SAND2017-3798J

Containment Sodium Chemistry Models in MELCOR

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Abstract

To meet regulatory needs for sodium fast reactors' future development, including licensing requirements, Sandia National Laboratories is modernizing MELCOR, a severe accident analysis computer code developed for the U.S. Nuclear Regulatory Commission (NRC). Specifically, Sandia is modernizing MELCOR to include the capability to model sodium reactors. However, Sandia's modernization effort primarily focuses on the containment response aspects of the sodium reactor accidents. Sandia began modernizing MELCOR in 2013 to allow a sodium coolant, rather than water, for conventional light water reactors. In the past three years, Sandia has been implementing the sodium chemistry containment models in CONTAIN-LMR, a legacy NRC code, into MELCOR. These chemistry models include spray fire, pool fire and atmosphere chemistry models. Only the first two chemistry models have been implemented though it is intended to implement all these models into MELCOR. A new package called "NAC" has been created to manage the sodium chemistry model more efficiently. In 2017 Sandia began validating the implemented models in MELCOR by simulating available experiments. The CONTAIN-LMR sodium models include sodium atmosphere chemistry and sodium-concrete interaction models. This paper presents sodium property models, the implemented models, implementation issues, and a path towards validation against existing experimental data.

Keywords:

MELCOR, sodium fast reactors, sodium chemistry, reactor safety, sodium spray fire, sodium pool fire

1 Introduction

This paper describes the implementation of the containment sodium chemistry models into MELCOR as a containment accident analysis tool to be used for analyzing sodium fast reactors (SFRs). MELCOR is currently employed by the NRC for light water reactor (LWR) source-term assessments, Level 2 and Level 3 probabilistic risk analyses, and containment design basis accident analysis [Tills 2008, Tills 2009 and Tills 2010].

To meet future design basis analysis needs [Schmidt 2011], sodium chemistry models are being implemented into the MELCOR code to simulate SFR designs. Many SFR sodium chemistry models have been incorporated into the CONTAIN-LMR code, a liquid metal reactor (LMR) version released in the 1990s [Murata 1993, Scholtyssek 1994]. CONTAIN-LMR has been used in many countries for analyzing the containment behavior of SFR accidents [Carroll 1990]. The implementation of the sodium models from CONTAIN-LMR into MELCOR was initiated as a part of the Advanced Reactor Technology Program at the U.S. Department of Energy (DOE). Starting in 2013, sodium properties were added into MELCOR as an alternative to a water coolant for LWR applications. Implementation of the CONTAIN-LMR sodium chemistry models for pool and spray fire models and related atmospheric chemistry reactions are expected to be completely implemented in 2017. The implementation approach includes porting the

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model subroutines from CONTAIN-LMR source code into MELCOR (including examining MELCOR code structures and the best suitable locations for implementations) and developing the associated interfaces to the MELCOR interface. The models implemented from CONTAIN-LMR include:

- Atmosphere chemistry model specifies the reactions of the sodium and sodium products to water and oxygen in the atmosphere, aerosol, and condensable film. This models uses a mechanistic model approach.
- Spray fire model specifies the reactions of the sodium droplets with oxygen. This model was based on the modeling from the NACOM code [Tsai 1980].
- Pool fire model specifies the reactions of sodium pool with oxygen. This model was based on the SOFIRE II code [Beiriger 1973].
- Sodium-concrete interaction (or reaction) model – this model is based on the SLAM code [Suo-Anttila 1983].

In this paper, the sodium properties and equation of state (EOS) in MELCOR is described first. Then this paper presents the CONTAIN-LMR sodium chemistry models to be implemented into MELCOR, including the development of a new package, “NAC,” which represents sodium chemistry. NAC is intended to house all sodium specific models. Section 4 describes the issues related to the implementation of the models into MELCOR and the subsequent re-mediations proposed to address these issues. Validation of the models is also in progress using available validation experiments. Section 6 describes several of these validation tests; however, results are preliminary and not included. Instead, we will discuss the limitation of the CONTAIN-LMR sodium models in MELCOR when modeling available experiments in Section 6.

2 Sodium Property Model

As described in Section 1 the default coolant in MELCOR must be changed from water to sodium to modernize MELCOR for analyzing SFR accidents. To do that, the implementation and testing of sodium properties into MELCOR began in 2013. 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 needed to be provided to replace those currently used for water. There are a considerable number of data sources for sodium thermophysical properties that could be implemented into MELCOR.As a part of SFR accident modeling effort, the Fusion Safety Database (FSD) [Merrill 2000] and SIMMER database [Schmidt 2010] as data sources for the sodium thermophysical properties implemented in MELCOR. Subsequent work in the SUMMER database includes the equation of state (EOS) from SAS4A [Calhalam 1994, Dunn 2012], but this work does not leverage a historical effort like the FSD and SIMMER EOSs.

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 redirected to the appropriate routines (SIMMER database) or tabular lookup (FSD database) for the sodium properties. To simplify code maintenance requirements and user input, the supporting code changes and input requirements for the SIMMER database and FSD database were structured so that they were as similar as possible. To activate the liquid metal capability, an unformatted file must be present in order to activate a particular fluid’s EOS for the simulation. For the FSD database, this unformatted file contains all properties needed for the simulation. Table 1 presents the corresponding fluid types and file names. As shown in Table 1, Fluid 7 and Fluid 20 are intended for sodium using FSD and SIMMER database, respectively.

Table 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

3 Sodium Chemistry Models

Once the fluid properties of sodium were in place, the development of the sodium chemistry models using these properties could be done. In this section the sodium chemistry models to be used to simulate SFR containment accidents are described. As previously described in Section 1, the sodium chemistry models were originated from the CONTAIN-LMR code. In addition to reviewing the CONTAIN-LMR manual [Murata 1993], the CONTAIN-LMR source code was also examined and tested to identify any discrepancy in the models and the model descriptions in the manual before implementing the models into MELCOR. CONTAIN-LMR sodium chemistry models can be divided into two types: interactions with the atmosphere constituents and interactions with the concrete constituents (see Figure 1). Sections 3.1 to 3.3 present the sodium interactions with atmospheric constituents followed by the discussions of the sodium-concrete interaction model in Section 3.4. The models involving the atmospheric constituents include the Atmospheric Chemistry model (see Section 3.1), Spray Fire model (see Section 3.2) and Pool Fire model (see Section 3.3). The sodium-concrete interaction model will not be discussed in detail since this model is still being implemented into MELCOR.

