 1980]. Note this model is also available in CONTAIN 2.

The sodium spray fire model described in this document is based on the phenomenological model developed in NACOM [Murata 1993]. In this model, the user specifies the mean droplet diameter for the sodium spray then an initial size distribution is determined using the Nukiyama-Tanasama correlation [Tsai 1980]. The current default mean droplet diameter is set at 0.001 m. This model also requires a user input fall height 'HITE'. In addition, this model requires the user to specify the mole fraction of Na_2O_2 produced by the spray fire. This mole fraction is currently set at 1.0 as default. Three main reactions are modeled:

$$\mathbf{2\ Na + 0.5\ O_2 \rightarrow Na_2O} \qquad [5\text{-}1]$$

$$\mathbf{2\ Na + O_2 \rightarrow Na_2O_2} \qquad [5\text{-}2]$$

$$\mathbf{2\ Na + 2\ H_2O \rightarrow 2\ NaOH + H_2} \qquad [5\text{-}3]$$

Note that Eq.[5-3] requires the presence of water vapor.

5.2.1 CONTAIN Coding

In both CONTAIN-LMR and CONTAIN2, the SPRAY routine documents the sodium spray fire model. The input routine for this model is through ISPRAY.

In the SPRAY routine, the following are included:

- Droplets are assumed at 1.015×10^5 Pa and saturation temperature.

- Mass fraction of Na_2O_2 is estimated based on the user specified input.
- Heat is estimated based on the above mass fraction.
- Selection of drop size distribution is based on the user specified mean droplet diameter.
- Determination of the spray source is based on the user specified data.
- Integration of the droplet fall and reactions is estimated.

The SPRAY routine only calls VELT routine for estimating the terminal velocity and Reynolds number. The SPRAY routine also calls SORSPR routine for the spray source.

5.2.2 MELCOR Code Modification

In MELCOR, the logical place to add the sodium spray model would be in the CVHRN3 routine where many recently developed models have been added, such as the H2C model. Since SPRAY is a self-contain module that only needs to interface with the atmosphere source, this routine can be ported to MELCOR with the only change to the data structures and interface variables. Also, another logical place for placing SPRAY is within tHydr_CVHRN1, since tHydr_CVHRN1 routine is used to calculate external sources of mass and energy. The chemical energy of the fire and the consumption of the oxygen from the gas space must be accounted for. In addition, the end products, such as Na_2O_2, and Na_2O must be added to the atmosphere of the control volume. However, the question is the re-direction of these species into the aerosol category of the gases. In this case, where these two sodium by-products are being treated as aerosols, it may be logical to treat the by-products as aerosol sources in the RN1_SOURCES routine.

5.3 Sodium Pool Modeling

A sodium pool may form in the reactor cavity area, which can play an essential role in LMR accident analyses. The modeling described here is limited to the heat transfer models within the sodium pool with hot surfaces, such as hot debris. Although sodium pool chemistry can take place, it is deferred to a topic on the sodium pool chemistry.

This model is associated with the sodium pool in the reactor cavity area. The lower cell input must be invoked in order to use this model. This modeling is to include any heat transfer equations that are specifically designed for sodium forming a lower cell pool.

In boiling heat transfer from the sodium pool is the saturation temperature, T_{sat} as a function of the pool pressure ($\mathbf{P_p}$ in Pascals). It is given as [Murata 1993]:

$$\mathbf{T_{sat}} = \frac{-1.2023\times10^4}{\log_{10}(P_p/10^6)-8.1185} \qquad [5\text{-}4]$$

For film boiling heat transfer, particularly for the surface below the sodium pool, T_{bot}(K) at the Leidenfrost point is given by [Murata 1993]. All units are in the MKS system:

$$\mathbf{T_{bot} - T_{sat}} = \frac{\Psi\lambda}{1-0.5c_{vf}\Psi} \qquad [5\text{-}5]$$

Where Ψ is given as:

$$\Psi = 0.086806 \left[\frac{\rho_{vf}\mu_{vf}^{1/3}}{k_{vf}}\right] \rho_l^{-5/6} \sigma^{1/2} \qquad [5\text{-}6]$$

where λ is the heat of vaporization of sodium at T_{sat}, c_{vf} is the vapor specific heat at constant pressure, ρ_{vf}, μ_{vf} and k_{vf} are the density, viscosity and conductivity of the vapor evaluated at the film temperature (where this temperature is average of T_{bot} and T_{pool}). σ is the sodium liquid surface tension evaluated at T_{sat}. ρ_l is the pool density. Thus the heat flux at the onset of film boiling is given:

$$q_{bot} = 0.15927 \cdot \rho_{vf}\, \lambda' \left(\frac{\sigma}{\rho_l}\right)^{1/4} \qquad [5\text{-}7]$$

where

$$\lambda' = \lambda + 0.5 c_{vf}(T_{bot} - T_{sat}) \qquad [5\text{-}8]$$

The critical heat flux used in CONTAIN-LMR is given by:

$$q_{chf} = 0.24775\, \lambda \cdot \rho_v^{1/2}\left(1 + 163.54 \cdot P_p^{-0.4}\right)(\sigma\rho_l)^{1/4} \qquad [5\text{-}9]$$

The equation used for T_{chf}, the surface temperature below the sodium pool evaluated at q_{chf} is defined as

$$T_{chf} - T_{sat} = 1814.6 \left[\frac{q_{chf}}{k_l}\right]^{0.3} \left[\frac{\lambda\rho_v}{c_l P}\right]^{0.7} \left[\frac{\sigma}{\rho_l}\right]^{1/2} \qquad [5\text{-}10]$$

The relation before this critical heat flux and the critical heat flux for a subcooled pool is given as

$$q_{chf,s} = q_{chf}\left[1 + 0.10714\, \frac{\left(\frac{\rho_l}{\rho_v}\right)^{3/4} \frac{c_l}{\lambda}(T_{sat} - T_{pool})}{1 + 163.54\, P^{-0.4}}\right] \qquad [5\text{-}11]$$

5.3.1 CONTAIN Coding

This model is associated with the sodium pool in the reactor cavity area. The lower cell input must be invoked in order to use this model. ICELL routine is the input controller for the cell level input models. It calls REBPLT routine a number of times for lower cell layers, such as concrete, intermediate, pool and atmosphere. REBPLT routine contains a number of sodium specified properties (such as surface tension for sodium), which includes the call of BOILER routine. Boiler routine includes correlations for boiling, film boiling, and critical heat flux equations for sodium. Critical temperature for the critical heat flux is also calculated in this routine.

5.3.2 MELCOR Code Modification

In MELCOR, Subroutine tHS_HSBOIL handles the boiling heat transfer for pools. Thus, the equations modeled in the BOILER routine of CONTAIN-LMR will be ported to tHS_HSBOIL routine of MELCOR. However, many constants as shown in the equations in Section 3.1 will be included as sensitivity coefficients. tHS_HSBOIL routine is called by tHS_HSTRAN routine,

which handles many heat and mass transfer from and to pool for MELCOR. The other two routines that call tHS_HSBOIL are COR_CORCNV and COR_CORRN1. Since the implementation task for this work is related to the containment analyses; therefore, no change will be made for these COR related routines.

5.4 Sodium Pool Fire

This sodium pool fire model is taken from the SOFIRE II code developed from the results of pool fire tests [Beiriger 1973]. SOFIRE II model was based on the verification of experiments, which included a large test vessel in a series of thermodynamic parameter tests to study the effect of oxygen concentration on the system pressure, sodium burning rates and heat transfer rates. This vessel has a diameter of 3.05 m (10 ft), with a high of 9.14 m(30 ft) and contains 62.3 m^3 (2200 ft^3) of gas at the standard condition. In the lower section of the vessel, a 0.5574 m^2 (6 ft^2) steel pan was installed on a spider off the floor of the vessel. The pan was insulated with fire brick and mounted below a feed line from an external sodium preheat tank. Thermocouples were mounted in or on the sodium pool volume, steel pan, pan insulation, gas volume and vessel walls. This experiment is referred as a one-cell experiment. A two-cell experiment was also used to validate this model [Beiriger 1973].

The main pool fire reaction for this model is given as:

$$(\mathbf{1+f_1})\cdot\mathbf{2}\cdot\mathbf{Na}+\ \mathbf{O_2}\rightarrow\mathbf{2}\cdot\mathbf{f_1}\cdot\mathbf{Na_2O}+(\mathbf{1-f_1})\cdot\mathbf{Na_2O_2}+\mathbf{q(reaction)} \qquad [5\text{-}12]$$

where f_1= fraction of total oxygen consumed that reacts to form monoxide and q(reaction) is 9.04540×10^6 and 1.09746×0^7 J/kg for the monoxide and peroxide, respectively [Murata 1993].

The above reaction requires oxygen in the air to diffuse to the sodium pool. CONTAIN-LMR uses a diffusion constant, D_O (m^2/s) for oxygen-nitrogen mixtures different than that of SOFIRE II [Murata 1993]:

$$\mathbf{D_O=6.4315\times10^{-5}\frac{T_{film}{}^{1.823}}{P}} \qquad [5\text{-}13]$$

where T_{film} = average temperature of the pool and atmosphere (K) and P = system pressure (Pa).

In this pool fire model, it is required to allocate the amount of the products and reaction energy to the pool and to the atmosphere layer of the cell. Thus, additional fractional inputs may be provided. The fractional inputs include:

- f_2 is the fraction of sensible heat from the reaction to the pool. The remainder will be directed to the atmosphere layer of the cell.
- f_3 is the fraction of Na_2O product that enters the pool as a solid after the fire. The remainder will be directed to the atmosphere as aerosols.
- f_4 is the fraction of Na_2O_2 product that enters the pool as a solid after the fire. The remainder will be allocated to the atmosphere as aerosols.

Note that the sodium burning rates calculated by this model depend on the temperature differences between the pool and the atmosphere. This difference is assumed to set up turbulent natural convection above the pool surface – the greater the differential, the greater the burning rate would be. Thus radiative heat transfer between the pool and its surrounding may result differences in the burning rate.

5.4.1 CONTAIN Coding

This sodium pool fire model is called within the lower-cell physics routines. In RHCNTR subroutine, where the lower cell controls are done, it calls lower cell layers to set up the physics, such as the intermediate and concrete layers. Then it calls the pool layer which calls the PFIRE routine to perform sodium pool fire calculations using Eq. [5-12] and the fractional inputs above. The calculations include mass and energy estimate of the reaction, including the estimate of the reactants, sodium from the pool and the oxygen from the atmosphere, via Eq. [5-13] for the diffusion rate, and the products, sodium monoxide and sodium peroxide. The allocation of the product masses to the pool and atmosphere are functions of the user-defined values or by default.

5.4.2 MELCOR Code Modification

To implement this model into MELCOR, a similar routine of PFIRE will be written based on the data structure of MELCOR for modeling aerosol. In terms of heat generation and heat transfer for this model may be similar to Section 5.3.2, which relies on subroutine tHS_HSBOIL for handling the boiling heat transfer for pools. For the chemical energy generated by the pool fire, the current CONTAIN model assumes that the user specifies the fraction of the chemical energy to pool. Then the rest of the energy would be directed to the gas space of the control volume. The similar methodology will be used for now until a more realistic model is developed for splitting this reaction energy. Using the same treatment as in the sodium spray fire model, tHydr_CVHRN1 routine may be used to direct the chemical energy from the pool fire to the gas space as well as to the pool space. Another logical place for this energy between the pool and atmosphere is in tHydr_CVHRN3 routine. In this routine, calling subroutine tHydr_CVHBL may be useful to account for the mass and energy of the sodium pool fire. Similarly to the sodium spray fire model, the treatment of the sodium fire by-products of peroxide and monoxide as gases or aerosols needs to be considered. As aerosols, these by-products may be treated as external aerosol sources which call the RN1_SOURCES routine.

