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STATUS OF MELCOR SODIUM MODELS DEVELOPMENT

David L.Y. Louie

Sandia National Laboratories
Albuquerque, New Mexico USA

Larry L. Humphries

Sandia National Laboratories
Albuquerque, New Mexico USA

ABSTRACT

A sodium coolant accident analysis code is necessary to provide regulators with a means of performing confirmatory analyses for future sodium reactor licensing submissions. MELCOR and CONTAIN, which have been employed by the U.S. Nuclear Regulatory Commission for light water reactor licensing, have been traditionally used for level 2 and level 3 probabilistic analyses as well as containment design basis accident analysis. To meet future regulatory needs, new models are being added to the MELCOR code for simulation of sodium reactor designs by integrating the existing models developed for separate effects codes into the MELCOR architecture. Sodium properties and equations of state, such as from the SAS4A code, have previously been implemented into MELCOR to replace the water properties and equation of state. Additional specific sodium-related models to address design basis accidents are now being implemented into MELCOR from CONTAIN-LMR. Although the codes are very different in the code architecture, the feasibility fit is being investigated, and the models for the sodium spray fire and the sodium pool fire have been integrated into MELCOR. A new package called Sodium Chemistry (NAC) has been added to MELCOR to handle all sodium related chemistry models for sodium reactor safety applications. Although MELCOR code requires the ambient condition to be above the freezing point of the coolant (e.g., sodium or water), the high relative freezing point of sodium requires MELCOR to handle situations, particularly far from the primary circuit, where the ambient temperatures are usually at room temperature. Because only a single coolant can be modeled in a problem at a time, any presence of water in the problem would be treated as a trace material, an aerosol, in MELCOR. This paper addresses and describe the integration of the sodium models from CONTAIN-LMR, and the testing of the sodium chemistry models in the NAC package of MELCOR that handles sodium type reactor accidents, using available sodium experiments on spray fire and pool fire. In addition, we describe the anticipated sodium models to be completed in the

coming year, such as the atmospheric chemistry model and sodium-concrete interaction model. Code-to-code comparison between MELCOR and CONTAIN-LMR results, in addition to the experiment code validations, will be demonstrated in the coming year.

INTRODUCTION

A sodium coolant accident analysis code is necessary to provide reactor designers and regulators with a means to perform containment and source term analyses for future advanced reactor applications, such as for 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 capability to model source terms and accidents involving the containment [1-2]. This gap was identified as a high priority during a subsequent review of gaps involving sodium technology, accident sequences and initiators, source terms, codes and models, and fuels and materials [3].

MELCOR [4-6] and CONTAIN [7], which have been 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 analyses as well as containment design basis accident (DBA) analysis [8-10]. Both codes were developed at Sandia National Laboratories (SNL) for the NRC. To meet future regulatory needs, new models are being added to the MELCOR code to simulate sodium reactor designs. Existing models developed for separate effects codes are also being integrated into the MELCOR architecture. Sodium properties and equations of state (EOS), such as from the SAS4A code [11-12], have been implemented into MELCOR to replace the water properties and its EOS as reported previously [13]. After the success of this implementation, additional specific sodium-related models to address DBA can be implemented into MELCOR. Figure 1 shows the sodium chemistry in the containment of a pool type SFR design. Much of the sodium chemistry phenomena (see

Fig. 1) for the containment have been modeled in CONTAIN-
LMR [14-15].