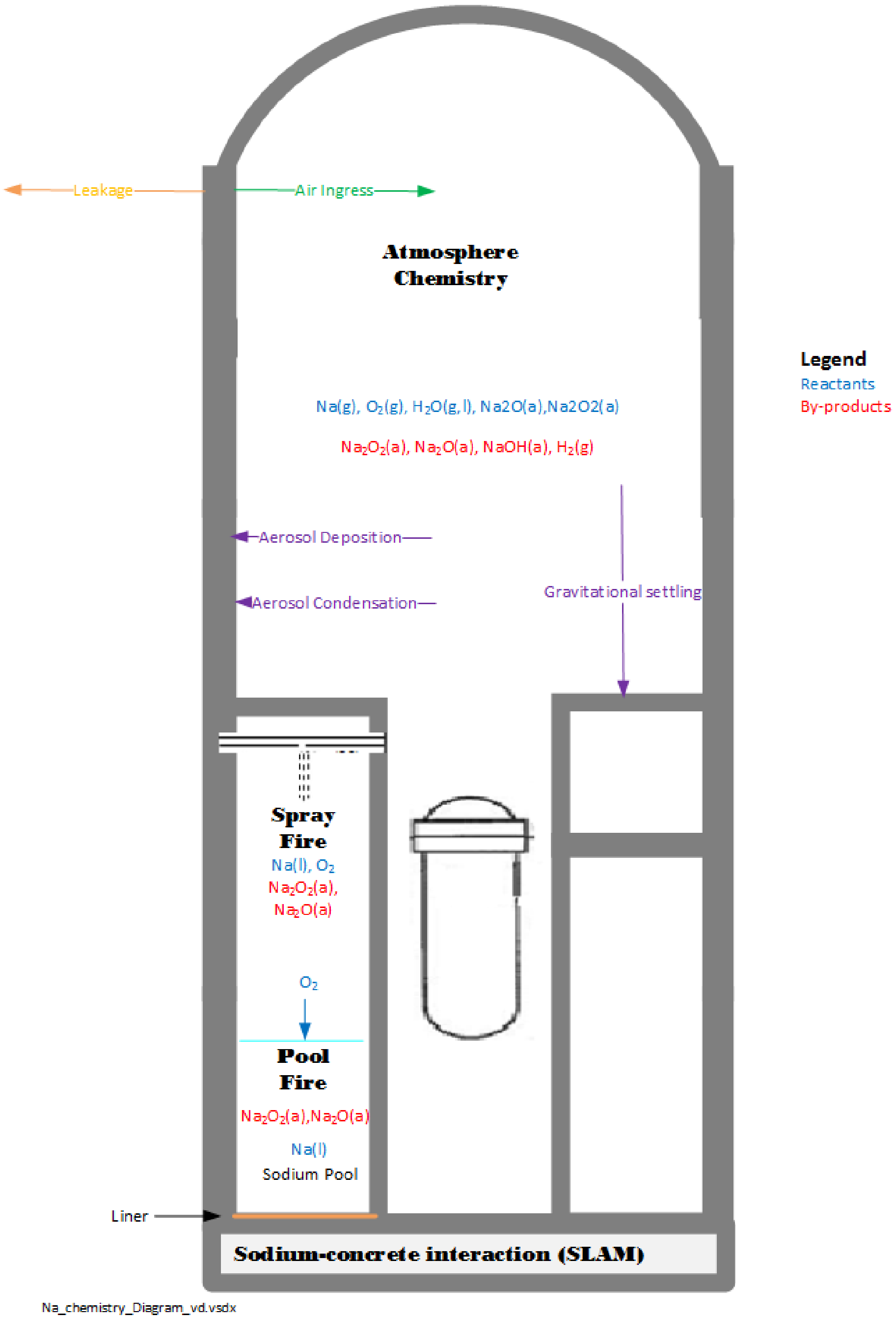

Figure 1. Sodium Chemistry Models.

3.1 Atmosphere Chemistry

When a breach of the primary coolant system occurs, the potential chemical reactions of sodium coolant with atmospheric constituents in the containment are of great interest in liquid metal reactors. Depending on the accident scenarios, the sodium vapor could react chemically with any oxygen or water present. These reactions are generally exothermic, which can add thermal load to the containment system. In addition, any hydrogen generated by the sodium chemical reactions may have additional consequences, such as hydrogen combustion or explosions.

3.1.1 Gas Chemistry

The first reaction is

$$\mathbf{Na + H_2O\ (l)\ \rightarrow NaOH + \frac{1}{2}H_2} \qquad (1)$$

Reaction (1) is assumed to occur only for liquid phase water (denoted as l in Equation 1) and sodium in contact with an aerosol particle, mingling aerosol deposits and condensate films on surfaces. Because the water is required to be liquid, the experimentally observed inhibiting effect of oxygen on reactions of water vapor and sodium is assumed to be inapplicable. This requirement assumes that either the temperature is relatively low (below the critical point of water) or the presence of a small amount of liquid water is traceable to numerical effects. As shown in this reaction, hydroxide is expected to be the principal reaction product with water at low temperatures or with excess water. Conversion from hydroxide to monoxide is not modeled.

For this reaction, Na species include Na (g) and NaOH. Other materials involve H_2O(l) and H_2.

The second reaction is:

$$\mathbf{2\ Na + H_2O\ (g)\ \rightarrow Na_2O + H_2} \qquad (2)$$

This reaction is used when the phase of water is vapor (denoted as g in Equation 2). It is presumably correct at high temperatures with excess sodium. At low temperatures (~200 C) with excess sodium [Wierman 1976], the use of reaction (2) may produce excess hydrogen per mole of water vapor. This reaction is also appropriate when water vapor is present, particularly when there is an excess of water vapor over oxygen. In this case, the water vapor is assumed to react not only with sodium vapor in the atmosphere, but also with sodium in aerosol form or in the form of aerosol deposits or films on surfaces. However, the reaction rate for reaction (2) at the surface with water is assumed to be limited by the evaporation rate of water from the surface. The sodium species include Na and Na_2O. Other species include H_2O (g) and H_2.

After the reactions with water, if any, oxygen in the atmosphere is assumed to react with sodium to form monoxide and peroxide, respectively, as follows:

$$\mathbf{2\ Na + \frac{1}{2}O_2\ \rightarrow Na_2O} \qquad (3a)$$

$$\mathbf{2\ Na + O_2\ \rightarrow Na_2O_2} \qquad (3b)$$

For reaction (3a) and (3b) for monoxide versus peroxide as products, this fraction relies on the input fraction parameter “$\mathbf{f_{ox}}$”, which represents the fraction of monoxide in the total reactions with oxygen. Thus reactions (3a) and (3b) can be rewritten as

$$2\ \mathbf{Na + (1 - 0.5 \cdot f_{ox})O_2\ \rightarrow f_{ox} \cdot Na_2O + (1 - 0.5 \cdot f_{ox}) \cdot Na_2O_2} \qquad (4)$$

Reactions (1) to (4) also are assumed to occur with sodium aerosols, sodium aerosol deposits, and sodium films, in that order.

Two subsequent reactions take place when peroxide and monoxide have been formed. The first subsequent reaction is peroxide reacting with sodium.

$$\mathbf{Na_2O_2 + 2\ Na \rightarrow 2\ Na_2O} \tag{5}$$

Reaction (5) is always assumed to occur if the peroxide and condensed sodium are in contact as a consequence of being present on the same aerosol particle or by the mingling of the aerosol deposits and condensate film on a surface. The order of reaction is aerosol particles first, and then aerosol deposits.

The second subsequent reaction is for sodium monoxide and peroxide to react with water, forming sodium hydroxide.

$$\mathbf{Na_2O + H_2O\ (g) \rightarrow 2\ NaOH} \tag{6}$$

$$\mathbf{Na_2O_2 + H_2O\ (g) \rightarrow 2\ NaOH + \frac{1}{2} O_2} \tag{7}$$

Water vapor is assumed to react with aerosol particles and aerosol deposits in that order. While the hydroxide is expected to be the principal reaction product with water at low temperatures or with excess water, the possible subsequent conversion of the hydroxide to the monoxide is not modeled if conditions change. The chemical reaction models presented here assume that all reaction heat is retained only by the gases present or by the structures; the models ignore the increase in the aerosols heat content or aerosol deposits due to an increase in temperature above the temperature of the formation. The heat generated by the surface reactions is assumed to be deposited at surface nodes of the structures involved. This treatment is regarded as conservative.