6 SUMMARY/CONCLUSIONS

This is a progress report for the MELCOR/CONTAIN LMR Integration Project, M3AR-13SN1701031. This report describes the preliminary design documentation of the sodium models from CONTAN-LMR code to be implemented into MELCOR 2.1. The sodium model to be completed in FY15 includes Two-Condensable Option (see Section 5.1), Sodium Spray Fire (see Section 5.2), Sodium Pool Heat Transfer Model (see Section 5.3), and Sodium Pool Fire (see Section 5.4). In these model descriptions, efforts have been made to document the subroutines and code information, in which will be used to be implemented into MELCOR 2.1. Additionally, preliminary testing for verification and validation of the selected sodium models for CONTAIN-LMR has been conducted. Although CONTAIN-LMR utilized the earlier version of CONTAIN code, additions of the missing sodium models from CONTAIN-LMR to CONTAIN 2 would represent a latest CONTAIN development tool for the code-to-code comparison to MELCOR 2.1, when the sodium models have been implemented.

Since this report is a "living" document, the prior year's accomplishment is also included in this report, such as the preliminary implementation of the sodium thermophysical properties into MELCOR 2.1 from both works done from INL as FSD database and the BRISC LDRD as SIMMER database. To minimize the impact, the implementation of the FSD was done by utilizing the detection of the data input file as a way to invoking the FSD. This methodology has been adapted currently for this work, but it may subject modification as the project becomes mature. The implementation of the initial stage of the sodium properties into MELCOR has been completed- all essential interfaces to replace water with sodium and all input processing. Additional work was done to ensure the FORTRAN coding of the sodium property subroutines, modules and functions are within the same code development guidelines as in MELCOR and is easily maintained. Documentation on the usage of the multi-fluid version of MELCOR is being developed. The equation sets and pertinent information on the sodium properties implemented into MELCOR have been provided in this report. Preliminary testing was performed to ensure that the sodium properties have been implemented properly. However, refinement of the properties and any interpolation of the ranges of the property correlation are still needed. In addition, a refinement of the sodium properties implemented in MELCOR will be performed with additional testing of the sodium models over a broad range of possible states.

In the coming FY, it is intended to implement all sodium models as described in Chapter 5 of this report into MELCOR 2.1. Validation testing will be done, including the use of existing available experiments, and latest experiments done at SNL. In the FY15 final report, a design document for the remaining sodium models, such as sodium atmospheric chemistry, sodium-concrete interaction, and sodium pool chemistry to MELCOR 2.1 will be included.

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APPENDIX A: INPUT/OUPTUT FILES FOR NALIBRARY PROGRAM

This appendix tabulates the input and output for the NaLibrary Program that is used with FSD data set. Table A-1 shows the INL data input file, Table A-2 shows output of the data limits and table statistics. Table A-3 shows an example of the saturation property table of temperature versus pressure. Table A-4 shows an example of the thermodynamic property table.

Table A-1. Input File

```
tpfna version 1.1.1, tables of thermodynamic properties of sodium

  84 temperatures as follows:

      371.
      400.   450.
      500.   550.
      600.   620.   640.   660.   680.
      700.   710.   720.   730.   740.   750.   760.   770.   780.   790.
      800.   810.   820.   830.   840.   850.   860.   870.   880.   890.
      900.   910.   920.   930.   940.   950.   960.   970.   980.   990.
     1000.  1010.  1020.  1030.  1040.  1050.  1060.  1070.  1080.  1090.
     1100.  1110.  1120.  1130.  1140.  1150.  1160.  1170.  1180.  1190.
     1200.  1220.  1240.  1260.  1280.
     1300.  1350.
     1400.  1450.
     1500.  1600.  1700.  1800.  1900.
     2000.  2100.
     2200.  2300.  2400. 2500. 2510.0 2600. 2800.0 3000.

  28 pressures as follows:

     2.13652E-05
     1.00e-4  5.00e-4
     1.00e-3  5.00e-3
     1.00e-2  5.00e-2
     1.00e-1  5.00e-1
     1.00e+0  5.00e+0
     1.00e+1  5.00e+1
     1.00e+2  5.00e+2
     1.00e+3  5.00e+3
     1.00e+4  5.00e+4
     1.00e+5  5.00e+5
     1.00e+6  5.00e+6
     1.0E+07
     2.0E+07
     25624700.0
     4.e7
     5.e7
```

Table A-2. Output File – Data Limits and Table Statistics

```
Data limits:

                                    temperature      pressure         volume
                                    -----------     -----------     -----------
   minimum allowed input value =    3.71000E+02     1.61000E-06         n/a
   maximum allowed input value =    3.00000E+03     5.00000E+07         n/a
   triple point value          =    3.71000E+02     2.11953E-05     1.07896E-03
   critical point value        =    2.45000E+03     3.20663E+07     6.32824E-03
Table statistics:
   number of temperatures            =    84
   number of pressures               =    28
   number of saturation temperatures =    79
   number of saturation pressures    =    26
   number of words in binary tables  = 15589
```

Table A-3. Output File – Example of Saturation Properties of Sodium (Temperature vs. Pressure)

temperature	pressure	state	specific volume	internal energy	thermal expansion	isothermal compress.	specific heat	entropy
3.71000E+02	2.11953E-05	liquid	1.07896E-03	2.05903E+05	2.96659E-04	1.95989E-10	1.19914E+03	2.62650E+03
		vapor	6.33173E+09	4.86030E+06	2.69542E-03	4.71803E+04	9.04333E+02	1.46920E+04
4.00000E+02	2.45341E-04	liquid	1.08827E-03	2.40575E+05	2.95561E-04	2.02010E-10	1.19228E+03	2.71649E+03
		vapor	5.89763E+08	4.87604E+06	2.50001E-03	4.07598E+03	9.04334E+02	1.38743E+04
4.50000E+02	7.91868E-03	liquid	1.10444E-03	2.99952E+05	2.94700E-04	2.12806E-10	1.18333E+03	2.85637E+03
		vapor	2.05560E+07	4.90316E+06	2.22230E-03	1.26285E+02	9.04345E+02	1.27240E+04
5.00000E+02	1.26705E-01	liquid	1.12083E-03	3.58957E+05	2.94929E-04	2.24191E-10	1.17732E+03	2.98071E+03
		vapor	1.42732E+06	4.93027E+06	2.00031E-03	7.89279E+00	9.04388E+02	1.18163E+04
5.50000E+02	1.21779E+00	liquid	1.13751E-03	4.17723E+05	2.96075E-04	2.36239E-10	1.17371E+03	3.09274E+03
		vapor	1.63321E+05	4.95732E+06	1.81907E-03	8.21304E-01	9.04509E+02	1.10838E+04
6.00000E+02	7.98980E+00	liquid	1.15453E-03	4.76362E+05	2.98021E-04	2.49029E-10	1.17213E+03	3.19478E+03
		vapor	2.71428E+04	4.98426E+06	1.66878E-03	1.25218E-01	9.04791E+02	1.04819E+04
6.20000E+02	1.55566E+01	liquid	1.16144E-03	4.99803E+05	2.99005E-04	2.54372E-10	1.17201E+03	3.23321E+03
		vapor	1.44005E+04	4.99498E+06	1.61576E-03	6.43230E-02	9.04974E+02	1.02704E+04
6.40000E+02	2.90363E+01	liquid	1.16842E-03	5.23244E+05	3.00101E-04	2.59853E-10	1.17215E+03	3.27042E+03
		vapor	7.96092E+03	5.00565E+06	1.56628E-03	3.44702E-02	9.05209E+02	1.00732E+04
6.60000E+02	5.21540E+01	liquid	1.17547E-03	5.46690E+05	3.01306E-04	2.65478E-10	1.17254E+03	3.30650E+03
		vapor	4.56831E+03	5.01627E+06	1.52006E-03	1.91968E-02	9.05507E+02	9.88899E+03
6.80000E+02	9.04556E+01	liquid	1.18259E-03	5.70147E+05	3.02618E-04	2.71254E-10	1.17319E+03	3.34151E+03
		vapor	2.71203E+03	5.02683E+06	1.47685E-03	1.10724E-02	9.05876E+02	9.71656E+03
7.00000E+02	1.51948E+02	liquid	1.18979E-03	5.93619E+05	3.04034E-04	2.77188E-10	1.17407E+03	3.37553E+03
		vapor	1.66068E+03	5.03730E+06	1.43643E-03	6.59448E-03	9.06328E+02	9.55487E+03
7.10000E+02	1.94752E+02	liquid	1.19341E-03	6.05363E+05	3.04781E-04	2.80216E-10	1.17460E+03	3.39219E+03
		vapor	1.31360E+03	5.04251E+06	1.41721E-03	5.14641E-03	9.06588E+02	9.47775E+03
7.20000E+02	2.47871E+02	liquid	1.19706E-03	6.17111E+05	3.05553E-04	2.83287E-10	1.17518E+03	3.40862E+03
		vapor	1.04612E+03	5.04769E+06	1.39862E-03	4.04469E-03	9.06872E+02	9.40298E+03
7.30000E+02	3.13364E+02	liquid	1.20073E-03	6.28866E+05	3.06351E-04	2.86400E-10	1.17582E+03	3.42484E+03
		vapor	8.38526E+02	5.05284E+06	1.38063E-03	3.20035E-03	9.07183E+02	9.33045E+03
7.40000E+02	3.93614E+02	liquid	1.20442E-03	6.40628E+05	3.07175E-04	2.89557E-10	1.17652E+03	3.44084E+03
		vapor	6.76320E+02	5.05797E+06	1.36322E-03	2.54872E-03	9.07520E+02	9.26007E+03
7.50000E+02	4.91364E+02	liquid	1.20813E-03	6.52397E+05	3.08024E-04	2.92759E-10	1.17727E+03	3.45663E+03
		vapor	5.48752E+02	5.06307E+06	1.34639E-03	2.04244E-03	9.07886E+02	9.19174E+03
7.60000E+02	6.09753E+02	liquid	1.21186E-03	6.64174E+05	3.08898E-04	2.96007E-10	1.17808E+03	3.47223E+03
		vapor	4.47799E+02	5.06814E+06	1.33011E-03	1.64653E-03	9.08282E+02	9.12538E+03
7.70000E+02	7.52358E+02	liquid	1.21562E-03	6.75958E+05	3.09797E-04	2.99302E-10	1.17894E+03	3.48764E+03
		vapor	3.67428E+02	5.07317E+06	1.31436E-03	1.33501E-03	9.08710E+02	9.06092E+03
7.80000E+02	9.23231E+02	liquid	1.21939E-03	6.87752E+05	3.10722E-04	3.02645E-10	1.17985E+03	3.50286E+03
		vapor	3.03075E+02	5.07816E+06	1.29913E-03	1.08842E-03	9.09170E+02	8.99827E+03
7.90000E+02	1.12694E+03	liquid	1.22319E-03	6.99556E+05	3.11672E-04	3.06037E-10	1.18081E+03	3.51789E+03
		vapor	2.51261E+02	5.08312E+06	1.28440E-03	8.92108E-04	9.09664E+02	8.93735E+03
8.00000E+02	1.36864E+03	liquid	1.22702E-03	7.11369E+05	3.12647E-04	3.09480E-10	1.18183E+03	3.53275E+03
		vapor	2.09321E+02	5.08804E+06	1.27016E-03	7.34953E-04	9.10193E+02	8.87812E+03

