SAND2020-1685C
Proceedings of the 2020 28th Conference on Nuclear Engineering
Joint with the ASME 2020 Power Conference
ICONE28-POWER2020
August 2-6, 2020, Anaheim, California, USA

ICONE28-POWER2020-14278

SODIUM FIRE ANALYSIS USING A SODIUM CHEMISTRY PACKAGE IN MELCOR

Mitsuhiro Aoyagi[1], Akihiro Uchibori, Takahi Takata
Japan Atomic Energy Agency
Oarai, Japan

David L.Y. Louie, Andrew J. Clark
Sandia National Laboratories
Albuquerque, NM

ABSTRACT

The Sodium Chemistry (NAC) package in MELCOR has been developed to enhance application to sodium cooled fast reactors. The models in the NAC package have been assessed through benchmark analyses. The F7-1 pool fire experimental analysis is conducted within the framework of the U.S.–Japan collaboration; Civil Nuclear Energy Research and Development Working Group. This study assesses the capability of the pool fire model in MELCOR and provides recommendations for future model improvements because the physics of sodium pool fire are complex. Based on the preliminary results, analytical conditions, such as heat transfer on the floor catch pan are modified. The current MELCOR analysis yields lower values than the experimental data in pool combustion rate and pool, catch pan, and gas temperature during early time. The current treatment of heat transfer for the catch pan is the primary cause of the difference in the results from the experimental data. After sodium discharge stopping, the pool combustion rate and temperature become higher than experimental data. This is caused by absence of a model for pool fire suppression due to the oxide layer buildup on the pool surface. Based on these results, recommendations for future works are needed, such as heat transfer modification in terms of the catch pan and consideration of the effects of the oxide layer for both the MELCOR input model and pool physic.

Keywords: Sodium fire, spray fire, pool fire, numerical analysis, MELCOR, NAC package, sodium fast reactors

NOMENCLATURE

A_S	Surface area of sodium pool [m^2]
D_{diff}	Gas diffusion coefficient [m^2/s]
f_{O2}	Fraction of the oxygen that forms Na_2O [-]
g	Gravity [m/s^2]
H_G	Gas transport coefficient [m/s]
$\dot{m}_{O2}$	Oxygen consumption rate for pool fire [kg/s]
$\dot{m}_{Na}$	Sodium pool combustion rate [kg/s]
S	Stochiometric ratio of sodium to oxygen [-]
Sc	Schmidt number [-]
T_g	Gas temperature [°C]
T_{surf}	Sodium pool surface temperature [°C]
Y_{O2}	Mass fraction of oxygen [-]
β	Coefficient of gas expansion [1/K]
ρ_g	Gas density [kg/m^3]
ν	Kinematic viscosity [m^2/s]

1. INTRODUCTION

MELCOR, developed by Sandia National Laboratories (Sandia) and employed by the U.S. Nuclear Regulatory Commission, is a system-level computer code for safety analysis of light water reactors (LWRs). Recently, the code has been enhanced to apply to advanced non-LWRs, such as sodium cooled fast reactors (SFRs) and high temperature gas reactors. [1] Sodium chemistry, such as sodium fire and sodium-concrete reaction is one of the great concerns in SFR plants. A new package named Sodium Chemistry (NAC) has been introduced into MELCOR to analyze sodium chemistry events. [2] Physical models related to sodium fire in the NAC package are adapted from CONTAIN-LMR [3], which is a legacy code for a liquid metal reactor (LMR). Sodium properties and equation of states in MELCOR are implemented from SIMMER code. [4] So far, basic verification of sodium fire models in MELCOR had been conducted through comparison with CONTAIN-LMR [1].

Sandia and Japan Atomic Energy Agency (JAEA) have exchanged information focusing on sodium fire modeling and related experimental data as a collaboration on the field of advanced reactor modeling and simulation within the Civil Nuclear Energy Research and Development Working Group (CNWG), established by the U.S.–Japan Bilateral Commission on Civil Nuclear Cooperation in 2012. In this collaborative work, benchmark analyses of sodium fire experiments have been

[1] Contact author: aoyagi.mitsuhiro@jaea.go.jp

conducted to validate sodium fire analysis codes in the United States and Japan.