The reaction energy of the reactions listed above is based on the enthalpy change of each reactant and byproducts in the reaction. All change of enthalpy ($\mathbf{\Delta H}$) in J/kg-mole are computed assuming a reference temperature, $\mathbf{T_{ref}}$= 298.15 K.

$$\mathbf{\Delta H_{H2O} = 2.86 \times 10^8 - 0.5 \cdot H_{O2}(T_{ref}) \cdot MW_{O2} - H_{H2O} \cdot MW_{H2O}} \tag{8}$$

$$\mathbf{\Delta H_{Na2O} = 4.16 \times 10^8 - 2 \cdot H_{Na}(T_{ref}) \cdot MW_{Na} - 0.5\ H_{O2} \cdot MW_{O2} + H_{Na2O} \cdot MW_{Na2O}} \tag{9}$$

$$\mathbf{\Delta H_{Na2O2} = 5.05 \times 10^8 - 2 \cdot H_{Na}(T_{ref}) \cdot MW_{Na} - H_{O2} \cdot MW_{O2} + H_{Na2O2} \cdot MW_{Na2O2}} \tag{10}$$

$$\mathbf{\Delta H_{NaOH} = 4.27 \times 10^8 - H_{Na}(T_{ref}) \cdot MW_{Na} - 0.5\ H_{O2} \cdot MW_{O2} - 0.5\ H_{H2} \cdot MW_{H2} + H_{NaOH} \cdot MW_{NaOH}} \tag{11}$$

The reaction heat per unit mole for the above reactions is provided in Table 2. As shown in this table, the reaction equations above are repeated in Column 2. Column 3 provides the location of the reactions. The last column in this table shows the heat generated in the reaction.

Table 2. Atmospheric Chemistry Reactions Data and Applications

#	Reaction	Locations	Reaction Heat
1	$Na + H_2O\ (l) \rightarrow NaOH + \frac{1}{2} H_2$	Reactions within aerosol particles or within aerosol deposit or condensable film	$\Delta H_{NaOH} - \Delta H_{H2O}$
2	$2\ Na + H_2O\ (g) \rightarrow Na_2O + H_2$	Reactions with gases,	$\Delta H_{Na2O} - \Delta H_{H2O}$

		aerosols with gases, and deposits or film with gases	
3	$2\,\mathrm{Na} + \frac{1}{2}\mathrm{O_2} \rightarrow \mathrm{Na_2O}$ $2\,\mathrm{Na} + \mathrm{O_2} \rightarrow \mathrm{Na_2O_2}$	See below	See below
4	$2\,\mathrm{Na} + (1 - 0.5 \cdot \mathrm{f_{ox}})\mathrm{O_2} \rightarrow \mathrm{f_{ox}} \cdot \mathrm{Na_2O} + (1 - 0.5 \cdot \mathrm{f_{ox}}) \cdot \mathrm{Na_2O_2}$	Reactions of gases with gases, aerosols, and deposits/film	$\mathrm{f_{ox}} \cdot \Delta\mathrm{H_{Na2O}} + (1 - \mathrm{f_{ox}}) \cdot \Delta\mathrm{H_{Na2O2}}$
5	$\mathrm{Na_2O_2} + 2\,\mathrm{Na} \rightarrow 2\,\mathrm{Na_2O}$	Contact reactions within an aerosol particle or within aerosol deposits or condensable film. aerosol reaction with excess sodium in the atmosphere, and aerosol reactions on the film	$\Delta\mathrm{H_{Na2O}} - 0.5\,\Delta\mathrm{H_{Na2O2}}$
6	$\mathrm{Na_2O} + \mathrm{H_2O}\ (\mathrm{g}) \rightarrow 2\,\mathrm{NaOH}$	Reactions within a repository, such as within an aerosol, aerosol deposit or condensable film, reactions of aerosol with gas, and reacting deposits or film with gases	$\Delta\mathrm{H_{NaOH}} - 0.5\,(\Delta\mathrm{H_{Na2O}} + \Delta\mathrm{H_{H2O}})$.
7	$\mathrm{Na_2O_2} + \mathrm{H_2O}\ (\mathrm{g}) \rightarrow 2\,\mathrm{NaOH} + \frac{1}{2}\mathrm{O_2}$		$\Delta\mathrm{H_{NaOH}} - 0.5(\Delta\mathrm{H_{Na2O2}} + \Delta\mathrm{H_{H2O}})$

This atmosphere chemistry model considers a number of reactions involving gases (oxygen, hydrogen, and sodium), aerosols (water, sodium, sodium hydroxide, sodium monoxide, and peroxide), and deposits and condensate film on the heat structures.

3.1.2 Combustion of Sodium Hydrogen Jets

A sodium-induced hydrogen deflagration model is included in this atmosphere chemistry model. The sodium-induced hydrogen deflagration model is used to consume the hydrogen in the presence of sodium. In this model, CONTAIN-LMR utilizes the standing flame model for hydrogen burn. If the standing flame model is active in the current volume, each flow path into the volume is monitored for temperatures and concentrations of hydrogen and sodium. If the flow entering has a temperature greater than 533.1 K, a hydrogen mole fraction greater than 0.1, and a sodium density greater than 0.006 kg per cubic meter of hydrogen, and there is at least 8% molar oxygen in the atmosphere, a burn is initiated. If sufficient oxygen is present, all the hydrogen entering with the sodium is consumed:

$$\mathbf{H_2(g) + 0.5O_2(g) \rightarrow H_2O(g)} \tag{12}$$

where the reaction energy is 1.43×10^8 J/kg of hydrogen consumed. This energy will be deposited in the atmosphere.

The sodium-induced hydrogen deflagration model requires the donor cell (or volume) information on flow and the state of the gases and aerosols coming into the present cell or volume. Thus this model is considered to be an inter-cell or inter-volume model, rather than an intra-cell (or intra-volume) model.

3.2 Spray Fire

The spray fire model is based on the phenomenological model used in NACOM, a code developed and tested at Brookhaven National Laboratory [Tsai 1980]. However, the model for the sodium reaction with water vapor in NACOM is not considered in MELCOR (the model adapted from CONTAIN-LMR). In this model an initial size distribution is assumed from a correlation using a specified mean droplet diameter. This correlation is based on the partitioning of the injected sodium spray source among 11 discrete droplet-size classes according to the Nukiyama-Tanasawa correlation [Tsai 1980]:

$$\mathbf{\frac{dF_v}{dD} = A^6 \frac{D^5}{120} \cdot EXP(-A \cdot D)} \tag{13}$$

where $\mathbf{A} = 3.915/\mathbf{\bar{D}}$, $\mathbf{\bar{D}}$=average droplet ($\mathbf{D}$), and $\mathbf{F_v}$= Volume fraction of spray which contains droplets of diameters smaller than $\mathbf{D}$.

A downward flow with a terminal velocity is generally assumed. The fall time of each droplet class is based on the user-specified fall height and its terminal velocity. The combustion rate of the spray fire is integrated over the droplet's fall to obtain the total sodium burned mass (as a function of droplet size), fall velocity, and atmospheric conditions (see Figure 2). The mass burn rate of the droplet is computed as:

$$\mathbf{D_n^2 = D_o^2 - K \cdot t} \tag{14}$$

Where $\mathbf{D_n}$= new time droplet diameter, $\mathbf{D_o}$= old time droplet diameter, $\mathbf{t}$ = time, and $\mathbf{K}$= reaction coefficient (or burn rate), which is given as:

$$\mathbf{K = \frac{8 \cdot k}{C_p \rho} ln(1 + B)} \tag{15}$$

Where $\mathbf{k}$= gas mixture heat conduction, $\mathbf{C_p}$= heat capacity of gas mixture, $\boldsymbol{\rho}$= density of the gas mixture, and $\mathbf{B}$ is defined as

$$\mathbf{B = \frac{C_p \cdot (T_g - T_s) + Q_c X_o}{h_{fg}}} \tag{16}$$

Where $\mathbf{T_g}$= gas temperature, $\mathbf{T_S}$= droplet temperature, $\mathbf{h_{fg}}$= heat of evaporation, $\mathbf{X_o}$= ambient oxygen mole fraction, and $\mathbf{Q_c}$= heat of combustion, which is depicted in Figure 2.