Table A-4. Output File – Example of Thermodynamic Properties of Sodium

pressure	temperature	state	specific volume	internal energy	thermal expansion	isothermal compress.	specific heat	entropy
2.13652E-05	3.71000E+02	liquid	1.07896E-03	2.05903E+05	2.96659E-04	1.95989E-10	1.19914E+03	2.62650E+03
	4.00000E+02	vapor	6.77237E+09	4.87604E+06	2.50000E-03	4.68051E+04	9.04333E+02	1.47572E+04
	4.50000E+02	vapor	7.61892E+09	4.90317E+06	2.22222E-03	4.68051E+04	9.04333E+02	1.48637E+04
	5.00000E+02	vapor	8.46546E+09	4.93030E+06	2.00000E-03	4.68051E+04	9.04333E+02	1.49590E+04
	5.50000E+02	vapor	9.31201E+09	4.95743E+06	1.81818E-03	4.68051E+04	9.04333E+02	1.50452E+04
	6.00000E+02	vapor	1.01586E+10	4.98456E+06	1.66667E-03	4.68051E+04	9.04333E+02	1.51239E+04
	6.20000E+02	vapor	1.04972E+10	4.99541E+06	1.61290E-03	4.68051E+04	9.04333E+02	1.51535E+04
	6.40000E+02	vapor	1.08358E+10	5.00626E+06	1.56250E-03	4.68051E+04	9.04333E+02	1.51823E+04
	6.60000E+02	vapor	1.11744E+10	5.01712E+06	1.51515E-03	4.68051E+04	9.04333E+02	1.52101E+04
	6.80000E+02	vapor	1.15130E+10	5.02797E+06	1.47059E-03	4.68051E+04	9.04332E+02	1.52371E+04
	7.00000E+02	vapor	1.18517E+10	5.03882E+06	1.42857E-03	4.68051E+04	9.04332E+02	1.52633E+04
	7.10000E+02	vapor	1.20210E+10	5.04425E+06	1.40845E-03	4.68051E+04	9.04332E+02	1.52761E+04
	7.20000E+02	vapor	1.21903E+10	5.04967E+06	1.38889E-03	4.68051E+04	9.04332E+02	1.52888E+04
	7.30000E+02	vapor	1.23596E+10	5.05510E+06	1.36986E-03	4.68051E+04	9.04332E+02	1.53012E+04
	7.40000E+02	vapor	1.25289E+10	5.06052E+06	1.35135E-03	4.68051E+04	9.04332E+02	1.53135E+04
	7.50000E+02	vapor	1.26982E+10	5.06595E+06	1.33333E-03	4.68051E+04	9.04332E+02	1.53257E+04
	7.60000E+02	vapor	1.28675E+10	5.07138E+06	1.31579E-03	4.68051E+04	9.04332E+02	1.53377E+04
	7.70000E+02	vapor	1.30368E+10	5.07680E+06	1.29870E-03	4.68051E+04	9.04332E+02	1.53495E+04
	7.80000E+02	vapor	1.32061E+10	5.08223E+06	1.28205E-03	4.68051E+04	9.04332E+02	1.53612E+04
	7.90000E+02	vapor	1.33754E+10	5.08765E+06	1.26582E-03	4.68051E+04	9.04332E+02	1.53727E+04
	8.00000E+02	vapor	1.35447E+10	5.09308E+06	1.25000E-03	4.68051E+04	9.04332E+02	1.53840E+04
	8.10000E+02	vapor	1.37141E+10	5.09851E+06	1.23457E-03	4.68051E+04	9.04332E+02	1.53953E+04
	8.20000E+02	vapor	1.38834E+10	5.10393E+06	1.21951E-03	4.68051E+04	9.04332E+02	1.54064E+04
	8.30000E+02	vapor	1.40527E+10	5.10936E+06	1.20482E-03	4.68051E+04	9.04332E+02	1.54173E+04
	8.40000E+02	vapor	1.42220E+10	5.11478E+06	1.19048E-03	4.68051E+04	9.04332E+02	1.54282E+04
	8.50000E+02	vapor	1.43913E+10	5.12021E+06	1.17647E-03	4.68051E+04	9.04332E+02	1.54389E+04
	8.60000E+02	vapor	1.45606E+10	5.12564E+06	1.16279E-03	4.68051E+04	9.04332E+02	1.54494E+04
	8.70000E+02	vapor	1.47299E+10	5.13106E+06	1.14943E-03	4.68051E+04	9.04332E+02	1.54599E+04
	8.80000E+02	vapor	1.48992E+10	5.13649E+06	1.13636E-03	4.68051E+04	9.04332E+02	1.54702E+04
	8.90000E+02	vapor	1.50685E+10	5.14191E+06	1.12360E-03	4.68051E+04	9.04332E+02	1.54805E+04
	9.00000E+02	vapor	1.52378E+10	5.14734E+06	1.11111E-03	4.68051E+04	9.04332E+02	1.54906E+04
	9.10000E+02	vapor	1.54072E+10	5.15277E+06	1.09890E-03	4.68051E+04	9.04332E+02	1.55006E+04
	9.20000E+02	vapor	1.55765E+10	5.15819E+06	1.08696E-03	4.68051E+04	9.04332E+02	1.55104E+04
	9.30000E+02	vapor	1.57458E+10	5.16362E+06	1.07527E-03	4.68051E+04	9.04332E+02	1.55202E+04
	9.40000E+02	vapor	1.59151E+10	5.16904E+06	1.06383E-03	4.68051E+04	9.04332E+02	1.55299E+04
	9.50000E+02	vapor	1.60844E+10	5.17447E+06	1.05263E-03	4.68051E+04	9.04332E+02	1.55395E+04
	9.60000E+02	vapor	1.62537E+10	5.17990E+06	1.04167E-03	4.68051E+04	9.04332E+02	1.55489E+04
	9.70000E+02	vapor	1.64230E+10	5.18532E+06	1.03093E-03	4.68051E+04	9.04332E+02	1.55583E+04
	9.80000E+02	vapor	1.65923E+10	5.19075E+06	1.02041E-03	4.68051E+04	9.04332E+02	1.55676E+04
	9.90000E+02	vapor	1.67616E+10	5.19617E+06	1.01010E-03	4.68051E+04	9.04332E+02	1.55768E+04
	1.00000E+03	vapor	1.69309E+10	5.20160E+06	1.00000E-03	4.68051E+04	9.04332E+02	1.55858E+04
	1.01000E+03	vapor	1.71002E+10	5.20703E+06	9.90099E-04	4.68051E+04	9.04332E+02	1.55948E+04
	1.02000E+03	vapor	1.72696E+10	5.21245E+06	9.80392E-04	4.68051E+04	9.04332E+02	1.56038E+04
	1.03000E+03	vapor	1.74389E+10	5.21788E+06	9.70874E-04	4.68051E+04	9.04332E+02	1.56126E+04

APPENDIX B: CONTAIN TESTING

This appendix documents the testing done to both CONTAIN-2 and CONTAIN-LMR codes after they were bought to the modern Software Quality Assurance practice. Table B-1 shows the list of the standard test problems were used to ensure CONTAIN-2 were upgraded correctly. For the CONTAIN-LMR code, there were no standard test problems designed for this code. The standard test problems used in CONTAIN-2 were designed for light water reactors, so these tests would not be suitable for testing CONTAIN-LMR code. However, we tested CONTAIN-LMR code with a test problem specifically designed for this code. Additionally, we provided demonstration problems to test out CONTAIN-LMR code for the specific sodium models as described in Chapter 5 of this document.

B.1 CONTAIN 2

This section discusses the testing for CONTAIN 2. Since there was no test result available, the testing is done by comparing the last time point calculation results from the outputs to those calculations done by the executables created in March 20, 2008 using a different Window Fortran compiler. Table B.1-1 shows the latest results using the STD tests conducted. As shown in this table, the latest version of CONTAIN 2 is working as indicated.

Table B.1-1. CONTAIN 2 Testing

STD Test No	Description	Run?	Comparison
1	ST01.ac --- condensation model w/forced convection, adapted from ac23(st)	Yes	Result is identical to existing executable*
2	ST02.af --- aerosol fall through check, adapted from af06(st)	Yes	Result is identical to existing executable*
3	ST03.af --- intercell aerosol flow test with fps, adapted from af07(st), and modified for light water reactors.	Yes	Result is identical to existing executable*
4	ST04.cf --- intercell gas flow test (adiabatic flow), adapted from cf09(st), but modified for light water reactors.	Yes	Result is identical to existing executable*
5	ST05.cv --- corcon/vanesa standard problem, adapted from cv04(st)	Yes	Existing executable* aborts on this input. Use last edit from CONTAIN 1.2 testing - results look very similar. Minor differences are observed.
6	ST06.ev --- engineered vent test, adpated from ev05(st)	Yes	Result is identical to existing executable*
7	ST07.ft --- fission product transport, adapted from ft02(st)	Yes	Result is identical to existing executable*
8	ST08.hb --- hydrogen burn test, adapted from hb04(st), but converted to thermal reactor	Yes	Result is identical to existing executable*
9	ST09.ic --- ice condenser test, adapted from ic02(st)	Yes	Result is similar to existing executable*up tp the point when all ices were melted. However, there should not be additional ice to be melted as predicted by the existing executable*. The latest executable predicts the ice melt and accumulation including vapor mass from atmosphere is correct.
10	ST10.ih --- test of fission product decay heating, adapted from ih11(st)	Yes	Result is identical to existing executable*
11	ST11.ih --- test of the engineered safety features, adapted from ih20(st)	Yes	Results are very similar to that of the existing executable*- minor differences in energy, mass and flow rates
12	ST12.ih --- fission product transport, adapted from ih22(st)	Yes	Result is identical to existing executable*
13	ST13.it --- integrated workshop problem, adapted from it01(st)	Yes	Results are very similar to that of the existing executable*- minor differences in energy, mass and flow rates

STD Test No	Description	Run?	Comparison
14	ST14.rh --- radiation enclosure problem, adapted from rh04(st)	Yes	Result is identical to existing executable*
15	ST15.bw --- bwr test, spv and srv with pool boiling, adapted from bw14(st)	Yes	Result is identical to existing executable*
16	ST16.cs --- connected structure option test, adapted from cs01	Yes	Result is identical to existing executable*
17	ST17.ff --- film flow test with fission products, adapted from ff01	Yes	Result is identical to existing executable*
18	ST18.ht --- condensation and ht test problems	Yes	Results are very similar to that of the existing executable* - minor differences in energy, aerosol, mass and flow rates
18a	ST18.ht --- condensation and ht test problems - slightly different cell elevation	Yes	Results are very similar to that of the existing executable*- minor differences in energy, aerosol, mass and flow rates
19	ST19.pt --- pool tracking test with drain-down, adapted from pt01	Yes	Results are very similar to that of the existing executable*- minor differences in energy, aerosol, mass and flow rates
20	ST20.pd --- grand gulf plant deck	Yes	Results are very similar to that of the existing executable*- very minor differences
21	ST21.df --- diffusion frame burn test, adapted from dfb05	Yes	Results are very similar to that of the executable from Beegees - very minor differences
22	ST22.eo --- non-ideal equation of state water test, adapted from eo01	Yes	Result is identical to existing executable*
23	ST23.fp --- fission product library test, adapted from fpd01	Yes	Results are very similar to that of the existing executable* - very minor differences in fp masses
24	ST24.lc --- lower cell heat conduction test, adapted from lch01	Yes	Result is identical to existing executable*

*Existing executable means the executable dated March 20, 2008.