SFR Sodium fast reactor
SLAM Sodium limestone ablation model

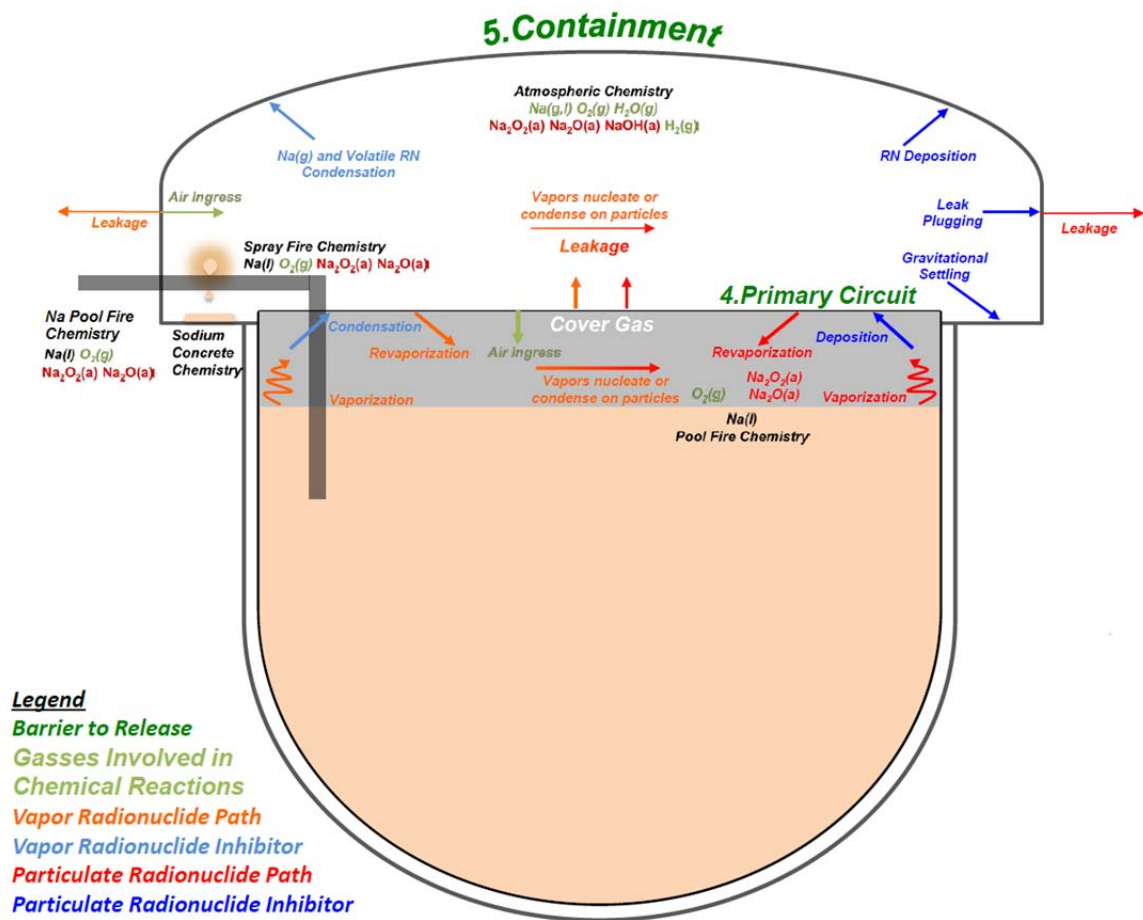


Figure 1 Graphical Representation of the Sodium Chemistry Models for Containment and Primary Circuit (adapted from [1]).

In this paper, we first describe the sodium models from CONTAIN-LMR being integrated into MELCOR. Then we describe the implementation status of these sodium models in MELCOR 2.1. Finally, we describe the testing of the implemented models in MELCOR.

NOMENCLATURE

AC	Atmosphere chemistry
CSTF	Containment System Test Facility
DBA	Design basis accident
EOS	Equation of state
FSD	Fusion Safety Database
LWR	Light water reactor
NAC	Sodium Chemistry Package
NaCL	NAC class
ndry	Number of dry nodes
Nfluid	Fluid identification as shown in Table 1
NRC	U.S. Nuclear Regulatory Commission

SNL Sandia National Laboratories
STD Standard temperature and pressure

Symbols

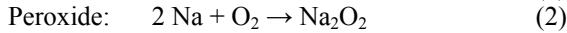
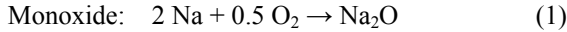
δ	Thickness of boundary layer
E	Combustion heat
F	Mole fraction: subscript peroxide for Na_2O_2
f_1	Fraction of total O_2 consumed
f_2	Fraction of sensible heat entering the pool
f_3	Fraction of Na_2O product entering the pool
f_4	Fraction of Na_2O_2 entering the pool
S	Correlated quantity given in Equation (3)

CONTAIN-LMR SODIUM MODELS

To simplify the sodium model development, the sodium models from CONTAIN-LMR are being integrated into MELCOR. The CONTAIN-LMR source code was examined and tested for changes from the models described in the CONTAIN-LMR manual [8] to identify and document any

missing information for the models. As of today, we have identified and integrated a number of sodium chemistry models from this code into MELCOR:

Spray fire models the leak of sodium in the air. This model is based on the phenomenological model used in NACOM, a code developed and tested at Brookhaven National Laboratory [16]. However, unlike NACOM, CONTAIN-LMR did not include the sodium reaction with water vapor. In the spray fire model, an initial size distribution is determined 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-Tanasama correlation [16]. An assumption is used to state the trajectory of the droplets, which is assumed to have a downward flow with a terminal velocity. The combustion rate of the spray fire is integrated over the droplet's fall to obtain the total sodium burned mass (as functions of droplet size), fall velocity and atmospheric conditions. In the spray fire model, the two chemical reactions of sodium droplet and oxygen in the air are:



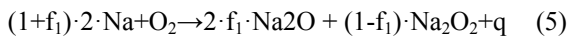
The combustion energy is computed based on the mole fraction of sodium (F_{peroxide}) to peroxide (Na_2O_2) as given by the following correlation:

$$S = (1.3478 \cdot F_{\text{peroxide}}) / (1.6957 - 0.3479 \cdot F_{\text{peroxide}}) \quad (3)$$

$$\text{Heat combustion, } E_{\text{spray}} \text{ (J) is then calculated as} \\ E_{\text{spray}} = (1 - S) \cdot 9.1797 \times 10^6 + S \cdot 10.46 \times 10^6 \quad (4)$$

The duration of this sodium source and the available oxygen determines the combustion time and the amount of the by-products (Na_2O and Na_2O_2 as aerosols) and 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 transferred to the atmosphere. The process continues until the droplet is either consumed or reaches the floor, forming a pool.

Pool fire models the accumulation of the sodium on the containment floor in the air environment. This model was taken from the SOFIRE II code developed empirically from pool fire experiments [15]. Reactions (1) and (2) are also considered in this model. However, the model reaction is given as:



Where f_1 = fraction of total O_2 consumed that reacts to form monoxide and $q = 9.0454 \times 10^6$ J/kg of monoxide and 1.09746×10^7 J/kg of peroxide. The above reaction requires

oxygen in the air to diffuse to the sodium pool. This diffusion is given by:

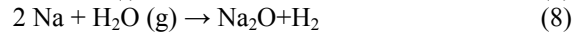
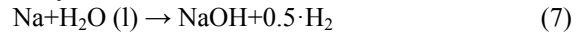
$$D = 6.4315 \times 10^{-5} T_{\text{film}}^{1.823} / P \quad (6)$$

Where T_{film} = average temperature of the pool and atmosphere (K), and P = system pressure (Pa). Although the CONTAIN_LMR manual [12] describes the heat transfer model for the sodium pool, the appropriate implementation of this model into MELCOR is still being investigated; therefore, it is not documented here further. Similar to the spray fire model, the by-products of the pool fire model are the aerosols of Na_2O and Na_2O_2 .

The pool fire model requires the allocation of the amount of the products and reaction energy to the pool and to the atmosphere layer of the cell. Thus, additional fractional inputs must 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.

Atmosphere chemistry models the interactions of the sodium aerosols, vapors and deposits in the atmosphere. In addition to the reactions (1) and (2) above, the atmosphere chemistry model includes additional reactions with water:



Reaction (7) is assumed to occur only for liquid phase water 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 liquid water is traceable to numerical effects and the amount is not significant. 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.

Reaction (8) is used when the phase of water is not liquid. It is appropriate at high temperatures with excess sodium. 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 this reaction at

the surface with water is assumed to be limited by the evaporation rate of water from the surface.

Note that reactions (7) and (8) with water dominate in the atmosphere over the reactions (1) and (2) with oxygen. Two additional reactions are considered to occur in the atmosphere, which relate to the reactions of the sodium monoxide and peroxide with water vapor in the atmosphere to form sodium hydroxide:



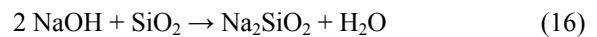
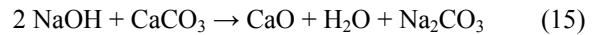
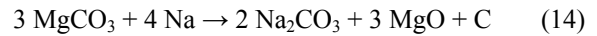
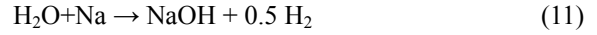
Water vapor is assumed to react with aerosol particles and aerosol deposits in that order. Again, the user should note that while the hydroxide is expected to be the principal reaction product with water at low temperatures or with excess water, the possible subsequent conversion of the hydroxide to 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 heat content of the aerosols 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.

A sodium-induced hydrogen deflagration model is included in this atmosphere chemistry model. It 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 of the hydrogen entering with the sodium is consumed. Note that this 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 as we have described so far.

Sodium-concrete interaction models the chemical reaction of the sodium with concrete. 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.

