# Validation Study of Sodium Pool Fire Modeling Efforts in MELCOR and SPHINCS Codes

David L.Y. Louie1, Mitsuhiro Aoyagi2, Akihiro Uchibori2, Takashi Takata2 and David L. Luxat1

1Sandia National Laboratories, Albuquerque, New Mexico, U.S.A.

2Japan Atomic Energy Agency, Oarai, Japan

Email contact of corresponding author: dllouie@sandia.gov

**Abstract**

Discharge of sodium coolant into containment from a sodium-cooled fast reactor (SFR) vessel can occur in the event of a pipe leak or break. In this situation, some of the liquid sodium droplets discharged from the reactor vessel will react with oxygen in the air before reaching the containment. This phase of the event is normally termed the sodium spray fire phase. Unreacted sodium droplets pool on the containment floor where continued reaction with containment atmospheric oxygen occurs. This phase of the event is normally termed the sodium pool fire phase. Both phases of these sodium-oxygen reactions (or fires) are important to model because of the heat addition and aerosol generation that occur. Any fission products trapped in the sodium coolant may also be released during this progression of events, which if released from containment could pose a health risk to workers and the public. The paper describes progress of an international collaborative research in the area of SFR sodium fire modeling between the United States and Japan under the framework of the Civil Nuclear Energy Research and Development Working Group (CNWG). In this collaboration between Sandia National Laboratories (SNL) and Japan Atomic Energy Agency (JAEA), the validation basis for and modeling capabilities of sodium spray and pool fires in MELCOR of SNL and SPHINCS of JAEA are being enhanced.

This study documents MELCOR and SPHINCS sodium pool fire model validation exercises against the JAEA’s sodium pool fire experiments, F7-1 and F7-2. The proposed enhancement of the sodium pool fire models in MELCOR through addition of thermal hydraulic and sodium spreading models that enable a better representation of experimental results is also described.

## INTRODUCTION

Discharge of sodium coolant into containment from a sodium-cooled fast reactor (SFR) vessel can occur in the event of a pipe leak or break. In this situation, some of the liquid sodium droplets discharged from the reactor vessel will react with oxygen in the air before reaching the containment. This phase of the event is normally termed the sodium spray fire phase. Unreacted sodium droplets pool on the containment floor where continued reaction with containment atmospheric oxygen occurs. This phase of the event is normally termed the sodium pool fire phase. Both phases of these sodium-oxygen reactions (or fires) are important to model because of the heat addition by the reactions and aerosol generation that occur. Any fission products trapped initially in the sodium coolant may also be released during this progression of events, which if released from containment could pose a health risk to workers and the public.

The advancement in the nuclear accident computer codes, such as MELCOR and SPHINCS led to models for these sodium fire phenomena. MELCOR is a severe accident code developed by Sandia National Laboratories (SNL) for the U.S. Nuclear Regulatory Commission (NRC). SPHINCS is a sodium fire accident code developed by Japan Atomic Energy Agency (JAEA). International collaborative research in the area of SFR sodium fire modeling using these codes has been established between the United States and Japan under the framework of the Civil Nuclear Energy Research and Development Working Group (CNWG). In this collaboration between SNL and JAEA, the validation basis for and modeling capabilities of sodium spray and pool fires in MELCOR of SNL and SPHINCS of JAEA are being enhanced.

In this paper, we present the MELCOR and SPHINCS sodium pool fire model validation exercises against the JAEA’s sodium pool fire experiments, F7-1 and F7-2. We also describe our proposed enhancement of the sodium pool fire models in MELCOR through addition of thermal hydraulic and sodium spreading models that enable a better representation of experimental results. For MELCOR, the model enhancement was done in MELCOR code input, rather than the software itself. MELCOR input allows a modeling capability via its powerful control function package [1]. A brief discussion of the F7 series experiments is provided followed by discussions on the numerical results of stimulating these experiments. A conclusion follows.

## Validation Experiments

To validate the pool fire model in both MELCOR from SNL and SPHINCS from JAEA, we used the data results from the JAEA’s F7 Series tests (F7-1 and F7-2) [1-2]. Fig. 1 shows the schematic of the test apparatus in the F7 Series test. The test apparatus consists of the stainless-steel vessel, the liquid sodium discharging system, the stainless-steel catch pan, the thermal insulator, the air ventilation (purge) line, and the measurement system. The test vessel is about 2.2 m in height and 1.3 m in diameter. The key difference between the F7-1 and F7-2 tests is the height of the nozzle exits, which are located at 0.1 m and 1.5 m from the catch pan, respectively. The thickness and area of the catch pans are 6 mm and 1 m2, respectively. The catch pan is attached to two 50 mm layers of thermal insulation. The liquid sodium is discharged with the average leak rate of 3.3 g/s for 1,500 seconds. The liquid sodium falls with a column shape and forms a pool on the catch pan. The final areas of the sodium pool are 0.28 m2 for F7-1 and 0.30 m2 for F7-2, respectively. The air in the vessel is ventilated with a steady flow of approximately 3.0 m3/min.