B.2 CONTAIN-LMR

B.2.1 Two Condensable Option

This section describes the demonstration input for the Two Condensable Option within the atmosphere input options (see Section 5.1). This option allows the modeling of both sodium and water condenses in the same problem. The keyword TWOCOND will activate this model. This keyword is placed in the MATERIAL block of the input. However, a keyword of FIRST and SECOND for each of condenses must be declared. Table B.2.1-1 shows the demonstration input deck for exercising this option. This deck was modified from the sample problem documented in SAND91-1490. The keyword to activate this model is “TWOCOND”. There was no experiment to be used for verifying or validating this model. Thus no further discussion of the option is provided.

Table B.2.1-1 Demonstration Input for the Two-Condensable Option

```
&& cray
&& slam-corcon-debris-bed test problem
&& (from appendix a of sand91-1490)
&& this problem is a modification of indb4. a .1 see slam
&& timestep is used to control limit cycles and assure
&& consistent slam results. the end time for slam is set
&& to 500 seconds and a transition to corcon is forced at
&& 10000 seconds, because slam cannot operate
&& concurrently with the debris bed, the debris bed is
&& introduced at 500 sec. the bed area has been modified
```

```
&& to allow quench at this time, and the bed power
&& increased to allow reasonable corcon interactions.
&&
&& --------------------- global input ---------------------------
control ncells=2 ntitl=2 ntzone=8 nsectn = 10 nac=4 eoi
material
compound h2 o2 co co2 h2ol h2ov fe n2 conc uo2 pu
  u mno mgo k2o nav nal uo2 puo2 cao ssox fel
  na2o2 na2o naoh na
  twocond
    first=nav
    second=h2ov
    cellcond nav nav
  eoi
times 60000. 0.
&& ---------- time zones ---------------
  5,   10,   1500.
  10.  30.   2400.
  5.   30.   3000.
  10.  60.   5000.
  10. 120.   9500.
  10.  30.  10000.
  10. 120.  16000.
  10. 120.  20000.
&& ----------------------------------
1. 1.
longedt 2

fast
flows
  area(1,2)=1. cfc(1,2)=.5 avl(1,2) =.5
  implicit
  dropout
aerosol
  deldif = 1.e-4 densty=300. tgas1=328. pgas1=1.e+5
  diam1 =1.e-8 tgas2=3000. pgas2=10.e+5
  na2o2=1.e-6 .531
  na2o=1.e-6 .531
  naoh=1.e-6 .531
  nal=1.e-6 .531
prlow-cl
prheat
prflow
praer
title
corcon/breeder test problem
       cna002 - mod - Two condensable demonstration
&& ------------ end of global input --------------
cell =2
 control
   nhtm =3 mxslab = 10 numtbc=2 maxtbc=3
   jconc =50 jint =2 jpool = 1 nraycc=50 ndblyr=4
 eoi
 geometry 1570. 9.4
 atmos=3 1.e+5 328.
        n2=.79 o2=.2 nav=.01
 condense
&& atmchem
&& h-bum
&& ------------- structures -----------------------
struc
&& --------------- cavity wall ---------------
cavwall wall cylinder 10 2 380. 9.4 0. 9.4
 7.30 7.40 7.50 7.60 7.70 7.80 7.90 8.00 8.10 8.20 8.30
 conc conc conc conc conc conc conc conc conc conc
&& --------------- cavity wall --------------------
cavwa12 wall cylinder 10 2 380. 9.4 0. 9.4
 7.30 7.40 7.50 7.60 7.70 7.80 7.90 8.00 8.10 8.20 8.30
 conc conc conc conc conc conc conc conc conc conc
&& --------------- cavity roof ---------------------
```

```
cavroof roof slab 10 2 380. 7.3 0. 167.
 0.00 0.10 0.20 0.30 0.40 0.50 0.60 0.70 0.80 0.90 1.00
 conc conc conc conc conc conc conc conc conc conc conc
&&
rad-heat
  emsvt .8 .8 .8 .8
  gaswal 7.4
eoi
ht-tran on on on on on
low-cell
  geometry 167. && floor area
  decay-ht=14.e+8
  dist-pwr 0. 1. 1. 0. 0. eoi
  concrete
&& concrete composition specification
&& use corcon's crbr concrete type, contain's generic
 compos = 1
  concrete = limena
    rhocon =2250. rebar =.14 tablat = 1650. emconc =.9
  eoi
  1.3e6 && concrete mass
  temp=300.
  physics
   na-conc
    model = slam
    times 0. 500. .1
   eoi
   corcon
    times 5000. 1
    20. 20. 100. 55000.
    geometry 0. 1.
      flatcyl
        0. 7.29 1.5 .5 10. 10. 10 10
    emisiv
      oxide
        time 2
          0. .9 6.e+8 .9
      metal
        time 2
          0. .9 6.e+8 .9
      surrnd
        time 2
          0. .9 6.e+8 .9
    eoi && terminate emisiv option
&& ischem && keyword for ideal solution chemistry
   eoi && terminate corcon option
&&
  eoi && terminate physics
&&
 eoi && terminate the layer
&& --------------- corcon melt layer specification -------------
 interm
  lay-nam = ccmelt
  compos = corcon
    oxides =4
      cao 2000.
      fe3o4 13128.1
      uo2 25278.
      puo2 1151.
    metals = 1
      fe 19557.
      toxide = 2000.
      tmetal=2500.
      layers=0
  eoi && terminate corcon compos
  temp = 2500.
  physics
    corestat
    0. 70.1851  2441. 0.
  eoi && terminate physics
```

```
 eoi && terminate the layer
 interm
  lay-name =debbed
  temp=2500.
  physics
    deb-bed && debris bed model
      times
        tdbstr=500. && debris start time
        timmlt= 10000. && debris remelt time
      eoi && terminate times block
      height
        total =.1875 && total debris bed height
        dry =.1875 && dry debris bed height
      eoi && terminate height block
      dbarea=50.
      dporos =.5 && bed porosity
      ddia = .005 && particle diameter
      tmpmlt=2550. && remelt temperature
      expmul = .01 && exposed bed ht. multiplier
    eoi && terminate debris input
  eoi && terminate physics
 eoi && terminate interm layer
 pool
  compos 1 nal 38000.
   temp 873.
   physics
    boil
    ht-coef
     name = atmos
     var-x=time x=2,0.,400000.
     var-y=coef y=2,22.,22.
    eoi
   eoi
 eoi && terminate the layer
 bc 300.
eoi && terminate lower cell input
&& ---------------------- end cell 2 ------------------------
cell = 1
 control
  nhtm =3 mxslab = 10
 eoi
 geometry 68500. 79.
 atmos=4 1.018e+5 300.
        n2=.74 o2=.15 nav=.01 h2ov=.10
 condense
&& ------------- structures -----------------------
struc
&& --------------- confinement wall --------------------
  conwall wall cylinder 5 6 300. 79. 0. 300. 79.
  25.00 25.08 25.15 25.23 25.30 25.38
  fe fe fe fe fe
&& --------------- confinement wall --------------------
  conwa12 wall cylinder 5 6 300. 79. 0. 300. 79.
  25.00 25.08 25.15 25.23 25.30 25.38
  fe fe fe fe fe
&& --------------- confinement roof ---------------------
  conroof roof slab 5 6 300. 7.3 0. 300. 167.
  0.00 0.08 0.15 0.23 0.30 0.38
  fe fe fe fe fe
&&
ht-tran on on on on on
eof
```

B.2.2 Atmosphere Chemistry

This section describes the demonstration input for the atmosphere chemistry. To invoke this model, the ATMCHEM keyword in the cell atmosphere block should be declared. Note that there were two principle chemical reactions considered in this model: $\mathrm{Na} + \mathrm{H_2O(l)} \rightarrow \mathrm{NaOH} +$

$0.5H_2$ and $2Na + H_2O(v) \rightarrow Na_2O + H_2$. Note that the second equation dominates if water vapor fraction is larger than the oxygen fraction in the atmosphere. Another option is that the user can enter the fraction of sodium that produces the monoxide versus the peroxide. Table B.2.2-1 shows the demonstration input deck for this model. As shown in this table, the model is activated in Cell 2, where the source of the sodium vapor is located. No experiment is available to validate this model. Thus no further discussion for this calculation is provided.