This model is based on experiments done at SNL regarding the sodium limestone ablation model (SLAM) [16-17]. SLAM uses a nodalized representation of the concrete with models for heat transfer, water migration, water and CO₂ evolution, and chemical ablation of the exposed concrete surface (see Figure

2). As shown in Figure 2, SLAM consists of three regions. The top 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. As shown in this figure, a number of constituents can be included within SLAM, which includes SiO₂, H₂O, Na, H₂, NaOH, Na₂SiO₃, Na₂CO₃, Na₂O, CaO, CaCO₃, CO₂, graphite, MgCO₃, MgO, inerts, steel and UO₂. The major reactions considered in SLAM are:



In SLAM, the boundary layer consists of 12 nodes, while the dry region consists of 15 nodes or more. Each node has the same thickness or size, which varies with the changing dimensions of the dry concrete region. A variable, “ δ ”, is the thickness of the boundary layer and dry concrete regions. This variable is subjected to change in terms of increasing or decreasing in the course of a problem. The initial δ is 0.003 m. The dry concrete region increases when the thermal penetration rate of the concrete exceeds the ablation rate and decreases when the converse is true. The bottom region is the wet concrete region where evaporable water may still be found in the concrete as shown in this figure. The number of nodes depends on the number of dry nodes which is given by $50 - \text{ndry} + 2$.

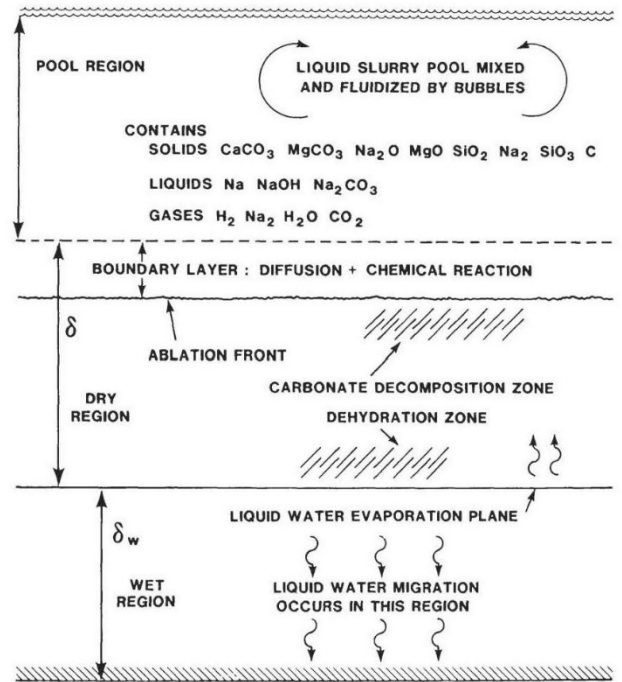


Figure 2. Schematic Diagram of SLAM [12].

With these three regions as shown in Figure 2, SLAM computes each region as time passes and penetration occurs, during which each region will change its size and position. The coordinate system of SLAM uses the moving Eulerian system (see more details in [14]). The 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 virtually isothermal. The pool changes in composition which results in swelling with time during penetration. 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 of 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 ablation. This region can swell or shrink (it 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 for the reaction species in the pool and dry regions in above three 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 CO₂ fluxes. Note that SLAM does not model the steel liner of the concrete.

Note that the above sodium models from CONTAIN-LMR are being implemented into MELCOR.

MELCOR SODIUM IMPLEMENTATION

In the previous section, the sodium chemistry models from CONTAIN-LMR were described. These models, including the subroutines from the CONTAIN-LMR source code are being implemented into MELCOR 2.1. Even though both MELCOR and CONTAIN-LMR are very different in terms of code architectures, the feasibility fit is being investigated. Note that CONTAIN-LMR code was written in Fortran 77 while MELCOR is written in Fortran 95. To be more efficient and better manage the sodium-related models, a new package “Sodium Chemistry” (NAC) package, which handles all sodium related chemistry models for sodium reactor safety applications has been added to MELCOR. This package will utilize these CONTAIN-LMR subroutines. All these subroutines will interface with CVH, CF, TF, HS and RN package variables for transferring chemistry related processes (both heat and mass), including sodium, oxygen, water and the creation of the by-products of sodium burn resulting from the reactions. A corresponding data structure for each of the implemented models has been created. Two models from CONTAIN-LMR have been integrated into MELCOR: sodium

spray fire and the sodium pool fire. The atmosphere chemistry model is partially implemented.