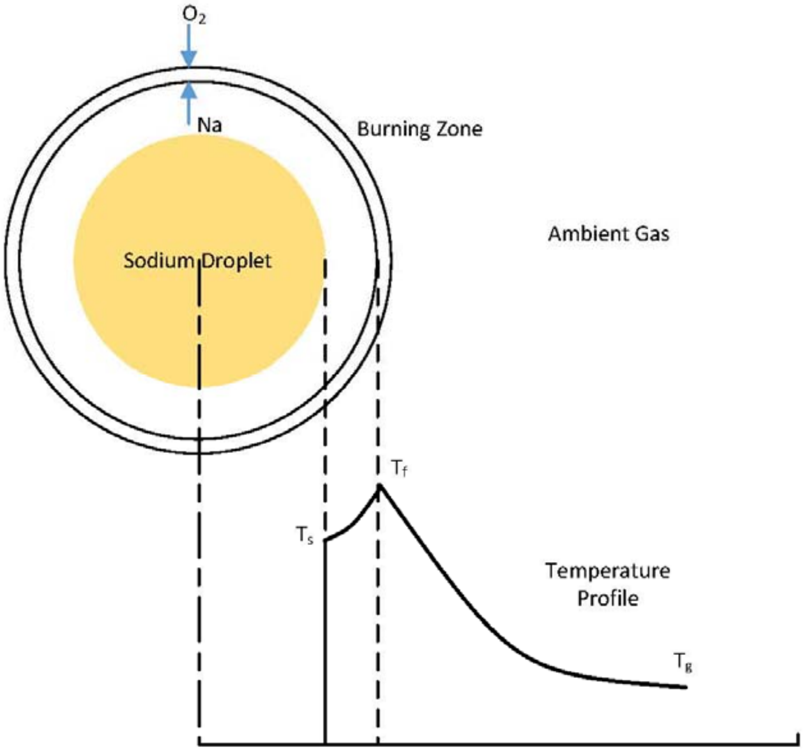

Figure 2. Schematic of a Burning Spray (Na) Droplet.

In the spray fire model, reactions (3a) and (3b) above are the two chemical reactions of sodium droplet and oxygen in the air.

The combustion energy is computed based on the mole fraction of sodium ($F_{peroxide}$) to peroxide (Na_2O_2) as given by the following correlation [Tsai 1980]

$$\mathbf{S} = (\mathbf{1.3478 \cdot Fperoxide})/(\mathbf{1.6957} - \mathbf{0.3479 \cdot Fperoxide}) \tag{17}$$

Heat combustion, $\mathbf{Q_c}$(J) is then calculated as [Tsai 1980]

$$\mathbf{Q_c} = (1\text{-}S)\cdot 9.1797\times10^6 + S\cdot 10.46\times10^6 \tag{18}$$

The duration of this sodium source and the available oxygen determines the combustion time and the amount of the byproducts (sodium monoxide and sodium peroxide as aerosols) and the reaction heat to be generated. If a droplet of a given size is not predicted to burn completely, a temporal, numerical integration of the droplet fall is performed (based on droplet terminal velocity). The time increment for the integration is taken as 1/8 of the fall time initially determined. Following each time increment of integration for the combustion equation, a resulting droplet diameter is determined for a new droplet terminal velocity. The combustion heat is reduced by the sensible heat required to raise the droplet mass to 1154 K (sodium boiling point at 1 atmosphere), and then the net energy is transferred to the atmosphere. This heat balance results in a new value for the droplet temperature. The process continues until the droplet is either consumed or reaches the floor, forming a pool.

Note that this model only models the spray in the downward direction. It does not model the upward direction of the spray. No interaction of the surface structure is modeled. Any unburned sodium from the spray fire model may fall onto a pool. In order to activate the pool fire in conjunction with the sodium spray, the pool fire model must be enabled (see Section 3.3).

3.3 Pool Fire

This sodium pool fire model is based on the SOFIRE II code [Beiriger 1973]. The SOFIRE II model was based on experiment verifications, 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. The test vessel had a diameter of 3.05 m (10 ft), with a height 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 hung above 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.

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

$$(\mathbf{1}+\mathbf{f_1})\cdot\mathbf{2}\cdot\mathbf{Na}+\ \mathbf{O_2}\rightarrow\mathbf{2}\cdot\mathbf{f_1}\cdot\mathbf{Na_2O}+(\mathbf{1}-\mathbf{f_1})\cdot\mathbf{Na_2O_2}+\mathbf{Q}(\mathbf{reaction}) \qquad (19)$$

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

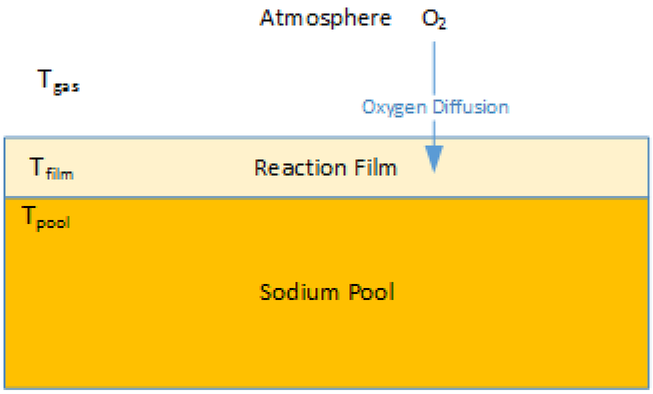

Figure 3. Pool Fire Chemistry Model Schematic.

The above reaction requires oxygen in the air to diffuse to the sodium pool (see Figure 3). CONTAIN-LMR uses a diffusion constant, $\mathbf{D_O}$ (m^2/s) for oxygen-nitrogen mixtures [Murata 1993]:

$$\mathbf{D_O}=\mathbf{6.4315}\times\mathbf{10^{-5}}\,\frac{\mathbf{T_{film}}^{\mathbf{1.823}}}{\mathbf{P}} \qquad (20)$$

where $\mathbf{T_{film}}$ = average temperature of the pool and atmosphere (K) and $\mathbf{P}$ = system pressure (Pa). Using Equation (20), the oxygen transport velocity ($\mathbf{v_{O2}}$) to the pool surface is given by [Beiriger 1973]:

$$\mathbf{v_{O2}}=\mathbf{0.14}\cdot\mathbf{D_O}\cdot\left(\frac{\mathbf{9.8}\cdot\frac{\boldsymbol{\mu}}{\mathbf{D_O}\cdot\bar{\mathbf{T}}}}{\boldsymbol{\mu}^{\mathbf{2}}}\left|\mathbf{T_p}-\mathbf{T_g}\right|\right)^{\mathbf{0.33333}} \qquad (21)$$

where $\mathbf{\mu}$= kinematic viscosity of the gas mixture evaluated at $\overline{\mathbf{T}}$, which is defined as an average of gas temperature ($\mathbf{T_g}$) and pool surface temperature ($\mathbf{T_p}$). Thus, the oxygen consumed rate, $\dot{\mathbf{m}}_{\mathbf{O2}}$, is computed as:

$$\dot{\mathbf{m}}_{\mathbf{O2}} = \mathbf{A_p} \cdot \mathbf{v_{O2}} \cdot \mathbf{\rho_g} \frac{\mathbf{m_{O2}}}{\mathbf{m_g}} \tag{22}$$

Where $\mathbf{A_p}$= pool area, $\mathbf{\rho_g}$= gas mixture density, $\mathbf{m_g}$= mass of total gas mixture, and $\mathbf{m_{O2}}$ = the mass of oxygen. The sodium burn rate can be calculated from Equation (22). There is a limit of the sodium burn rate initially, which is one-half of the initial pool mass divided by the incremental time step in CONTAIN-LMR.