Table B.2.2-1 Demonstration Input for Atmosphere Chemistry Model

```
&& cray
&& ------------------------- clmrdb4 ----------------------------
&&          contain lmr/1 test problem db4
&&
&& model atmosphere chemistry
&&     to activate h2 generation, h2ov mole fraction > that of o2
&&
&& original cell 1 is divided into 5 cells
&&
&& --------------------- global input --------------------------
control ncells=6 ntitl=2 ntzone=7  nsectn=10  nac=4 eoi
material
compound h2 o2 co co2 h2ol h2ov fe n2 conc uo2 pu
   u mno mgo k2o nav nal uo2 puo2 cao ssox  ss fel
   na2o2 na2o naoh na
times 60000.0   0.
&& ---------- time zones ---------------
  5.0   10.0       10.
  10.0   30.0     3000.
  10.0   60.0     5000.
  10.0  120.0     9500.
  10.0   30.0    12000.
  10.0  120.0    15000.
  10.0  120.0    20000.
&& --------------------------------------
1.0 1.0 1.0 1.0 1.0 1.0  && cell timestep fraction
&&    debug 5 cvtoat medboil pool slam pooldf  1100.  1200.
longedt 2
fast
&& thermo
flows
  area(1,2)=160.0  cfc(1,2)=0.01  avl(1,2)=0.50   && area is the roof area of cell2
  elevcl(2)=4.7  elevcl(1)=20.0  elevfp(1,2)=9.4 elevfp(2,1)=9.4

  area(1,4)=162.7  cfc(1,4)=0.01  avl(1,4)=0.50
  elevcl(1)=20.0  elevcl(4)=16.5  elevfp(1,4)=16.5    elevfp(4,1)=16.5

  area(1,3)=162.7  cfc(1,3)=0.01  avl(1,3)=0.50
  elevcl(1)=20.0  elevcl(3)=16.5  elevfp(1,3)=16.5    elevfp(3,1)=16.5

  area(4,5)=242.5  cfc(4,5)=0.01  avl(4,5)=0.50
  elevcl(4)=16.5 elevcl(5)=5.85  elevfp(4,5)=9.4    elevfp(5,4)=9.4

  area(3,6)=242.5  cfc(3,6)=0.01  avl(3,6)=0.50
  elevcl(3)=16.5 elevcl(6)=5.85  elevfp(3,6)=9.4    elevfp(6,3)=9.4

  area(2,5)=3.5   cfc(2,5)=0.01  avl(2,5)=0.50
  elevcl(2)=4.7  elevcl(5)=5.85  elevfp(2,5)=5.85    elevfp(5,2)=5.85

  area(2,6)=3.5   cfc(2,6)=0.01  avl(2,6)=0.50
  elevcl(2)=4.7  elevcl(6)=5.85  elevfp(2,6)=5.85    elevfp(6,2)=5.85


  implicit
  dropout
aerosol
   deldif=1.0e-4  densty=300.
```

```
   diam1=1.0e-08   tgas2=3000.0   pgas2=10.0e+5
   na2o2=1.0e-6  0.531
   na2o=1.0e-6   0.531
   naoh=1.0e-6   0.531
   nal =1.0e-6   0.531
prlow-cl
prheat
prflow
prburn   && print option for burn
praer
title
   contain lmr - snl
     model atmosphere chemistry
&& ------------ end of global input --------------
cell=2
control
  nhtm=3  mxslab=10 numtbc=2  maxtbc=3
  jconc=5  jint=1  jpool=1            && nraycc=50 ndblyr=4
  nsoatm=1 nspatm=4     && number of atm source, entry for table
eoi
geometry  1570.0  9.4   && volume and height
atmos=4  1.018e+5  378.0
   n2=0.75  o2=0.10  nav=0.0 h2ov=0.15  && initial condition to allow 2*na+h2o=na2o+h2
   condense
  atmchem
  frna2o=0.5
  h-burn
  eoi
  source=1  && number of table
    nav=4 iflag=1
      t=0.0   250.0 500.0 1000.0
      mass=5.0 5.0 5.0 5.0
      temp=600.0 600.0 600.0 600.0
&& ------------- structures ----------------------
struc
&& --------------- cavity wall --------------------
  cavwal1 wall  cylinder  10 2 328. 9.4 0. 9.4
  7.30  7.40  7.50  7.60  7.70  7.80  7.90  8.00  8.10  8.20  8.30
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&& --------------- cavity wall --------------------
  cavwal2 wall  cylinder  10 2 328. 9.4 0. 9.4
  7.30  7.40  7.50  7.60  7.70  7.80  7.90  8.00  8.10  8.20  8.30
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&& --------------- cavity roof ---------------------
  cavroof  roof  slab  10  2  328.  7.3  0.  167.
   0.00  0.10  0.20  0.30  0.40  0.50  0.60  0.70  0.80  0.90  1.00
   ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&&
rad-heat
     emsvt .8 .8 .8 .65   && nhtm+pool surface
     gaswal   7.4
eoi

ht-tran  on  on  on  on  on


low-cell
     geometry  167.0  && floor area

&& ---------------- concrete specification, inc. interaction model
     concrete
&&              concrete composition specification
&&      use corcon's crbr concrete type, contain's generic
           compos=1   concrete=limecc rhocon=2250   && concrete=limena   rhocon=2250.
             rebar=.140  tablat=5000.  emconc=0.9
           eoi
&&               concrete mass
           1.3e6
           temp=300.0  && initial temp
```

```
        eoi    &&  terminate the layer
&& ---------------- stainless liner specification ---------------
    interm
          lay-nam = liner
          compos = 1 ss  266.87 && assume mass here

          temp=400.

    eoi   &&  terminate the layer

     pool
        compos  1  nal   1000.
            temp  400.
            physics
              boil
          eoi    &&   terminate physics
    eoi   &&  terminate the layer
        bc  300.0  0.85e5
eoi  &&  terminate cell 1 input
&& ----------------------- end cell 1 ------------------------
cell=1
control
  nhtm=1  mxslab=10
eoi
geometry  3540.4  21.2
atmos=3  1.018e+5  378.0
   n2=0.75   o2=0.10  h2ov=0.15
  condense
&& ------------- structures -----------------------
struc

&& ---------------- confinement roof (center)---------------------
 conroof  roof  slab   10  10  328.  14.4 0.0  300.0  167.0
  0.00  0.10  0.20  0.30  0.40  0.50  0.60  0.70  0.80  0.90  1.00
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&&
ht-tran on  on  on  on  on

&& ----------------------- end cell 3 ------------------------
cell=3
control
  nhtm=2  mxslab=10
eoi
geometry  3443.4  14.1
atmos=3  1.018e+5  378.0
   n2=0.75   o2=0.10  h2ov=0.15
  condense
&& ------------- structures -----------------------
struc

&& ---------------- confinement wall --------------------
  conwal3 wall  cylinder   10 10 328. 14.1 0. 300.0 14.1
  14.40  14.50  14.60  14.70  14.80  14.90  15.00  15.10  15.20  15.30 15.4
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&& ---------------- confinement roof ---------------------
  conroof3  roof  slab   10  10  328.  14.1  0.  300.0 242.22
  0.00  0.10  0.20  0.30  0.40  0.50  0.60  0.70  0.80  0.90  1.00
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&&
ht-tran on  on  on  on  on

&& ----------------------- end cell 4 ------------------------
cell=4
control
  nhtm=2  mxslab=10
eoi
geometry  3443.4   14.1
atmos=3  1.018e+5  378.0
   n2=0.75   o2=0.10  h2ov=0.15
  condense
```

```
&& ------------- structures -----------------------
struc
&& --------------- confinement wall --------------------
  conwal4 wall  cylinder   10 10 328. 14.1 0. 300.0 14.1
  14.40  14.50  14.60  14.70  14.80  14.90  15.00  15.10  15.20  15.30 15.4
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc

&& --------------- confinement roof ---------------------
  conroof4  roof  slab   10  10  328.  14.1  0.  300.0 242.22
   0.00  0.10  0.20  0.30  0.40  0.50  0.60  0.70  0.80  0.90  1.00
   ss  ss  conc  conc  conc  conc  conc  conc  conc  conc
&&
ht-tran on  on  on  on  on

&& ------------------------ end cell 5 ------------------------
cell=5
control
  nhtm=1  mxslab=10
eoi
geometry  1721.4  7.1
atmos=3  1.018e+5  378.0
    n2=0.75   o2=0.10  h2ov=0.15
   condense
&& ------------- structures -----------------------
struc

&& --------------- confinement wall --------------------
  conwal5 wall  cylinder   10 10 328. 7.1 0. 300.0 7.1
  14.40  14.50  14.60  14.70  14.80  14.90  15.00  15.10  15.20  15.30 15.4
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc

ht-tran on  on  on  on  on

&& ------------------------ end cell 6 ------------------------
cell=6
control
  nhtm=1  mxslab=10
eoi
geometry  1721.43  7.1
atmos=3  1.018e+5  378.0
    n2=0.75   o2=0.10  h2ov=0.15
   condense
&& ------------- structures -----------------------
struc
&& --------------- confinement wall --------------------
  conwal6 wall  cylinder   10 10 328. 7.1 0. 300.0 7.1
  14.40  14.50  14.60  14.70  14.80  14.90  15.00  15.10  15.20  15.30 15.4
  ss  ss  conc  conc  conc  conc  conc  conc  conc  conc

&&
ht-tran on  on  on  on  on

eof
```

B.2.3 Sodium Spray Fire

This section describes the demonstration input for the sodium spray fire model (see the model details in Section 5.2). This model is a part of the atmospheric physics model. To invoke this model, the keyword "SPRAFIRE" is required. Once this model is activated, the user can specific the fall height of the sodium spray, mean sodium droplet diameter, the mole fraction of sodium peroxide by the fire, and the source of the sodium for the spray.

To verify and validate this model, ABCOVE AB5 experiment is used [Souto 1994]. The brief description of the experiment is provided. The primary objective of the ABCOVE test AB5 was

to provide experimental data for use in validating aerosol behavior computer codes for the case of a moderate-duration, strong, single-component aerosol source generated by a sodium spray in an air atmosphere. A secondary objective was to provide experimental data on the temperature and pressure in the containment vessel and its atmosphere, for use in validating containment response codes. The experimental apparatus is given in Figure B.2.3-1. As shown in this figure, the experimental vessel is a round headed cylindrical vessel, which are built with steel and surrounded with insulation to minimize the heat loss. The sodium spray is injected about 5.1 m above the vessel bottom. A pan catch is in place to allow aerosol settling and liquid collection.

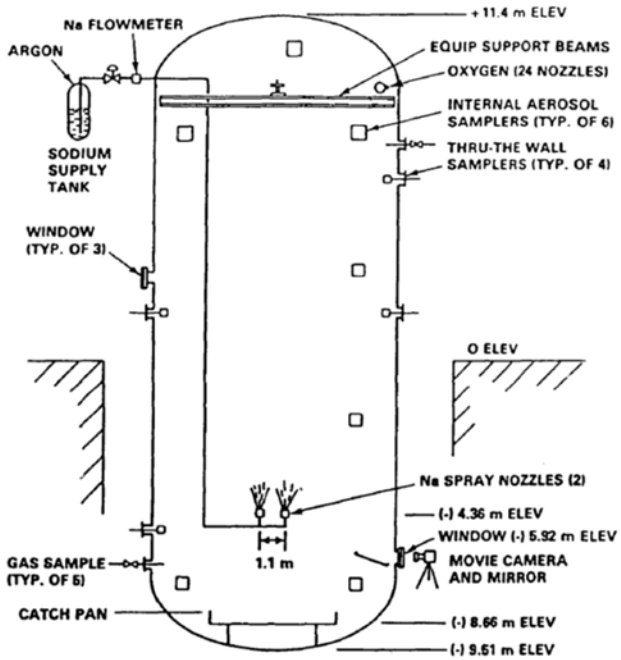


Figure B.2.3-1 CSTF Arrangement for ABCOVE AB5 Test [Souto 1994]

For the CONTAIN model, a single cell is used for this vessel. Walls, floor and roof of the vessel are modeled, including the internal deposition components. A summary of the Test AB5 is provided in Table B.2.3-1. The input deck for this experiment is shown in Table B.2.3-2. As shown in this table, the thermodynamic conditions of the experiment were modeled, including the sources of the sodium and oxygen. Since the aerosol results showed no monoxide formed (60% Na_2O_2 and 40% NaOH), the input value for the peroxide is set to 1.0. In order to model NaOH formation, the water vapor mass of the dew point from the test was included.

The preliminary comparison between calculated results from CONTAIN-LMR and the available test results is shown in Table B.2.3-3. Even though with the amount of water vapors modeled, CONTAIN-LMR did not predict any NaOH production. In the experiment, all sourced sodium was reacted. However, CONTAIN-LMR estimated that a portion of the sodium did not react and fall into the pool.

Table B.2.3-1 Test Conditions for ABCOVE AB5 [Souto 1994]

INITIAL CONTAINMENT ATMOSPHERE	***PARAMETER***
Oxygen Concentration	23.3±0.2%
Temperature (mean)	302.25K
Pressure	0.122MPa
Dew Point	289.15±2K
Nominal Leak Rate	1%/day at 68.9kPa
Na SPRAY	***PARAMETER***
Na Spray Rate	256±15g/s
Spray Start Time	13s
Spray Stop Time	885 s
Total Na Sprayed	223±11 kg
Na Temperature	836.15 K
Spray Drop Size, MMD	1030±50 µm
Spray Size Geom. Std. Dev., GSD	1.4
OXYGEN CONCENTRATION	***PARAMETER***
Initial O_2 Concentration	23.3±0.2 vol %
Final O_2 Concentration	19.4±0.2 vol %
Oxygen Injection Start	60 s
Oxygen Injection Stop	840 s
Total O_2	47.6 m^3 (STD)
CONTAINMENT CONDITIONS DURING TESTS	***PARAMETER***
Maximum Average Atmosphere Temperature	552.15 K
Maximum Average Steel Vessel Temperature	366.65 K
Maximum Pressure	213.9 kPa
Final Dew Point	271.65 K
AEROSOL GENERATION	***PARAMETER***
Generation Rate	445 g/s
Mass Ratio, Total Na	1.74
Material Density	2.50 g/cm^3
Initial Suspended Concentration	0
Source Mass Median Dia.	0.50 µm
Source Sigma, σ_g	1.5
Maximum Suspended Mass Concentration	170 g/m^3
Suspended Conc. Steady-State Value	110±17 g/m^3