There are several issues related to the implementation of the CONTAIN-LMR models into MELCOR:

- When replacing the water coolant as sodium coolant, no other condensable can be modeled (i.e., water). Thus the two-condensable option from CONTAIN-LMR may not be easily implemented. Substantial modification to MELCOR architecture may be required.
- To treat the existence of water in the MELCOR-Na code, water is assumed to be a trace element (or aerosol) which does not affect the thermo-dynamic materials.
- Because the design of the water EOS in MELCOR in such a way, only liquid and vapor phases can be modeled. Thus the solid phase may not be easily implemented in the EOS. There is a similar situation for sodium as a coolant, since the melting temperature of sodium is 371 K. If the ambient atmosphere can be less than the sodium freezing temperature, it poses challenge to MELCOR.
 - The properties for the liquid phase are extrapolated for sub-frozen temperatures.
 - Coding needs to be modified for ‘small’ sodium pool.
- Aerosol class re-assignment is required for modeling sodium as coolant. Class 2 (Cs) includes Na as the list of elements included. Since the replacement of the water to sodium, now Class 14 (H₂O) becomes the sodium.

The next section provides a description of the NAC package development.

NAC PACKAGE DEVELOPMENT

To be more efficient and better manage the sodium-related models, a new package “Sodium Chemistry” (NAC) package is being added to MELCOR. In order to activate this package, the fluid material number (Nfluid) must be either 7 for the Fusion Safety Database (FSD) or 20 for the SIMMER (SAS4A) database as described in Table 1 for the sodium coolant [11].

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		

¹Refer to FSD data set

²Refer to SIMMER data set

This package includes a number of subroutines from CONTAIN-LMR, which include SPRAY for the spray fire model, PFIRE for the pool fire model, and CHEMRX, CHMAER, CHMGAS, CHMREP and CHMDEP for the atmosphere chemistry model. Additional subroutines will be

included in the coming year for modeling the sodium-concrete interaction. All these subroutines will interface with various packages in MELCOR, for example:

- NCG – O₂ and H₂
- HS – condensate and deposits
- CVH – Na and reaction energies
- RN – aerosol interactions: H₂O, Na, NaOH, Na₂O₂ and Na₂O

Na models as a condensable and water is modeled as aerosol. Thus a new water class must be created as H₂O_A.

This package contains the following subroutines and modules which have been implemented in MELCOR:

- M_NAC – data structure module and specialized subroutines for data processing and for supporting various chemistry model routines
 - o NAC classes (NaCL) to map to the RN classes (water, Na, NaOH, Na₂O₂ and Na₂O in that order)
 - o Old-new variables for each chemistry models and input parameters
- NAC_GENERATEDB – Subroutine for the MELGEN
- NAC_NACDBD –Executive level routine to call NACRUN
- NAC_NACRUN – High level subroutine to run various chemistry models
 - o Calling sequence for the NAC model executions looping over the control volumes.
- NAC_PFIRE – Pool fire run routine
- NAC_RW – MELGEN input processing for all NAC MELGEN inputs, and restarts
- NAC_SPRAY – Spray fire run routine
- NAC_CHEMRX – Atmospheric chemistry (AC) main routine, which calls NAC_CHMAER, NAC_CHMDEP, NAC_CHMGAS, and NAC_CHMREP. Not completely implemented yet.
- NAC_CHMAER – Aerosol chemistry routine
- NAC_CHMDEP – Deposited chemistry routine
- NAC_CHMGAS – Gas chemistry routine
- NAC_CHMREP – Repository chemistry routine
- NAC_EDIT – Editing routine for NAC models. Currently only spray fire and pool fire outputs are provided.

As well as the above additions, various interface and code modifications to the EXEC package were done in order to run the NAC package appropriately. Note that NAC package is intended to model the intra-volume process. The sodium-induced hydrogen deflagration in the atmosphere chemistry model will be in the BUR package as a separate model.

For the MELGEN input processing, the calling of the NAC package will be included in the EXEC package. The current designed input records for the NAC package are:

- NAC_INPUT
 - o Test if Nfluid=7 or Nfluid=20
- NAC_RNCLASS – Mapping NAC classes to RN classes
- NAC_ATMCHEM – Atmosphere chemistry model input record
- NAC_SPRAY – Spray fire model input record
- NAC_PFIRE – Pool fire model input record
- NAC_COND – Two-condensable option, which will not be implemented in the near future.
- NAC_SLAM – Sodium-concrete interaction model input, which will be implemented in the coming year.
- NAC_SC – NAC specified sensitivity coefficient, which will be implemented in the coming year.