 *FIG. 1. Schematic of JAEA’s F7 Series test apparatus*

## Numerical Method

The numerical conditions of MELCOR and SPHINCS is modeled in accordance with the experimental condition described in the previous section. A brief description of the numerical methods for these codes is provided and the reader is encouraged to peruse the details in the literature [1-2].

### MELCOR

MELCOR is developed by SNL. Several improvements have been implemented into MELCOR to address accidents for advanced reactor designs, including SFRs. In this paper, we describe the current sodium pool fire model and the proposed enhancement via the input model here.

#### Current pool fire model

The current sodium pool fire model in MELCOR was implemented from CONTAIN-LMR, a legacy reactor containment code, which was also developed at SNL. This fire model was originally based on the SOFIRE II code [3]. The details of this fire model, including parametric model inputs can be found in the literature [1]. The brief model description of the input parameters for MELCOR is provided here. Because this model was developed as a parametric model, the enhancement of this model can be done through inputs via user-specified control functions. The user-specified control function provides flexibility in the testing of uncertain inputs of the current pool fire model without altering the source code. Table 1 lists the important input parameters that are entered as constant for the current sodium fire pool model in MELCOR. For this study, a control function capability was added to each of these input parameters. This capability, as indicated before, allows the implementation of a complicated model function that varies with physical parameters to better represent the phenomena physically.

TABLE 1. Important Input Parameter for MELCOR Pool Fire Model

|  |  |
| --- | --- |
| **Input Parameter** | **Definition** |
| DAB | Oxygen diffusion coefficient that determines the reaction rate between oxygen and liquid sodium |
| FNA2O | Fraction of the Na2O remaining in the pool during a fire. |
| FNA2O2 | Fraction of the Na2O2 remaining in the pool. The balance will be applied to the atmosphere as aerosols |
| FO2 | Fraction of the oxygen consumed to form monoxide in the reaction |
| FHEAT | Fraction of the sensible heat from the fire to be added to the pool. |
| \* The balance will be applied to the atmosphere as aerosols |

#### Model Enhancement

In this paper, we describe the enhancement on the modeling of the oxygen diffusion coefficient (DAB) in the MELCOR sodium pool fire model as described in the previous section. The detail of this DAB improvement is fully described in the literature [1]. Equation 1 was implemented as a control function model [1].

|  |  |
| --- | --- |
| $D\_{diff} = \frac{\left(\frac{Sh}{L}\right)\left(\frac{D }{1+{δ}/{∆\_{l}}}\right)}{0.14\left(g S\_{c}\frac{β}{ν^{2}} \left|T\_{surf} - T\_{g}\right|\right)^{\frac{1}{3}}}$, |  (1) |

where Sh is the Sherwood number, L is the pool diameter, D is the gas diffusion coefficient, $δ$ is the oxide layer thickness, which is normalized by the characteristic length scale ($∆\_{l}$), g is the acceleration due to gravity, Sc is the Schmidt number, β is the coefficient of gas expansion, ν is the kinematic viscosity, Tsurf is the sodium pool surface temperature, and Tg is the gas temperature.

Liquid sodium spreading is an important phenomenon because it can influence the sodium fire intensity and its reaction rate with oxygen. A pancake radial spreading model is used to describe the liquid sodium behavior as it falls downward onto the center of the pool; it then spreads outward. The radial spreading is influenced by both viscous and gravitational forces. The final radial spreading distance as implemented is shown below

|  |  |
| --- | --- |
| $$R(t+Δt)=\sqrt[8]{R(t)^{8}+C\_{1}∙ \frac{g}{μ π^{3}ρ^{2}}m^{3}Δt}$$ | (2) |

where $μ, ρ$ and $C\_{1}$ are the sodium viscosity, density, and empirical constant, respectively. Including the effect of solids in the liquid sodium, the enhanced sodium viscosity $μ$ is given as the function of the fraction of the sodium oxides ($ε$) by:

|  |  |
| --- | --- |
| $$μ=μ\_{0}∙exp⁡(2.5 C\_{2}∙ε)$$ |  (3) |

$C\_{2}$ in Equation (3) is an empirical constant. The Ramacciotti correlation has been used extensively for modeling corium experiments, which has allowed determination of an appropriate $C\_{2}$. $μ\_{0}$ is the liquid sodium viscosity.

The MELCOR model results as shown in the result section in this paper were based on implementing these equations into control function models. The descriptions of these control function models are given in the literature [1].