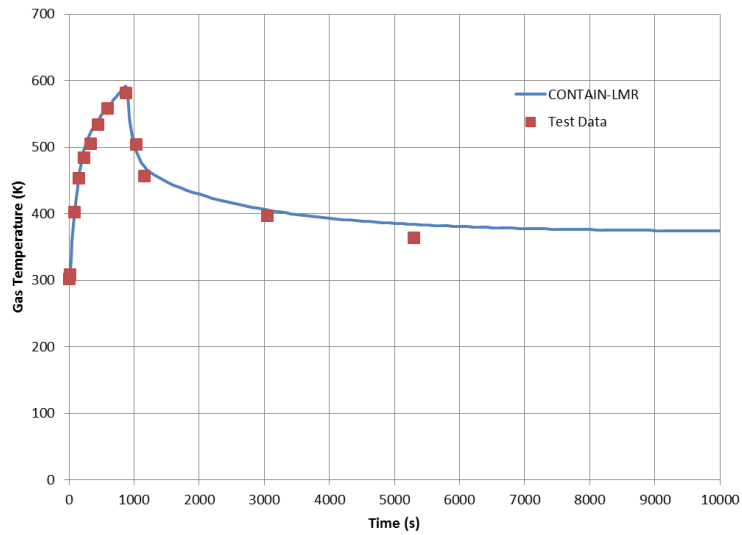
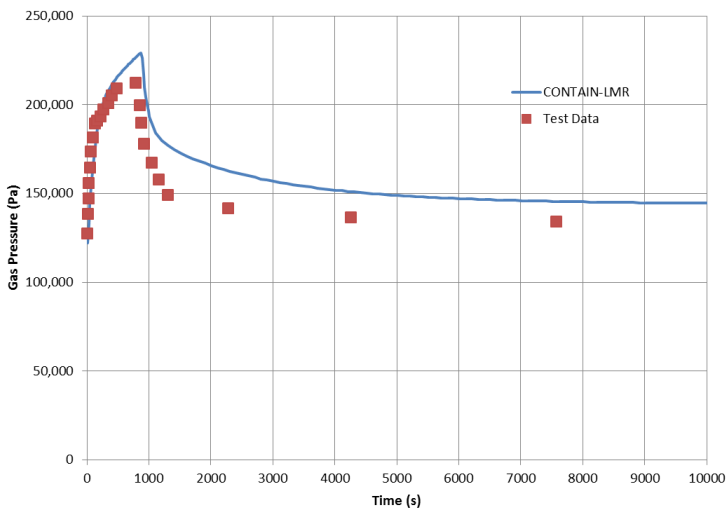
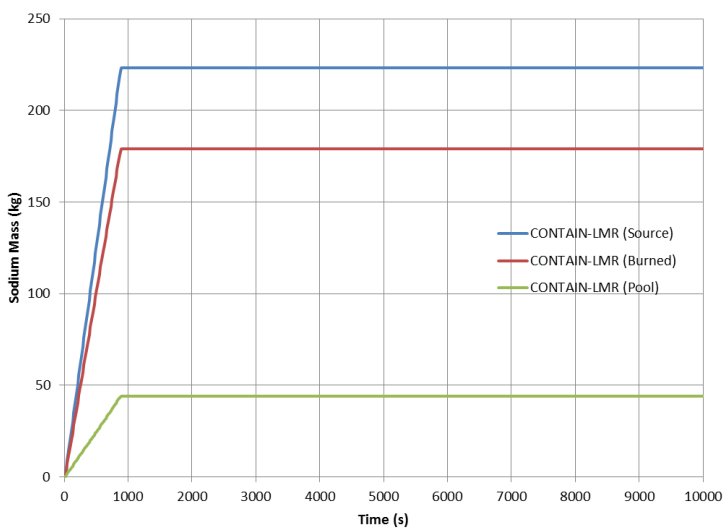
Table B.2.3-2. Demonstrated Input For ABCOVE AB5

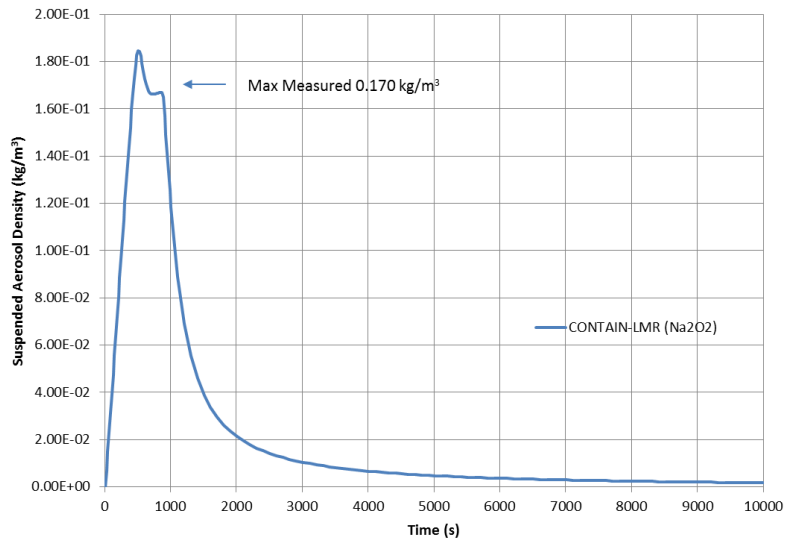
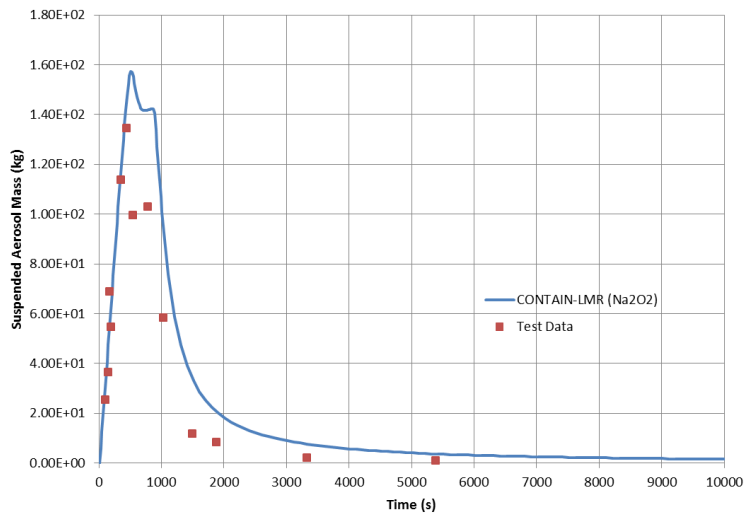
```
&& cray
&& ------------------------- AB5 ----------------------------
&&          contain lmr/1 test problem AB5
&&
&& model sodium spray fire - AB5
&& The experiment was modeled as two cells.
&&     cell 1 represents CSTF

&& Heat structures are modeled in 5:
&&     1 the CSTF top head
&&     2 CSTF cylindrical walls
&&     3 internal components for aerosol plating
&&     4 CSTF bottom head
&&     5 internal componets for aerosol settling
&&
&& Sodium is injected at 5.15 m above the tank bottom.
&& a total of 223 kg over 872 s.  All sodium converted to
&& 60%na2o2 and 40%naoh.
&& Results: maximum P=214kPa, MeanT=553.15K, max 843.15K
&& max suspended aerosol density 170g/m3 after 383s initiated Na inj
&& -------------------- global input ---------------------------
control ncells=1 ntitl=2 ntzone=4  nsectn=10  nac=4 eoi
material
compound h2 o2 co co2 h2ol h2ov fe n2 conc uo2 pu
```

```
   u mno mgo k2o nav nal uo2 puo2 cao ssox  ss fel
   na2o2 na2o naoh na
times 60000.0   0.
&& ---------- time zones ---------------
  5.0   10.0        10.
  10.0   30.0     3000.
  10.0   60.0     5000.
  10.0  120.0    10000.
&& ---------------------------------------
1.0  && cell timestep fraction
&&
longedt 2
fast
thermo

&& aerosol
&& generation rate 445 g/s, material density=2.5g/cc
&& mass median radius=0.25 um, sigma=1.5
aerosol
   densty=2500.
   tgas2=3000.0   pgas2=10.0e+5
   na2o2=0.250e-6  1.5
   na2o=0.250e-6  1.5
   naoh=0.250e-6  1.5
   na  =0.250e-6  1.5
prlow-cl
prheat
prflow
prspray   && print option for sodium spray fire
praer
title
   contain lmr/1 test abcove AB5
     model sodium spray fire
&& ------------ end of global input --------------

&& ------------ cell 1 - CSTF ----------------
cell=1  && CSTF
control
  nhtm=5  mxslab=10 numtbc=2  maxtbc=3 nsoatm=1  nspatm=3
  jint=1  jpool=1            && nraycc=50 ndblyr=4
  nsospr=1 nspspr=3     && number of spray source, entry for table
eoi
geometry  852.0  20.3   && volume and height
atmos=3  1.22e+5  302.25  && 0.122 MPa, 302.25 K
   n2=0.752  o2=0.233 h2ov=0.015  && initial o2 23.3vol%
   source=1  && model o2 injection rate, ts=60, tend=840s
            && 47.6 m3 (STD), 0.02241 m3= 1mole -> 2123.67 moles of O2
            && total injected 68 kgs. 0.08718 kg/s
     o2=3 iflag=1
     t=0.0  60.0 840.0
     mass=0.0 0.08718 0.08718
     temp=293.0 293.0 293.0



&& ------------- structures ------------------------
struc
&& --------------- Top Head ------------------
  tophead  roof  slab  2  0  303.45  7.62  1.0 0.0 63.0   && insulated
   0.00  0.00905 0.0181
   ss  ss
&& ---------------  walls    ------------------
  wall1 wall  cylinder 2  0  301.55  7.62  1.0 0.0 1.9    && insulated
  3.81 3.82145 3.8329
  ss  ss
&&
  wall2 wall  cylinder 2  0  301.55  7.62  1.0 0.0 1.9    && insulated
  3.81 3.82145 3.8329
  ss  ss
&& --------------- Internal    -------------------
```

```
  intern1  wall  slab  2  1  302.25  7.62  1.0  232.0
   0.00  0.0017 0.0034
   ss  ss
&& --------------- Internal  ---------------------
  intern2  floor  slab  2  1  302.25  7.62  1.0  42.696
   0.00  0.0017 0.0034
   ss  ss

&&
rad-heat
     emsvt .9 .9 .9 0.9 0.9 .65   && nhtm+pool surface
     gaswal   7.4
eoi

ht-tran  on  on  on  on  on

&&
&& sodium spray fire input
&&
&& assume fall height of 10.0, since
sprafire   hite=5.15  dme=0.00103  fna2o2=1.0  && 1030 um, fna2o2, default
  source=1  && number of table
    nal=3 iflag=1
    t=0.0   13.0 885.0
    mass=0.0 0.256 0.256
    temp=836.15 836.15 836.15
  eoi

low-cell
     geometry  45.604  && floor area (bottom head)


&& ---------------- stainless bottom head specification ---------------
     interm
         lay-nam = bothead
         compos = 1 ss  8753.0 && bottom head mass
         temp=301.55
         physics
         ht-coef name=bas-mat var-x=time
           x=2 0.0 10000.0
           y=2 0.0 0.0
         eoi
       eoi
     eoi   &&  terminate the layer

      pool
         compos  1  nal   0.
             temp  301.55
             physics
                boil
           eoi    &&   terminate physics
     eoi   &&  terminate the layer
         bc  300.0  0.85e5
eoi  &&  terminate cell 1 input
&& ------------------------ end cell 1 -------------------------

eof
```

Table B.2.3-3. Calculation Results for ABCOVE AB5

	As shown the gas temperature results, the code matches closely with the experiment. However, not all sodium reacted, which means the gas temperature may be higher for CONTAIN-LMR, if all sodium reacted. Note that although the majority of the reaction energy is added to the atmosphere, a small portion of the reaction energy is also added to the pool.
	The pressure results show some agreements between the code and experimental data.
	As shown in this figure, the total sourced sodium is 223 kg, and the amount sodium burned is 179 kg. The unburned sodium was relocated to the pool.