TESTING

Once the sodium models were implemented into MELCOR, testing was conducted. To enable the sodium coolant in MELCOR, an input file was required to activate the MELCOR sodium model. A number of the experiments have been identified to test the spray fire model and the pool fire model. For the spray fire model, the ABCOVE AB5 [20] was used. Additional tests, such as Sandia Surtsey T3 [21] tests will be used. For the pool fire model, the ABCOVE AB1 [22] will be used. The first model to be tested was the spray fire model. Utilizing the existing input decks from the MELCOR 2.1 assessment problems [6], the ABCOVE AB5 test was first. 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 Fig. 3 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.

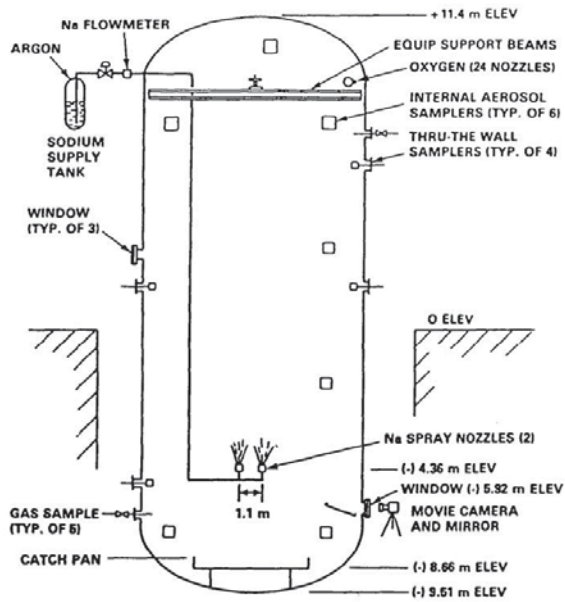


Figure 3. Schematics of ABCOVE Sodium Spray Fire Test [20]

The initial sodium spray mass of 223 kg at 836 K was injected into a vessel of 852 m³ filled with air and O₂ makeup. The validation goals were to observe the sodium combustion during sodium spray, and the calculated combustion energy, and aerosol generation. The effect of the pressure and temperature response in the vessel was also of interest. The test conditions and other specifications for this AB5 test are listed in Table 2. As shown in this table, the ambient vessel temperature was at 302 K, which is below the freezing point of sodium. The sodium spray characteristics are provided in this table. Note that the spray was pointed upward, so the current spray fire model will not correctly capture the sodium residence time since the spray points downward. Nonetheless, for this test a spray fall height was assumed to be 5.15 m from the vessel bottom. To sustain the combustion, a continuous flow of oxygen was provided as shown in this table. Figures 4 to 9 show the preliminary results of the use of the spray fire model and comparison to CONTAIN-LMR and calculations assumed no sodium modeled in MELCOR 2.1 and MELCOR 1.8.6. The comparison of the results from MELCOR (NAC package) with CONTAIN-LMR on the prediction of the sodium burned, oxygen consumed, and combustion energy as shown from Figures 4 to 6, respectively, show that the two codes are very similar. In terms of the temperature and pressures, MELCOR-Na predicts slightly lower temperature and pressure than test data and CONTAIN-LMR (see Figures 7-8). More analyses will be done to investigate these differences. In terms of the suspended aerosols as shown in Figure 9 MELCOR-Na predicts well with the test data. Note that the experiment result indicated that no monoxide was formed and only 60% peroxide and 40% hydroxide were obtained. Therefore, the spray fire model input model only assumes 100% peroxide, and no NaOH is modeled, since the spray fire model only models reactions (1-

2). Note that in order to model the experiment properly, the spray fire model needs to incorporate upward spraying and the terminal velocity of the droplet needs to be reflected in this change.

Table 2. Test Conditions for ABCOVE AB5 [20]

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

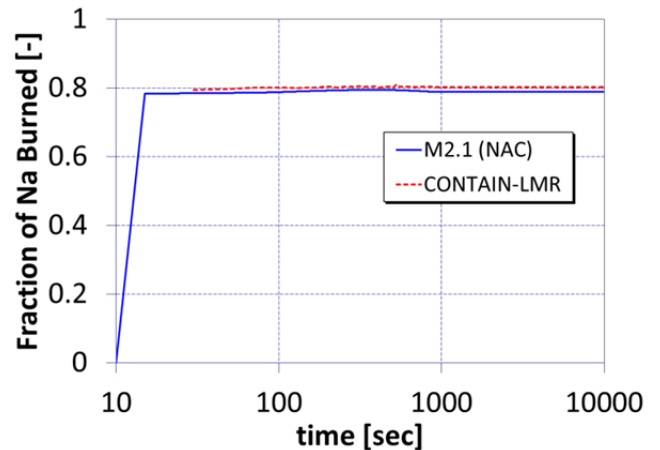


Figure 4. Preliminary MELCOR Prediction on Na Fractional Consumed for ABCOVE AB5.