### SPHINCS

SPHINCS [4] is developed by JAEA as a sodium fire analysis code with a lumped mass model and a 1-D flow network model for thermal-hydraulics in control volumes, which is similar to MELCOR. The flame sheet model is employed considering the pool combustion occurs in the flame sheet layer with zero thickness on the sodium pool. This model consists of conservation equations in terms of mass and energy transfer on the flame sheet layer: molar flux of sodium vapor and oxygen, heat transfer between the pool and the flame sheet, and between the atmosphere and the flame sheet. By solving these equations, source terms of mass and energy transportation due to pool fire are obtained. SPHINCS also can simulate the effect of the oxide layer on the pool combustion. The pool combustion rate is multiplied by the liquid sodium fraction over the total pool mass that includes the mass of the oxide.

The sodium pool spreading in SPHINCS is modeled based on the balance of the surface tension and the gravitational force. Once the pool area reaches the maximum value, which can be specified in the input deck, the expansion of the pool stops, and the pool height starts increasing.

Heat transfer between the pool and the floor is calculated in the 2-D system in SPHINCS to simulate heat transfer accurately between the pool and the floor where temperature becomes higher under the pool. The computational mesh is divided into the ring-shaped coordinate system in the radial and depth directions.

## NUMERICAL RESULT

Using F7 Series test data, we were able to enhance our sodium pool fire model in MELCOR based on the phenomena observed from the test data and other similar pool fire tests [1]. The representation of the F7 Series test chamber for both MELCOR and SPHINCS is given in Fig. 1. The results of sodium pool fire combustion rate and pool temperature results are shown in Fig. 3 and Fig. 4, respectively. As shown in these two figures, both codes predicted similar results before the sodium discharge was completed in comparison to the experimental data. In the recent enhancement of MELCOR, the catch pan temperature was divided into two regions corresponding to under the pool and outside the pool. As the result of this model improvement, the pool combustion rate and temperature correspond reasonably with the results of SPHINCS, which has a 2D heat transfer model for the radial and depth directions.



*FIG. 2.* *MELCOR and SPHINCS representation of test chamber in the JAEA’s F7 Series tests*

|  |  |
| --- | --- |
|  |  |
| *(a) F7-1*  | *(b) F7-2* |

*FIG. 3. Pool combustion rate results*

|  |  |
| --- | --- |
|  |  |
| *(a) F7-1* | *(b) F7-2* |

*FIG. 4. Pool temperature result (r in the legend is the radial distance measured from the pool center)*

The difference in the peak of the combustion rate is mainly caused by the different pool spreading models in the two codes. Once the pool area reaches the maximum value specified in the input deck in SPHINCS, the pool spreading stops suddenly. Therefore, the pool combustion rate in SPHINCS has a sharp peak. Because the pool spreading in MELCOR becomes slower in proportion to the amount of the oxide on the pool as shown in Equations (2) and (3), the pool combustion rate in MELCOR changes gradually.

The pool combustion rate decreases rapidly after the end of the sodium discharge phase in the tests. This is caused by oxide layer build-up on the pool surface. Although both codes have the model for the pool combustion suppression due to the oxide, its modeling is still being refined. Consequently, additional modeling improvements after the discharge may be needed.

The aerosol concentration results are depicted in Fig. 5. Additional enhancement of the aerosol prediction based on the combustion and oxide build-up may be needed. During sodium discharge, the calculated aerosol concentration is smaller than the test data. One effective improvement would be adding a realistic oxide buildup model that could influence the oxygen diffusion to the pool to react with the liquid sodium. Currently, the oxide buildup as fraction of sodium aerosol remained in the pool is given, as the constant parameter in both codes. The overestimation of the airborne aerosol concentration after the end of the sodium discharge may be resolved through improvements in the oxide layer modeling and its effect on the pool combustion rate. At the beginning of the pool combustion, very little sodium aerosol remains in the pool which leads to more suspended aerosol. As more accumulation of sodium aerosol in the pool that forms an oxide layer could reduce the oxygen to diffuse the layer to react the sodium underneath. Thus, the aerosol generation rate is directly impacted to combustion rate, which was also too high during this phase.

|  |  |
| --- | --- |
|  |  |
| *(a) F7-1* | *(b) F7-2* |

*FIG. 5. Aerosol concentration results*

## CONCLUSION

This study enabled us to develop the enhancements, which establish a refined means to characterize key phenomena observed in the sodium pool fire experiments. With these enhancements, both MELCOR and SPHINCS can capture the F7-1 and F7-2 experimental data well in the area of thermal hydraulics. In addition, to the assessment of the sodium pool fire dynamics, additional analysis of the sodium fire aerosol generation is reported in this validation study. Despite limited experimental data being available, the relevant sodium aerosol generation trends are characterized to develop insights of relevance to the design of future experimental campaigns.

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