	Although no NaOH was predicted, the aerosol density predicted by CONTAIN-LMR is within the bulk part of the experimental data of 170 g/m^3 maximum.
	This figure shows that CONTAIN-LMR predicts similar results as from the experiment.

B.2.4 Sodium Pool Fire

This section describes the demonstration input for the sodium pool fire model (see the model details in Section 5.4). An effort has been made to benchmark the model with existing experiment. An experiment used to verify SOFIRE II code was used – one-cell experiment [Beiriger 1973]. In this experiment, a large test vessel (LTV) with a dimension of 3.048 m (10 ft) in diameter, 9.14 m (30 ft) in height and a gas volume of 62.3 m^3 (2200 ft^3). This gas volume contained gases at standard conditions. In the lower portion of the vessel, a 0.55742 m^2 (6 ft^2) steel pan was installed on a spider off the floor of the vessel. The pan was insulated with fire brick and mounted below a feed line from an external sodium pre-heat tank. A number of thermocouples were placed in the experiment. The test conditions of this one-cell experiment are shown in Table B.2.4-1. As shown in this table, three tests were done. The initial sodium mass sourced in the pool is 22.68 kg (50 lbs) for all cases. The only differences among these tests were the initial oxygen content, and pool temperatures which yield slightly different in the system pressure. In addition, this table provides the experimental oxide fraction of peroxide after the experiment. This would be used as an input condition for the CONTAIN-LMR calculation.

Because there was no specific additional information about the vessel, other than the dimensions, the heat structures modeled in CONTAIN-LMR for this experiment were assumed. Even though the experiment indicated that the steel pan holding the sodium was insulated with fire brick, a constant and small heat transfer rate from the pan to the base mat was assumed. Tables B.2.4-2 to B.2.4-4 show the input decks for Test 4, Test 5 and Test 6, respectively. The results shown in this section are preliminary. Further evaluations of the models and the experiment may be required to identify any model and/or experiment shortcomings.

For Test 4, CONTAIN-LMR predicts general trend of the experiment data. The finding is provided in Table B.2.4-5.

For Test 5, additional runs were conducted to check the sensitivity of the assumed fraction of monoxide and peroxide. By assuming 100% reaction for the monoxide, the CONTAIN-LMR greed generally with the experiment than the base case and 100% reaction for peroxide. Table B.2.4-6 provided the preliminary finding.

For Test 6, the assumed 50% reaction for peroxide yields higher pressure than the experiment data. The slope of the sodium pool's pool temperature is more pronounce for the experiment than CONTAIN-LMR. Table B.2.4-7 shows the preliminary finding for this test.

In general, the demonstration runs show that the model of the sodium pool fire in CONTAIN-LMR is working. Also the modeling of the aerosol generation from the sodium pool fire is working for CONTAIN-LMR. Additional model refinement and experiment comparison may be needed, particularly if no detail information is available for the experiments shown here.

Table B.2.4-1. Test Conditions and Data of the One-Cell Experiment [Beiriger 1973]

Parameter	Test 4	Test 5	Test 6
Weight of sodium introduced (kg)	22.68	22.68	22.68
Introduced sodium temperature (K)	811	866	866
Initial pool temperature with sodium (K)	566.6	616.5	699.8
Initial vessel oxygen (%)	21	9.25	2.0
Initial vessel pressure (kPa)	121.7	123.0	125.9
Pan Thickness (m)	0.0064	0.0064	0.00025
Sodium peroxide fraction (experimental)	0.39	0.78	-
Oxygen consumed (%)	10.7	5.3	0.34
Average gas temperature rise* (C)	48.3	27.2	7.2
Peak pressure rise (kPa)	19	10.9	2.8
Maximum bulk sodium temperature (K)	977-1037	750	700
*It was reported as in °F, but converted and recalculated using standard condition temperature of 20 °C or 68 °F			

Table B.2.4-2. Test 4 Input for CONTAIN-LMR

```
&&
&& ------------------------- one-cell---------------------------
&&          contain lmr/1 test problem 1cell – Test4
&&
&& model na pool fire –
&& using one cell experiment in AI-AEC-13055
&&   Test 4 – oxide fraction of peroxide = 0.39
```

```
&&            f1=1-0.39=0.61
&&            O2 consumed=10.7%
&&            Peak delP=2.77 psi (1.9098e4 Pa)
&&            Bulk Na T=1300-1400 F(917.6-1037.15K)
&&            Gas T Rise=87 F
&&
&&
&& --------------------- global input ---------------------------
control ncells=1 ntitl=2 ntzone=4  nsectn=10  nac=4 eoi
material
compound h2 o2 co co2 h2ol h2ov fe n2 conc uo2 pu
   u mno mgo k2o nav nal uo2 puo2 cao ssox  ss fel
   na2o2 na2o naoh na
times 60000.0   0.
&& ---------- time zones ---------------
  5.0   10.0        10.
  10.0   20.0     1000.
  10.0   20.0     2000.
  10.0   50.0     4320.

&& --------------------------------------
0.0    && cell timestep fraction


longedt 2

fast

thermo

aerosol
   deldif=1.0e-4  densty=300.
   Diam1=1.0e-08   tgas2=3000.0   pgas2=10.0e+5
   na2o2=1.0e-6  0.531
   na2o=1.0e-6   0.531
   naoh=1.0e-6   0.531
   na  =1.0e-6   0.531


prlow-cl
prheat

praer  && aerosol print
title
   contain lmr/1 test4 One-cell
     model pool fire
&& ------------ end of global input --------------
&& cell 1 models the LTV, height = 30 ft (9.14 m)
&&                        volume = 2200 ft3 (62.3 m3)
&&      1 ft3=28.3168e-3 m3
cell=1
control
  nhtm=3  mxslab=10 numtbc=2  maxtbc=3
    jint=1  jpool=1            &&
eoi
geometry  62.3  9.14   && volume and height
atmos=2  1.21685e+5  293.  && STD: 20 C, 101.325 kPa
   n2=0.79  o2=0.21
   condense
&&  atmchem
&&   h-burn
&& ------------- structures -----------------------
struc
&& --------------- vessel wall --------------------
&& name   istr  ishape  nslab ibc tint chrl vufac bctr heit
  veswal1 wall cylinder 5      0  293. 9.14 0.0 0.0 9.14 && 566.48 9.14 0.  0.   9.14
  1.524 1.534 1.544 1.555 1.565 1.575
  ss  ss  ss  ss  ss
&& --------------- cavity wall --------------------
  veswal2 wall cylinder 5      0  293. 9.14 0.0 0.0 9.14 && 566.48 9.14 0.  0.   9.144
```

```
  1.524 1.534 1.544 1.555 1.565 1.575
  ss  ss  ss  ss  ss
&& --------------- vessel roof ---------------------
  vesroof  roof slab    5      0  293. 9.14 0.0 0.0 6.82 && 566.48 9.14 0.  0.   6.82
   0.0     0.01  0.02  0.03  0.04 0.05


   ss  ss  ss  ss  ss
&&
rad-heat
     emsvt .8 .8 .8 .8   && nhtm+pool surface
     gaswal   7.4
eoi
ht-tran  on  on  on  on  on
low-cell
     geometry  0.55742  && floor area, 6 ft2


&& ---------------- stainless liner specification ---------------
     interm
       lay-nam = liner
       compos = 1 ss  28.52 && based on pan thickness of 0.25”x6ft2x503 lb/ft3 density

       temp=293.
       Physics
         ht-coef name=bas-mat var-x=time
           x=2 0.0 10000.0
           y=2 1.0e+1 1.0e+1
         eoi
       eoi


     eoi   &&  terminate the layer

      pool
         compos  1  nal   22.68 && 50 lbs
             temp  566.5   && 560 F
             physics
&&                  boil
&&
&& sodium pool fire –
               poolfire
                 ratios  0.61  0.5  0.5 0.5   &&
               eoi

           eoi    &&   terminate physics
     eoi   &&  terminate the layer
         bc  293.
Eoi  &&  terminate cell 1 input
&& ----------------------- end cell 1 ------------------------



eof
```

Table B.2.4-3. Test 5 Input for CONTAIN-LMR

```
&&
&& ------------------------- one-cell----------------------------
&&            contain lmr/1 test problem 1cell -Test5
&&
&& model na pool fire -
&& using one cell experiment in AI-AEC-13055
&&   Test 5 - oxide fraction of peroxide = 0.78
&&             f1=1-0.78=0.22
&&            initial p=3.2 psig (2.2063e4 Pa)
&&            initial T=300 K (assumed at STD)
&&            peak delP=1.59 psi (1.0962 Pa)
&&            gas T rise=49 F
&&
```

```
&&
&& --------------------- global input ---------------------------
control ncells=1 ntitl=2 ntzone=4  nsectn=10  nac=4 eoi
material
compound h2 o2 co co2 h2ol h2ov fe n2 conc uo2 pu
   u mno mgo k2o nav nal uo2 puo2 cao ssox  ss fel
   na2o2 na2o naoh na
times 60000.0   0.
&& ---------- time zones ---------------
  5.0   10.0        10.
  10.0   20.0     1000.
  10.0   20.0     2000.
  10.0   50.0     7200.

&& --------------------------------------
1.0   && cell timestep fraction

longedt 2

fast

thermo

aerosol
   deldif=1.0e-4  densty=300.
   diam1=1.0e-08   tgas2=3000.0   pgas2=10.0e+5
   na2o2=1.0e-6  0.531
   na2o=1.0e-6   0.531
   naoh=1.0e-6   0.531
   na  =1.0e-6   0.531


prlow-cl
prheat

praer  && aerosol print
title
   contain lmr/1 test4 One-cell
     model pool fire
&& ------------ end of global input --------------
&& cell 1 models the LTV, height = 30 ft (9.14 m)
&&                        volume = 2200 ft3 (62.3 m3)
&&      1 ft3=28.3168e-3 m3
cell=1
control
  nhtm=3  mxslab=10 numtbc=2  maxtbc=3
    jint=1  jpool=1            &&
eoi
geometry  62.3  9.14   && volume and height
atmos=2  1.2306e+5   293.  && STD: 20 C, 101.325 kPa
   n2=0.9075  o2=0.0925
   condense
&&  atmchem
&&   h-burn
&& ------------- structures -----------------------
struc
&& --------------- vessel wall --------------------
&& name   istr  ishape  nslab ibc tint chrl vufac bctr heit
  veswal1 wall cylinder 5      0  293.0 9.14 0.0 0.0 9.14 && 566.48 9.14 0.  0.   9.14
  1.524 1.534 1.544 1.555 1.565 1.575
  ss  ss  ss  ss  ss
&& --------------- cavity wall ---------------------
  veswal2 wall cylinder 5      0  293.0 9.14 0.0 0.0 9.14 && 566.48 9.14 0.  0.   9.144
  1.524 1.534 1.544 1.555 1.565 1.575
  ss  ss  ss  ss  ss
&& --------------- vessel roof ----------------------
  vesroof  roof slab    5      0  293.0 9.14 0.0 0.0 6.82 && 566.48 9.14 0.  0.   6.82
   0.00  0.01  0.02  0.03  0.04 0.05
   ss  ss  ss  ss  ss
&&
```

```
rad-heat
    emsvt .8 .8 .8 .8   && nhtm+pool surface
    gaswal   7.4
eoi
ht-tran  on  on  on  on  on
low-cell
    geometry  0.55742  && floor area, 6 ft2


&& ---------------- stainless liner specification ---------------
    interm
      lay-nam = liner
      compos = 1 ss  28.52 && based on pan thickness of 0.25"x6ft2x503 lb/ft3 density

      temp=293.0
      physics
        ht-coef name=bas-mat var-x=time
          x=2 0.0 10000.0
          y=2 1.0e+1 1.0e+1
        eoi
      eoi


    eoi   &&  terminate the layer

     pool
        compos  1  nal   22.68 && 50 lbs
            temp  616.5   && 650 F
            physics
&&                boil
&&
&& sodium pool fire -
              poolfire
                ratios  0.22  0.5  0.5 0.5   &&
              eoi

           eoi    &&   terminate physics
    eoi   &&  terminate the layer
        bc  293.0
eoi  &&  terminate cell 1 input
&& ----------------------- end cell 1 ------------------------



eof
```