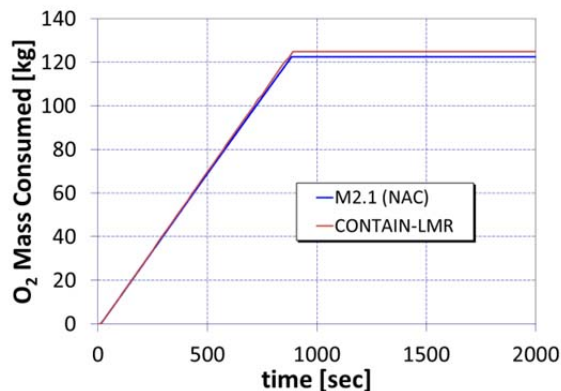


Figure 5. Preliminary MELCOR Prediction on O₂ Mass Consumed for ABCOVE AB5.

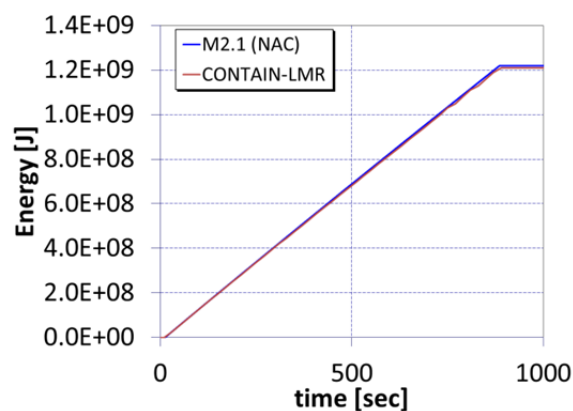


Figure 6. Preliminary MELCOR Prediction on Combustion Energy for ABCOVE AB5.

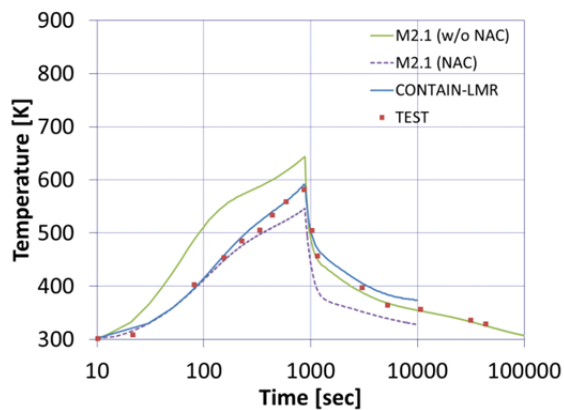


Figure 7. Preliminary Comparison of MELCOR on Gas Temperature for ABCOVE AB5.

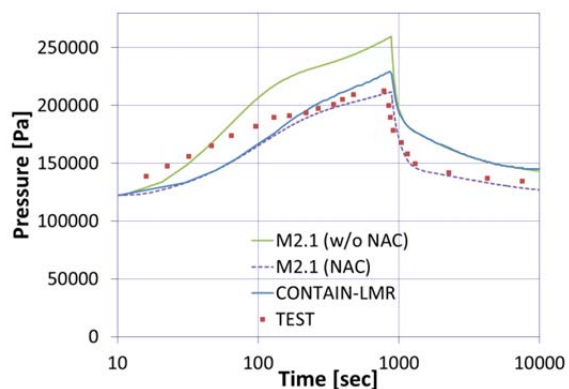


Figure 8. Preliminary Comparison of MELCOR on Gas Pressure for ABCOVE AB5.

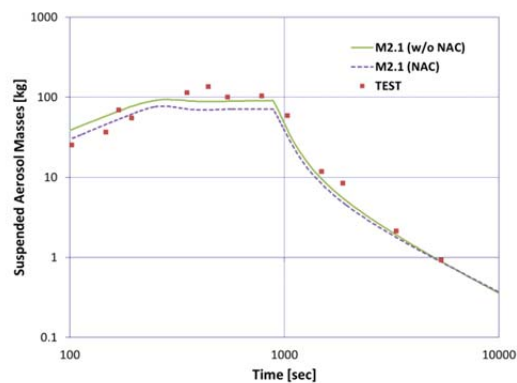


Figure 9. Preliminary Comparison of MELCOR on Suspended Aerosols for ABCOVE AB5.