Our research is also intended to validate the sodium fire models of the NAC package in MELCOR within the flamework of the CNWG collaboration. The preliminary validation study on the sodium pool fire model has already been started [5] through a benchmark analysis of the JAEA F7-1 pool fire experiment. [6] The report of this preliminary study provides several suggestions for improvement of the simulation and modelling based on the result of validation analysis. This paper describes the F7-1 analysis with some modification in analytical conditions and models based on the suggestion of the preliminary study. Capability of MELCOR's pool fire model is assessed. Current issues and recommendations from the modified analysis are provided for additional improvements to the models.

2. ANALYTICAL METHODS

To benchmark and assess the sodium pool fire model in MELCOR, an experimental benchmark is a good approach. In this section, we briefly describe a F7-1 pool fire experiment. Then we describe a sodium fire model and MELCOR input model.

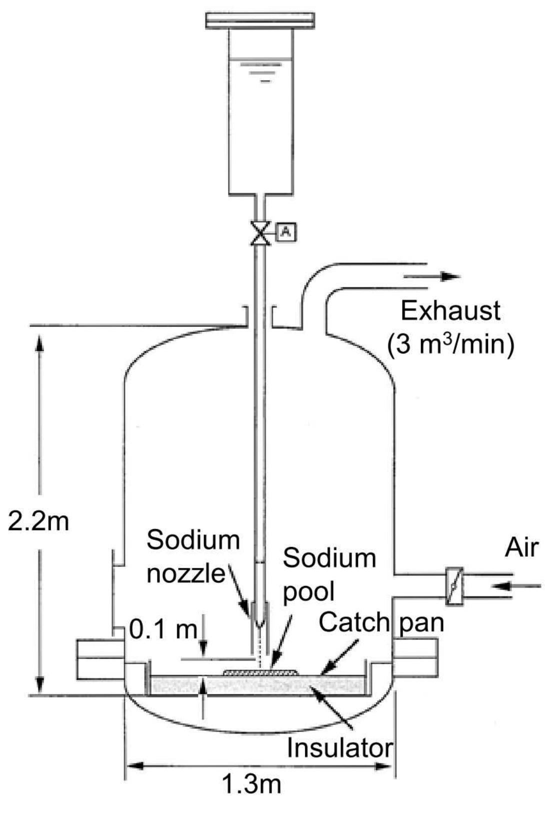

FIGURE 1: Test apparatus "FRAT" vessel (This figure is modified from the original in the report [6])

TABLE 1: Experimental and analytical conditions

	Experiment	Analysis
Sodium temperature	505°C	
Sodium leak form	Column (Nozzle dia.:4.35 mm)	Spray (Mean dia.: 4.5mm)
Sodium leak height	0.1 m from catch pan	
Sodium leak duration	1505 s	
Average sodium leak rate	3.28 g/s	
Total leak quantity of sodium	4.94 kg	
Oxygen concentration	20.8%vol (Initial)	
Gas temperature	12.7°C (Initial)	
Relative humidity	49.2% (Initial)	0.0%
Exhaust flow rate	3.0 m^3/min	

2.1 F7-1 Pool Fire Experiment

FIGURE 1 illustrates the test apparatus consisting of the stainless-steel vessel, the liquid sodium discharging system, the catch pan with the thermal insulator, the air ventilation (purge) lines, and the measurement system of the F7-1 test [6]. The height, diameter and volume of the test vessel were about 2.2 m, 1.3 m and 3 m^3, respectively. Thickness and area of the catch-pan were 6 mm and 1.0 m^2, respectively. The bottom of the catch pan was attached to the thermal insulator consisting of two 50 mm layers. The 505°C liquid sodium was discharged at 0.1 m height from the catch pan with the average leak rate of 3.28 g/s for 1505 s. The liquid sodium fell with a column shape and formed a pool at the center of the catch pan. The sodium liquid spread outward on the pan, while burning. The final area of the sodium pool was 0.28 m^2, which corresponds to 0.3 m in radius. The air in the vessel was ventilated with a steady flow of approximately 3 m^3/min at the exhaust to keep constant oxygen concentration in the vessel. The test conditions are summarized in TABLE 1.