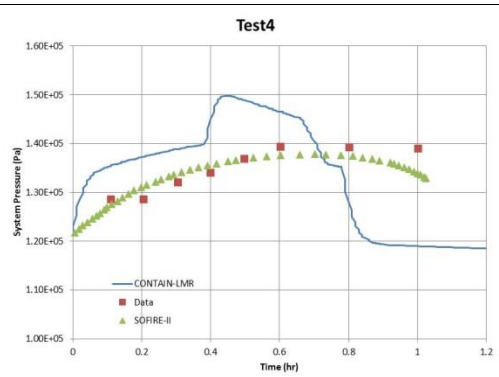
Table B.2.4-4. Test 6 Input for CONTAIN-LMR

```
&&
&& ------------------------- one-cell----------------------------
&&          contain lmr/1 test problem 1cell -Test6
&&
&& model na pool fire -
&& using one cell experiment in AI-AEC-13055
&&   Test 6 - oxide fraction of peroxide =
&&
&&          initial p=3.6 psig (2.4821e4 Pa)
&&          initial T=300 K, 80.33 F (assumed at STD)
&&          peak delP=0.41 psi (2827 Pa)
&&          gas T rise=13 F
&&
&&
&& --------------------- global input ---------------------------
control ncells=1 ntitl=2 ntzone=4  nsectn=10  nac=4 eoi
material
compound h2 o2 co co2 h2ol h2ov fe n2 conc uo2 pu
   u mno mgo k2o nav nal uo2 puo2 cao ssox  ss fel
   na2o2 na2o naoh na
times 60000.0   0.
```

```
&& ---------- time zones ---------------
  5.0   10.0        10.
  10.0   20.0     1000.
  10.0   20.0     2000.
  10.0   50.0     3600.

&& ---------------------------------------
1.0   && cell timestep fraction

longedt 2

fast

thermo

aerosol
   deldif=1.0e-4  densty=300.
   diam1=1.0e-08   tgas2=3000.0   pgas2=10.0e+5
   na2o2=1.0e-6  0.531
   na2o=1.0e-6   0.531
   naoh=1.0e-6   0.531
   na  =1.0e-6   0.531


prlow-cl
prheat

praer  && aerosol print
title
   contain lmr/1 test4 One-cell
     model pool fire
&& ------------ end of global input --------------
&& cell 1 models the LTV, height = 30 ft (9.14 m)
&&                        volume = 2200 ft3 (62.3 m3)
&&      1 ft3=28.3168e-3 m3
cell=1
control
  nhtm=3  mxslab=10 numtbc=2  maxtbc=3
    jint=1  jpool=1            &&
eoi
geometry  62.3  9.14   && volume and height
atmos=2  1.2588e+5  293.0  &&
   n2=0.98  o2=0.02
   condense
&&  atmchem
&&   h-burn
&& ------------- structures ------------------------
struc
&& --------------- vessel wall --------------------
&& name   istr  ishape  nslab ibc tint chrl vufac bctr heit
  veswal1 wall cylinder 5      0  293. 9.14 0.0 0.0 9.14 && 566.48 9.14 0.  0.   9.14
  1.524 1.534 1.544 1.555 1.565 1.575
  ss  ss  ss  ss  ss
&& --------------- cavity wall ---------------------
  veswal2 wall cylinder 5      0  293. 9.14 0.0 0.0 9.14 && 566.48 9.14 0.  0.   9.144
  1.524 1.534 1.544 1.555 1.565 1.575
  ss  ss  ss  ss  ss
&& --------------- vessel roof ----------------------
  vesroof  roof slab    5      0  293. 9.14 0.0 0.0 6.82 && 566.48 9.14 0.  0.   6.82
   0.00  0.01  0.02  0.03  0.04 0.05
   ss  ss  ss  ss  ss
&&
rad-heat
     emsvt .8 .8 .8 .8   && nhtm+pool surface
     gaswal   7.4
eoi
ht-tran  on  on  on  on  on
low-cell
     geometry  0.55742  && floor area, 6 ft2
```

```
&& ---------------- stainless liner specification ---------------
    interm
      lay-nam = liner
      compos = 1 ss  28.52 && based on pan thickness of 0.25"x6ft2x503 lb/ft3 density

      temp=293.
      physics
        ht-coef name=bas-mat var-x=time
          x=2 0.0 10000.0
          y=2 1.0e+1 1.0e+1
        eoi
      eoi


    eoi   &&  terminate the layer

     pool
        compos  1  nal   22.68 && 50 lbs
            temp  699.8   && 800 F
            physics
&&                boil
&&
&& sodium pool fire -
              poolfire
                ratios  1.0  0.5  0.5 0.5   &&
              eoi

          eoi    &&   terminate physics
    eoi   &&  terminate the layer
        bc  293.
eoi  &&  terminate cell 1 input
&& ----------------------- end cell 1 ------------------------



eof
```

Table B.2.4-5. Calculation Results for Test 4 [Beiriger 1973].

	CONTAIN-LMR seems to over-predict the pressures to about 0.7 hour before under-predict the pressures. In CONTAIN-LMR, the heat structures were modeled

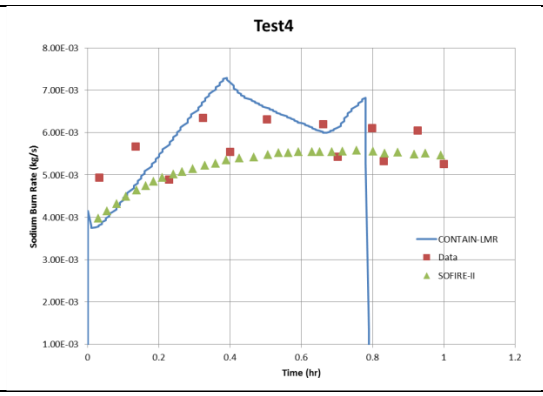
	In terms of the burn rate, CONTAIN-LMR underestimates the values at the start, but it exceeds the data at about 0.4 hour then started to decrease closely with the data, but reaction dropped off quickly at about 0.8 hour, which is limited by the model that is subjected further analysis. The percentage of oxygen consumed predicted by CONTAIN-LMR is about 6.22, significantly lower than that of the experiment and SOFIRE-II code.

Table B.2.4-6. Calculation Results for Test 5 [Beiriger 1973].

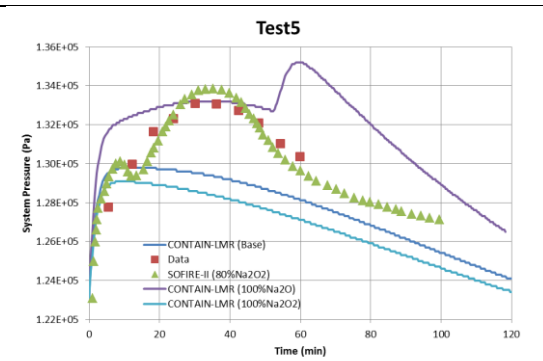
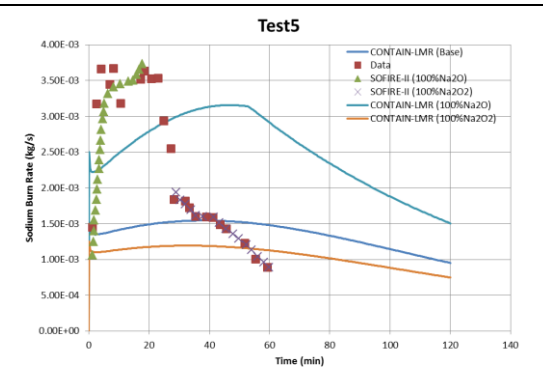
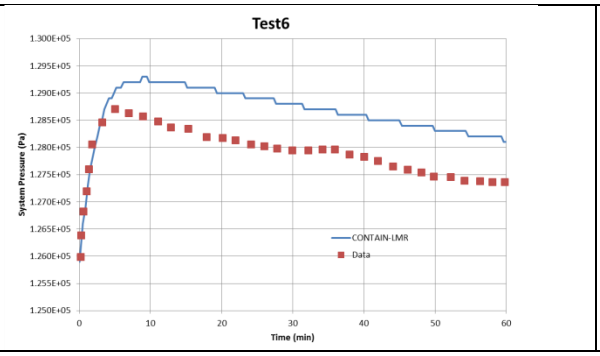
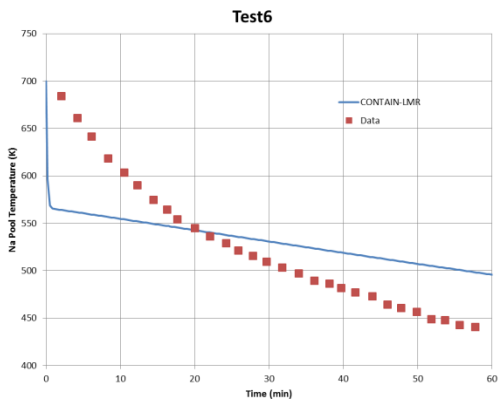
	In this case, three CONTAIN-LMR runs were conducted and results were compared with the experimental data. The base case uses the measured fraction of the monoxide. The other two cases as a sensitivity study examine if only 100% of monoxide or peroxide. The results show that the base case falls between the two sensitivity cases. Assuming 100% monoxide yields a better pressure results, because of the reaction rate. Assuming 100% peroxide under-predicts the system pressure.
	In terms of the burn rate, CONTAIN-LMR calculations underestimate the rate for the first 20 minutes of the experiment. Then the calculations overestimate the results after that time. Assuming 100% monoxide for CONTAIN-LMR yields a better burn rate, than the CONTAIN-LMR base case and 100% peroxide case. The percentage of oxygen consumed was predicted by CONTAIN-LMR is about 5.3 for the base case, 5 for the peroxide case and 6 for monoxide case.

Table B.2.4-7. Calculation Results for Test 6 [Beiriger 1973].

	CONTAIN-LMR estimates the oxygen consumed is 0.52 percent where the data yields only 0.34 percent. In terms of prediction in system pressure, CONTAIN-LMR yields a slightly high over pressure trend.

	In terms of the sodium pool temperature, CONTAIN-LMR predicts the pool temperature decreases rapidly as it conducts to the heat the pan, which was assumed to have a 293 K. In the experiment, the pool temperature was measured after the spill, so the pan may have a similar temperature as the sodium pool. In terms of the slope of the temperature decreases, the experiment predicts deeper slope than that of CONTAIN-LMR. If the pan was insulated, the only mode of rapid temperature decrease is due to heat transfer to the structure, since the pressure of the experiment seems to be lower than CONTAIN-LMR. The gas temperature from the experiment after the fire was 308 K, where CONTAIN-LMR calculated the maximum gas temperature of 301 K. Additional sensitivity studies may be required to benchmark this test.

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