A final calculation of the ABCOVE AB5 for testing the spray fire model in MELCOR will be done. Once it is completed, the subsequent Surtsey T-3 spray fire test will be conducted (see Fig. 10 for the test schematic).

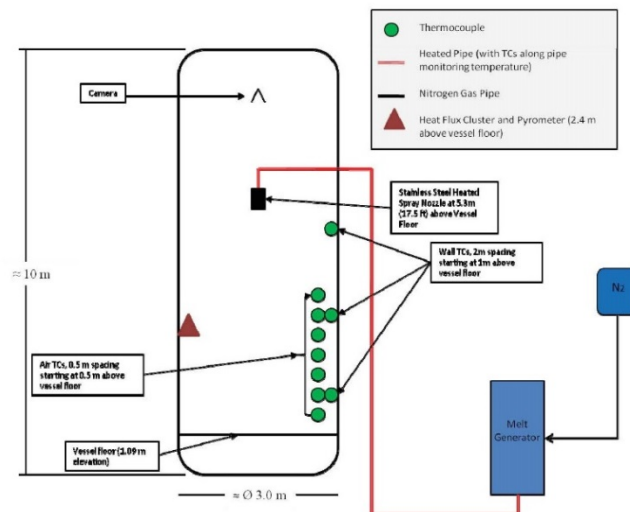


Figure 10. Sandia Surtsey Schematics for Sodium Spray Fire Tests [19]

The primary goal of this the T3 test is to examine the thermal dynamic behavior of the atmosphere in terms of temperature and pressure rise (see Table 3 for the test data).

Table 3. SURTSEY T-3 Spray Fire Test Data [19]

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

In addition to this test, an ABCOVE AB1 pool fire test will be used to validate the pool fire model implemented in MELCOR. This test uses the same CSTF volume to model the pool fire. Figure 11 shows the schematic of the ABCOVE AB1 test. Table 4 shows the test conditions for AB1. As shown in this table, the pool fire test contains on steam injection. However, there is some moisture in the atmosphere which allows the formation of NaOH. To estimate the NaOH formation, the atmosphere chemistry model must be working. Once this model is implemented completely, more accurate predictions can be provided for this test and for the other tests mentioned in this paper.

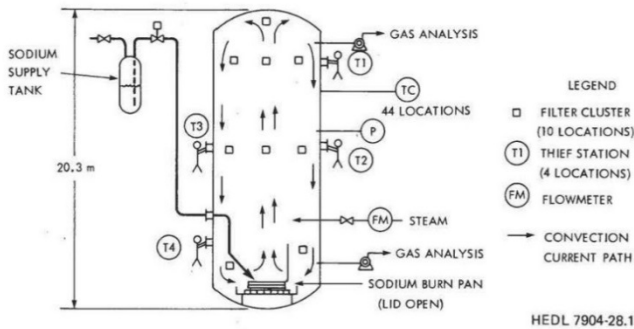


Figure 11. Schematic of ABCOVE AB1 Pool Fire Test [22]

Table 4. Test Conditions for AB1 Test [22]

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

SUMMARY AND CONCLUSION

This paper summarizes the development status of MELCOR sodium models. This sodium code utilizes the existing containment sodium chemistry models from CONTAIN-LMR and previously implemented sodium properties. In addition, we have begun to implement the sodium chemistry models: spray fire, pool fire and atmosphere chemistry models, and created a new packaged called "NAC" to manage the sodium chemistry model more efficiently. Currently only the spray and pool fire models are implemented. Using the ABCOVE AB5 test, the testing of the spray fire model has begun. The preliminary results of this test for the spray fire model seem to indicate that the model agrees well with the test data and the results from CONTAIN-LMR. Additional tests are being planned including the Surtsey spray fire test at SNL and pool fire test of ABCOVE AB1. These tests are in progress.

In addition to the above, the implementation of the atmosphere chemistry model should be completed in early 2017. Once it is done, the above tests should 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 implemented in 2017 and be completed in 2017. Once the sodium-concrete interaction model is completed and tested, the MELCOR's NAC package is ready to be applied for analyzing the containment accident conditions of metallic fuel types of SFRs.

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