In this pool fire model, the amount of the products and reaction energy to the pool and to the atmosphere of the volume are partitioned through three additional fractional inputs:

- $\mathbf{f_2}$ is the fraction of sensible heat from the reaction to the pool. The remainder will be directed to the atmosphere layer of the cell.
- $\mathbf{f_3}$ 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.
- $\mathbf{f_4}$ 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.

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 surroundings may result in differences in the burning rate.

A sodium pool may form in the reactor cavity area or a room where a possible sodium leakage is postulated, which can play an essential role in SFR accident analyses. The modeling described in this paper is limited to the heat transfer models within the sodium pool with hot surfaces, such as hot debris.

3.4 Sodium-Concrete Interaction

When sodium leaks onto a concrete floor, there is a potential chemical reaction between the sodium and the concrete material. Although the concrete is normally lined with steel to protect against the direct contact of the sodium, there are heat transfers between the liquid sodium and the liners that could potentially heat up the concrete floor, which will cause the concrete to dry out. Both carbon dioxide and moisture released from the concrete can interact with sodium if the liner is penetrated. Thus, sodium-concrete interaction can occur. The model treatment in CONTAIN-LMR is based on the experiments done at Sandia regarding the sodium limestone ablation model (SLAM) [Suo-Anttila 1983, Westrich 1983]. This report provides only a brief description of SLAM.

SLAM uses a nodalized representation of the concrete with models for heat transfer, water migration, water and CO_2 evolution, and chemical ablation of exposed concrete surface (see Figure 4). As shown Figure 4, SLAM consists of three regions. The topmost region is the pool region, but the nodalization is associated with the boundary layer where the ablation occurs. Below this region is the dry concrete region. Below the dry concrete region is the wet concrete region. Also shown in this figure, the constituents that can be included within SLAM includes SiO_2, Na_2SiO_3, Na_2O, CaO, $CaCO_3$, graphite, $MgCO_3$, and MgO as solid; Na, NaOH and Na_2CO_3 as liquid; and H_2, H_2O and CO_2 as gases. The major reactions considered in SLAM are given as:

$$H_2O + Na \rightarrow NaOH + \frac{1}{2} H_2 \tag{23}$$

$$CO_2 + 2\ Na \rightarrow 4\ Na_2O + C \tag{24}$$

$$3\ CaCO_3 + 4\ Na \rightarrow 2\ Na_2CO_3 + 3\ CaO + C \tag{25}$$

$$3\ MgCO_3 + 4\ Na \rightarrow 2\ Na_2CO_3 + 3\ MgO + C \tag{26}$$

$$2\ NaOH + CaCO_3 \rightarrow CaO + H_2O + Na_2CO_3 \tag{27}$$

$$2\ NaOH + SiO_3 \rightarrow H_2O + Na_2SiCO_3 \tag{28}$$

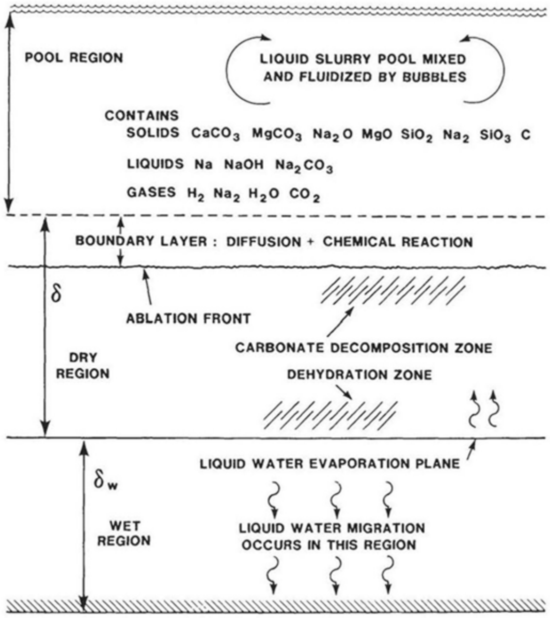

Figure 4. Schematic Diagram of SLAM [Suo-Anttila 1983].

Detailed descriptions of these three regions are:

Pool region: The pool region contains a sodium pool region with all of the reaction products from the sodium-concrete interaction. Materials are assumed to be well-mixed and isothermal. The pool changes composition which results in swelling with time during SLAM. The swelling is caused by the addition of gases and reaction products of lower density than the reactants.

Dry region: The dry region contains the dehydrated concrete region and the boundary layer of the pool region. Almost all the important reactions occur within the boundary layer of the dry region. At the interface, the ablation is presumed to occur by two mechanisms: dissolution and reaction. This region can swell or shrink (this region moves with the penetration front).

Wet region: The wet region is the concrete region that contains water. The distribution of the water is important because it determines the amount which can be evaporated and available for the reactions with sodium at the boundary layer.

The SLAM model solves the conservation equations, taking into account the reaction species in the pool and dry regions. The model will provide the average dry zone temperature, concrete reaction heat, heat flux into the wet zone, ablation velocity, dry zone growth rate, dry zone water, and CO_2 fluxes. SLAM does not model the steel liner of the concrete. In SLAM (see Figure 5), the boundary layer (between dry and pool layers) consists of 12 nodes, while the dry region consists of 15 nodes. Each node has the same thickness or size; each node can vary with the changing dimensions of the dry concrete region. The thickness of the boundary layer is subjected to change in terms of increasing or decreasing in the course of a problem. The dry concrete region will increase when the thermal penetration rate of the concrete exceeds the ablation rate and will decrease when the converse is true. The bottom most region is the wet concrete region where evaporable water may still be found in the concrete as shown in Figure 5. The number of equations depends on the number of dry nodes, which is given by 50 – ndry + 2.

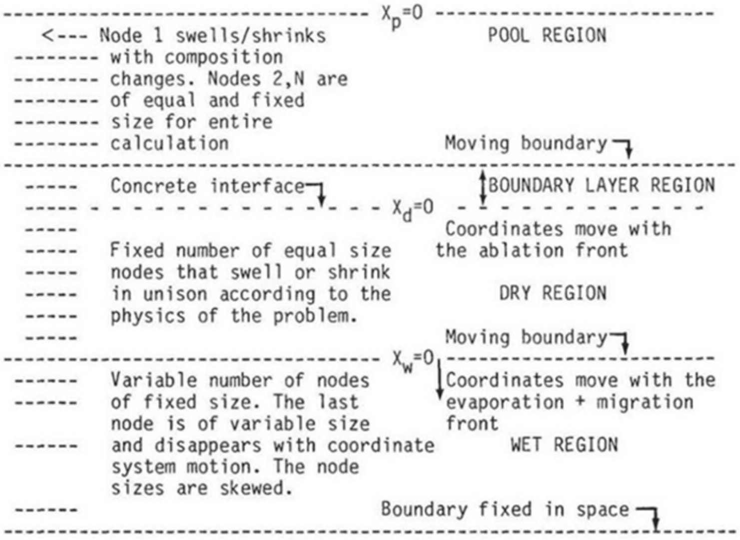

Figure 5. The SLAM Systems
(subscripts p, d, and w refer to pool, dry, and wet respectively) [Suo-Anttila 1983].