Temperature was measured with the thermocouples at the test vessel surface, the atmosphere, the pool, the bottom surface of the catch pan, and the surface between the two thermal insulating layers. The concentrations of the oxygen, the hydrogen, and the aerosol were also measured in this test. The measured values used for comparison with the computational results in the following section are all shown in the report [6].

2.2 Sodium Fire Model

Sodium spray and pool fire is modeled in the NAC package in MELCOR. The burning rate of sodium with oxygen is assumed to have a constant diffusion of oxygen to the pool surface. The oxygen mass consumption rate for a pool fire is expressed as:

$$\dot{m}_{O2} = A_S H_G \rho_g Y_{O2}, \tag{1}$$

Where the coefficients are:

$$H_G = 0.14 D_{diff} \left(g\, Sc \frac{\beta}{\nu^2} \left| T_{surf} - T_g \right| \right)^{\frac{1}{3}}, \quad (2)$$

$$D_{diff} = \frac{6.4312\times10^{-5}}{P_g} \left[\frac{1}{2} \left(T_{surf} + T_g \right) \right]^{1.823}, \quad (3)$$

$$Sc = \nu / D_{diff}, \quad (4)$$

$$\beta = \left\{ \frac{1}{2} \left(T_{surf} + T_g \right) \right\}^{-1}. \quad (5)$$

The sodium burning rate in the pool is expressed by the product of the oxygen mass consumption rate and the stoichiometric combustion ratio of sodium to oxygen as:

$$\dot{m}_{Na} = \dot{m}_{O2} S, \quad (6)$$

$$S = 2.88 f_{O2} + 1.44(1 - f_{O2}). \quad (7)$$

Here, f_{O2} is the fraction of the total consumed oxygen that forms Na_2O as defined in the user input. An upper limit is imposed on $\dot{m}_{Na}$ such that the amount of sodium burned may not exceed one half of the pool mass within a single timestep.

As the result of combustion, energy and masses of Na_2O and Na_2O_2 are assumed to be released to both the pool and the atmosphere by input fractions. The fractions of the energy and masses remaining in the pool are defined in the user input. To provide flexibility of the pool fire model, many of the input parameters described in the equations above can be implemented as control functions, which allows flexibility to improve the pool fire model, such as oxide layer buildup. [7]

Aerosols in MELCOR are being treated as trace materials, which are assumed to transfer with the fluid but have no thermal mass. However, if a larger quantity of aerosols is presented in the problem compared to the other thermal-dynamic materials, ignoring the thermal capability of these aerosols may not be accurate. For sodium fire, which are significant sodium aerosols can be expected, the proper inclusion of the heat capacity of the sodium aerosols may be important.

2.3 MELCOR Model and Condition

The MELCOR input model consists of three control volumes and two flow paths, as shown in FIG. 2. The control volume "FRAT" corresponds to the test vessel illustrated in FIG. 1. Height and volume of "FRAT" are 2.2 m and 3.0 m^3, respectively. The volumes "PREENV" and "ENV" correspond to the atmospheric environment to give boundary parameters for the "FRAT" volume. All parameters, such as temperature, pressure, and gas composition are constant in the two volumes. Velocity at the flow path connected to the "ENV" volume is kept to 5.74 m/s throughout the computation. This velocity corresponds to 3.0 m^3/min in the pipe with the cross-sectional area of 8.71×10^{-3} m^2. The velocity of the flow path between "FRAT" and "ENV" was kept at a constant rate of 5.74 m/s.

Liquid sodium is discharged as droplets at 0.1 m height from the catch pan for 1,505 s. Flow rate, mean diameter and temperature of the sodium droplets are 3.28 g/s, 4.5 mm, and 505°C, respectively. A sodium pool is formed on the catch pan by unburnt sodium droplets. To model the droplet combustion, the sodium spray fire model of MELCOR has been invoked. An assumption of an initial sodium pool of 0.2 mm in height, which corresponds to 0.25 kg, is configured in this analysis to avoid cut-off of pool heat transfer to the catch pan in MELCOR. As an input, the surface area of the pool is controlled by the pool spreading model. [5] When the sodium flow stops, the final pool area of 0.28 m^2 is calculated.