In SLAM, the gas generation of carbonate dioxide and water vapor is due to the heat that is generated in the reaction zone and conducted into the concrete. When the concrete temperatures reach a few hundred degrees Celsius, chemically bound water is released from the cement paste. A number of correlations were developed to assume the release rates as a function of temperature only. The decomposition of $MgCO_3$ is estimated from the $CaCO_3$ decomposition. However, gCO_3 decomposes at lower temperature than $CaCO_3$ [Suo-Anttila 1983].

$$\mathrm{S_{CO_2}} = \rho_{\mathrm{CaCO_3}} 3.3 \times 10^{5} \mathrm{e}^{-19362/\mathrm{T}} \tag{29}$$

$$\mathrm{S_{CO_2}} = \rho_{\mathrm{MgCO_3}} 4.2 \times 10^{8} \mathrm{e}^{-19362/\mathrm{T}} \tag{30}$$

$$\mathrm{S_{H_2O}} = \rho_{\mathrm{H_2O}} 3.3 \times 10^{10} \mathrm{e}^{-20560/\mathrm{T}} \tag{31}$$

Where S is the release rate in kg/m^3-sec, ρ =density of the gas or binding material (kg/m^3), and T = temperature (K). Note that these gas generation rates cause the concrete to degas at any temperature.

In CONTAIN-LMR, a user has the ability to prescribe the SLAM reaction by providing a start and end time and maximum internal timestep. A user can also provide a layer temperature for the steel liner to be failed to start SLAM reaction. However, the liner is assumed to disappear from the problem when the failure occurs. The major subroutines from CONTAIN-LMR to be implemented into MELCOR include:

- SLAM –This is the major physics routine for this model. It is called by CONCRM subroutine.
- CONEQS – This routine calculates the water release and heat transfer in the concrete, including both interface heat flux from the middle and bottom layers of concrete. It also does the integration of the heat transfer and mass changes. It calls set up Gaussian integration and then estimates the average diffusion coefficient for reactants and by-products at the average temperature of the layers.
- SORGAS – This routine computes the CO_2 and H_2O gas release.
- CONCRM – controlling routine for modeling SLAM in a concrete layer in the CONTAIN-LMR lower cell. It is used to set up the boundary layer between the pool and concrete regions. CONCRM first calls chemical reaction data for SLAM and initialization of the SLAM calculations. Then it computes the initial set of the SLAM coordinate system, including the water migration coordinates. CONCRM requires that no more than 33% of the pool mass is involved in the reaction and, if this condition is met, then SLAM computes the sodium-concrete interaction physics.

4 Implementation Issues

MELCOR only allows a single coolant in a given problem. In MELCOR, the water equation of state was replaced or substituted with the sodium equation of state. Unlike in MELCOR, CONTAIN allows two condensables, such as water and sodium in the problem. However, CONTAIN does restrict that only a single coolant can be modeled in a given volume or cell.

In that case, without the ability to add water as a condensable, the only way to model both sodium and water in a given problem is to treat water as an aerosol. Water aerosol has its vapor pressure from liquid to gas. Therefore, it does not affect the hydrodynamic materials. Thus, water in the case is assumed to be a traceable amount.

Further complicating the sodium implementation in MELCOR is the treatment or the definition of the ambient temperature. For water reactors, the typical ambient temperature in the containment or experiment room is about 290 to 300 K, which is below the boiling point of water and above the freezing point of 273 K. For sodium reactors, particularly in the containment volume, the ambient temperature in the volume may be on the order of 290 to 300 K, while the freezing point of sodium is 371 K. This poses an issue with MELCOR, due to the assumption that the ambient temperature is above the coolant’s freezing point. In order to model a coolant room with the presence of water, MELCOR requires a user flag that enables CVH_ALLOWCOOLATM to model this situation. When sodium appears in the problem, the atmosphere temperature needs to be above the coolant’s freezing point. If not, the code will abort. This poses a development issue to ensure that the amount of the sodium introduced into the spray fire must have an associated energy source. Also this energy source is large enough to heat the atmosphere above the freezing point of sodium and that any transport of sodium to the adjacent volume is examined. To overcome this issue, MELCOR has been modified to allow the sodium coolant in the problem at atmospheric temperature below its freezing point. This process requires a code review to ensure that the new changes do not compromise water reactor applications.

In addition, because the sodium-concrete interaction model in CONTAIN-LMR is linked to the debris model in the cavity (CORCON), sodium freezing may complicate porting the subroutine SLAM and other calling routines for use within MELCOR. The cavity package in MELCOR is expecting conditions consistent with core-concrete interaction phenomena. Since the sodium-concrete interaction may not occur in the cavity volume in the SFRs, the location of the sodium-concrete interaction model, without the CORCON model activation, is being investigated. If necessary, the SLAM model may be included in the NAC package.

5 NAC Package Development

To efficiently manage the sodium-related models, a package, the "Sodium Chemistry" (NAC) package, has been added to MELCOR. In order to activate this package, the fluid material number (Nfluid) for the sodium coolant must be either 7 for the FSD or 20 for the SIMMER (SAS4A) database, as described in Table 1.

This new package contains new routines that have been adapted from CONTAIN-LMR to model the pool fire, spray fire, and atmospheric chemistry. These new models will interface with various packages in MELCOR, for example:

- NCG – O_2 and H_2
- HS – condensate and deposits
- CVH – Na and reaction energies
- RN – aerosol interactions: H_2O, Na, NaOH, Na_2O_2, and Na_2O.

Na is modeled as a condensable and water is modeled as an aerosol. Thus, a new water class must be created as H2OA to distinguish it from the default water aerosol class. The NAC package is intended to model the intra-volume process. The atmospheric chemistry models for sodium-induced hydrogen deflagration will be transferred to the BUR package as a separate model. At this time, both major subroutines from the spray fire and pool fire models from CONTAIN-LMR have been implemented into MELCOR. The development of the input records and the run subroutines for MELCOR has been implemented and the testing of these models is in progress. The implementation of the atmosphere chemistry model from CONTAIN-LMR should be completed early in 2017. The treatment of the sodium reactions with water vapor is especially challenging because both sodium and water vapor cannot be modeled, and the use of the water vapor as an aerosol for reactions is inconsistent with water condensation on the heat structure surfaces.

6 CONTAIN-LMR Sodium Models Validation

To validate the sodium models in CONTAIN-LMR, a number of available sodium experiments for validating these models were identified. Although experimental validations have begun, the validation process is preliminary. Section 6 describes each of the experiments used to validate the individual sodium chemistry models implemented into MELCOR.

For the spray fire model, MELCOR has been validated against the ABCOVE AB5 [Souto 1994]; but additional tests, such as Sandia Surtsey T3 [Olivier 2010] tests, will be incorporated into the validation matrix as time progresses. For the pool fire model, MELCOR has been validated against the ABCOVE AB1 [Hillard 1979]. The first model to be tested was the spray fire model. The ABCOVE AB5 presented below utilized the existing input decks from the MELCOR 2.1 assessment problems [Humphries 2015].

6.1 ABCOVE AB5

The purpose of this experiment was to provide experimental data for validating aerosol behavior of computer codes during a sodium spray fire scenario. This experiment was conducted at the Containment

Systems Test Facility (CSTF) at Hanford Engineering Development Laboratory (see Figure 6 for the apparatus setup). Although the existing MELCOR model was intended for examining the aerosol behavior rather than the sodium reactions, it can be modified easily to include the sodium spray model parameters. The CONTAIN-LMR model was also developed from this MELCOR model.

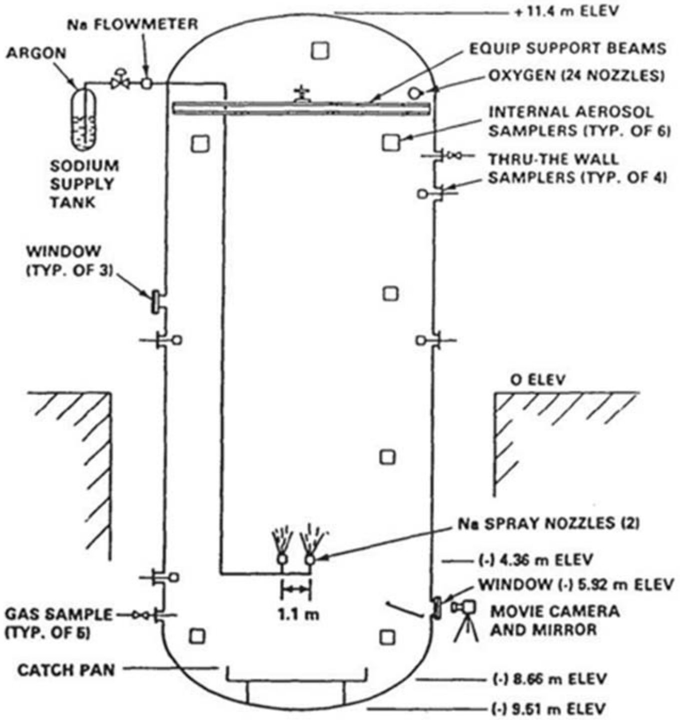

Figure 6. Schematics of ABCOVE Sodium Spray Fire Test [Souto 1994].

Table 3. 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 Oxygen Injection Stop Total O_2	60 s 840 s 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

The initial sodium spray mass of 223 kg at 836 K was injected into a vessel of 852 m^3 filled with air and O_2 makeup. The validation goals were to observe the sodium combustion during sodium spray, the calculated combustion energy, and the aerosol generation. The effect of the pressure and temperature response in the vessel was also of interest. Note that the initial temperature of the containment is below the freezing of sodium (see Section 4 for remediation of this issue in MELCOR). The experiment's results indicate that not only the sodium peroxide is formed, but some amount of NaOH is formed due the presence of moisture in the air. The current spray fire model in MELCOR does not model the formation of NaOH. However, the activation of the atmosphere chemistry may enable the modeling of the NaOH formation, if sodium vapor resides in the atmosphere. Thus, it may be important to include the reaction of the water vapor in the atmosphere to form NaOH in additional to oxygen. The inclusion of NaOH when modeling the aerosol generated would enhance the quantification of the aerosol results from the experiment. Also, the spray direction of the AB5 test is upward, rather than downward, as currently modeled in the spray model implemented in MELCOR. The proper treatment of the droplet rise and drop is very important for the time that the droplet may react with the atmosphere. Sandia received the code modification from the Japanese Atomic Energy Agency (JAEA) [Takata 2016] to be considered for updating MELCOR spray fire models to capture non-terminal velocity flow. Other modeling information for sodium spray fires will also be considered [Sathiah 2014a].

6.2 Surtsey T-3

This test conducted at Sandia is a downward spray experiment (see Figure 7 for the test schematic), which should be well suited for the current spray model in MELCOR. The primary goal of the Surtsey T-3 test is to examine the thermal dynamic behavior of the atmosphere in terms of temperature and pressure rise. Although the test is not well characterized in terms of the aerosols generated, the temperature and pressure data may validate the thermodynamic behavior of the spray model in MELCOR.

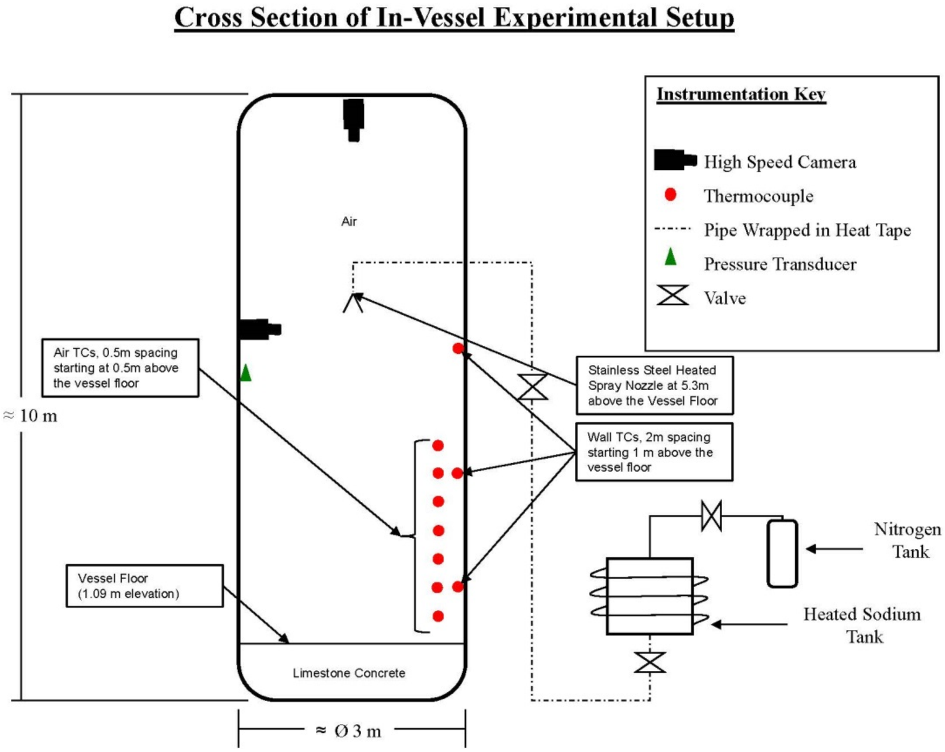

Figure 7. Sandia National Laboratories Surtsey Schematics for Sodium Spray Fire Tests Adapted from [Olivier 2010].

Table 4. Test Conditions for Surtsey T-3 Test [Olivier 2010].

SURTSEY DIMENSION	***PARAMETER***
Vessel Free Volume	99 m^3
Vessel Wall and Heads Thickness	1 cm
Na SPRAY	***PARAMETER***
Na Spray Rate	1 kg/s
Spray Start Time	0 s
Spray Stop Time	20 s
Total Na Sprayed	20 kg
Na Temperature	473.15 K
Spray Drop Size, diameter	3-5 mm
Spray Height	5.3 m
VESSEL CONDITIONS DURING TESTS	***PARAMETER***
Peak Air Temperature (0.33 m from wall)	753.15 K

Peak Overpressure	0.006 MPa
Peak Heat Flux (1.46 m from center)	< 1 kW/m^2

6.3 ABCOVE AB1

This test models the pool fire inside CSTF as in the ABCOVE AB5 test above. This test studies the pool fire burning and aerosol generations (see Figure 8 for the experiment schematic and Table 5 for the test conditions). As shown in Figure 8 and Table 5, the pool fire ends in one hour when covered with a lid on the pan. In order to capture the NaOH formation, the atmosphere chemistry model in MELCOR is activated. In order to model the entire duration of the experiment, the pool fire model needs to be turned off in one hour. An input parameter to permit turning off this model was added to model the testing protocol.