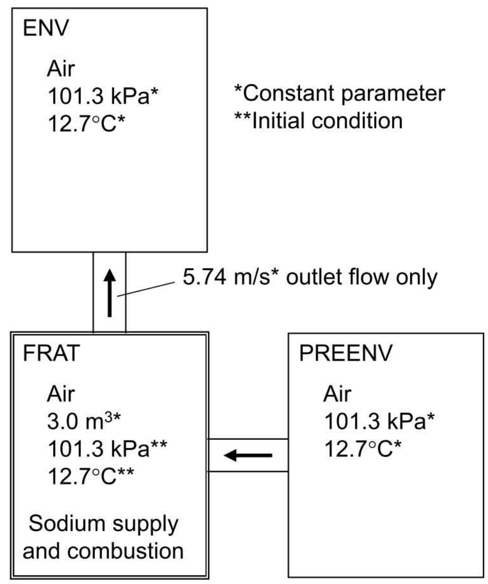

FIGURE 2: MELCOR model for control volumes

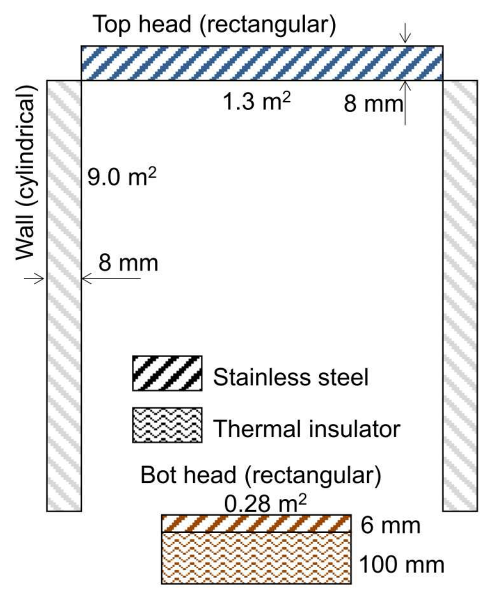

FIGURE 3: MELCOR model for heat structures

There are three heat structures; "top head," "wall," and "bot head" (catch pan) as shown in FIG. 3. The top head and wall have thermal properties of stainless steel. The "bot head" is divided into the stainless-steel pan and the thermal insulation layer. Surface area of the bot head is reduced to 0.28 m^2 from 1.0

m^2 in the previous analysis [5] to simulate the proper heat transfer under the pool as illustrated in FIG. 4.

FIGURE 4: Schematics of temperature distribution in a steel liner during pool fire where temperature rise in the steel liner occurs just under the sodium pool

Closely related to the experiment, a natural convective heat transfer coefficient (HTC) for the top head and the wall surfaces is set to 6.08 W/(m·K). For the bot head where the sodium pool resides, the proper treatment of liquid and gas HTCs was needed, because MELCOR uses the equation of natural, forced, or mixed convection heat transfer depending on Reynolds and Grashof numbers of the fluid. In this study, we implemented the HTCs, if the liquid sodium was present. In sodium fire, thermal radiation (TR) is important. There are two TR models in MELCOR, gray gas (simple) and enclosure (detailed) models. Note that the gray gas model only radiates to and from the atmospheric gases. The enclosure model includes the gray gas model and radiate to and from the aerosol as well. In this study, we used the gray gas model, with the consideration of the view factors. Emissivity of the heat structure and pool surfaces are 0.9 and 0.98, respectively in this study. The view factors of the top head and the wall are 0.04 and 0.96, respectively, according to their ratio of solid angle from the pool center. This is also the improvement over the preliminary analysis [5]. The boundary conditions for outside the heat structures are adiabatic.