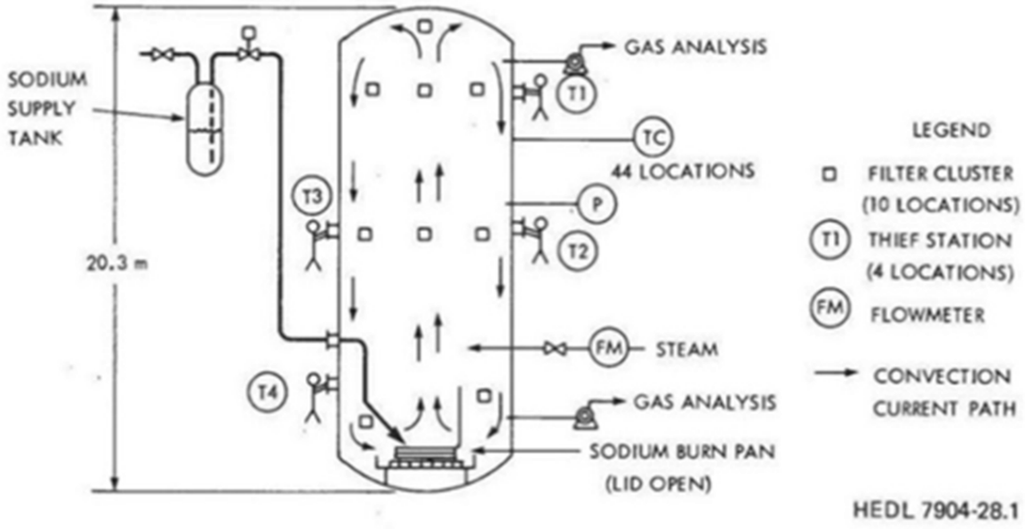

Figure 8. Schematic of ABCOVE AB1 Pool Fire Test [Hillard 1979].

Table 5. Test Conditions for the AB1 Test [Hillard 1979].

INITIAL CONTAINMENT ATMOSPHERE	***PARAMETER***
Oxygen Concentration	19.8%
Temperature (mean)	299.65K
Pressure	0.125MPa
Dew Point	283.15K
Na POOL	***PARAMETER***
Na Source Rate	11.1 g/s
Source Start Time	0 s
Spray Stop Time	3600 s
Total Na Spilled	410 kg
Initial Na Temperature	873.15 K
Burn Pan Surface Area	4.4 m^2
Burn Time	3600 s

Total Sodium Oxidized	157 kg
OXYGEN CONCENTRATION	***PARAMETER***
Initial O_2 Concentration	19.8 vol %
Final O_2 Concentration	14.7 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	0.142 MPa
Final Dew Point	233.15 K
Total Aerosol Released as Na	39.9 kg
Fraction of Oxidized Na Released	0.255

6.4 JAEA RUN F7

This test models the pool fire test by dropping sodium onto a pan that allows the spreading of the sodium on the pan. The pool fire test experiments were conducted at the Japan Atomic Energy Agency (JAEA) [Nishimura 2007]. Figure 9 shows the test schematic. As shown in Figure 9, the sodium leak rate is from 0.1 to 1.5 m above the insulated catch pan. The sodium on the pan spread toward the edge of the pan as evidenced in the thermocouple measurement distributed throughout the entire area of the pan. The pool fire model in CONTAIN-LMR assumes a constant pool area (an assumption of water spreading); thus, it would overestimate the pool fire for this experiment. The ability to spread the sodium pool is needed in order to model the pool fire experiment correctly. Adaption of the molten corium spreading model in the cavity (CAV) package of MELCOR may be necessary. This molten pool model is a 1-D spreading model based on the balance of viscous flow and gravity [Humphries 2015b].

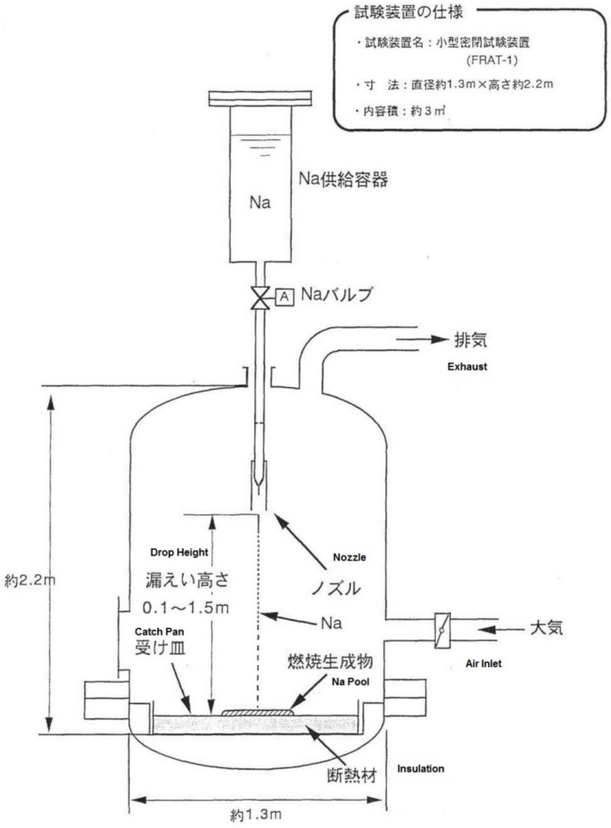

Figure 9. Schematic of JAEA Pool Fire Run F7 Tests [Nishimura 2007].

6.5 Sodium-Concrete Interaction (Reaction) Experiments

There were only a few large-scale sodium-concrete interaction experiments conducted in the 1980s. Among them, the sodium-concrete interaction experiments conducted at Sandia included the development of computer modeling to study this interaction [Randich 1983, Suo-Anttila 1983] The SLAM model in CONTAIN-LMR was based on these experiments and model developments conducted at Sandia. The model was based on experiments with sodium and limestone concrete interactions. Other concrete could be used instead of limestone concrete in other countries, including siliceous concrete used in Korea and Japan. Since the principal reactions may be different between limestone and siliceous concretes, the reaction between sodium and siliceous concrete needs to be added to MELCOR. For example, several researchers discuss the importance of sodium and silica reactions for tight sands concrete and siliceous concretes [Kikuchi 2015a, Kikuchi 2015b, Bae 1998]. No detailed discussion is presented here for the additional experiments described in [Kikuchi 2015a, Kikuchi 2015b, Bae 1998]. Once this SLAM model for the interaction with the limestone concrete is implemented into MELCOR, additional interaction models can be added into MELCOR for analyzing interaction with concrete other than the limestone concrete type. Summary and Conclusion

7 Summary and Conclusion

This paper summarizes the development status of MELCOR sodium chemistry models. MELCOR code utilizes the existing containment sodium chemistry models from CONTAIN-LMR and previously implemented sodium properties. Sodium chemistry models—spray fire, pool fire, and atmosphere chemistry models—are being implemented into MELCOR and validated against experiments. A new packaged called "NAC" has been created to manage the sodium chemistry model more efficiently. Currently only the spray fire and pool fire models have been completely implemented in MELCOR. Using the ABCOVE AB5 test, the testing of the spray fire model has begun. Additional tests are being planned including the SURTSEY spray fire test at Sandia National Laboratories and the pool fire test of ABCOVE AB1. Model validations are in progress.

In addition to the above, the atmosphere chemistry model should be completely implemented in early 2017. Once completed, the above tests will be re-simulated to account for the generation of NaOH, since both spray and pool fire models do not account for the reaction with moisture to form NaOH. Also the sodium-concrete interaction model will be completed in 2017. Once the sodium-concrete interaction model is completed and tested, the MELCOR's NAC package will be ready to be applied for analyzing the containment accident conditions of metallic fuel types of SFRs.

8 Acknowledgements

This work is funded by the Office of Nuclear Energy of the U.S. Department of Energy, Work Package AT-16SN170204.

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