3. RESULTS AND DISCUSSION

In this section, we discuss the MELCOR results and compare them to the experimental data of the F7-1 test. Even though both sodium spray fire and pool fire models in MELCOR have been invoked, our discussion herein only considers the pool fire model. The spray fire should contribute to the increase in temperature and sodium aerosol generation. However, we don't discuss this spray fire results in this paper.

3.1 Combustion rate

FIGURE 5 shows pool combustion rate. In the experiment, two different combustion rates were estimated by changes in enthalpy and oxygen consumption, respectively [6]. The enthalpy was evaluated from temperature measurements at the structures, the pool, and the atmosphere. Then, the mass of burnt sodium was estimated from the chemical reaction heat with an assumption that the products fractions of Na_2O and Na_2O_2 were 60% and 40%, respectively. The oxygen consumption was evaluated from the difference in oxygen concentration between the inlet and outlet ducts. The mass of burnt sodium was estimated with the same assumption for the fractions of the oxides. The report concluded the evaluation by oxygen consumption was more reliable. [6]

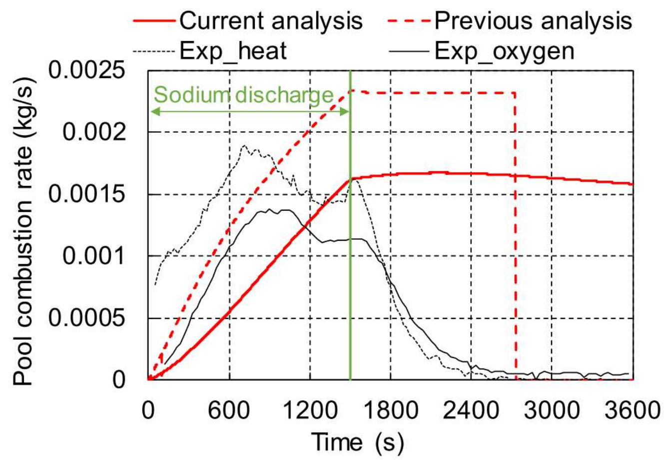

FIGURE 5: Pool combustion rate for the current and previous [5] MELCOR analyses, and experimental estimations

As shown in FIG 5, the sodium source discharge is stopped about 1,500 s. The comparison of the MELCOR results to the experimental data can be divided into two regions: during sodium discharge, and after the discharge. The combustion rate in the current analysis is lower than the two experimental estimations in its value and also in its increasing rate until around 1,000 s. The difference from the oxygen-based estimation is about 30%. The change in the pool combustion rate is proportional to pool temperature (T_{surf}) according to Eqs. (1)-(6). The main reason for the difference is the low pool temperature predicted by MELCOR, which is 100-400°C lower than the experimental result until 1,200 s, as discussed later. On the other hand, the combustion rate of the previous analysis showed good agreement with the oxygen-based estimation until 800 s. The pool temperature in the previous analysis was up to 100-200°C higher than the experimental data. This means that if the higher pool temperature could be calculated in MELCOR, the pool combustion rate would be matched more closely to the experimental data. One improvement to the current analysis is to model the proper heat transfer between the sodium pool and the bot head (catch pan).

After the sodium discharge stops at 1,505 s, the combustion rate is overpredicted by MELCOR. In the current modelling, pool surface area reacting with oxygen is kept at the final value 0.28 m^2 despite the small pool mass and oxide accumulation on the pool after the sodium discharge stops. In reality, the sodium oxide layer will form on the unburned sodium pool and this layer will slow the oxygen diffusion to the sodium. [5] The inclusion of this layer in the pool fire model may alleviate this overprediction. The effect of the oxide layers will be examined in future work.

3.2 Pool Temperature

FIGURE 6 shows the pool temperature results. Pool temperature predicted by MELCOR current analysis is much lower than the experimental data. The small combustion rate due to the low pool temperature escalates this situation. Modeling of a single catch pan is the primary cause of the difference. In reality, heat conduction between the sodium liquid and catch pan would be high and heat conduction in the horizontal direction in the catch pan would be lower as illustrated in FIG. 4. However, the heat structure model for the catch pan has just a single radial temperature node currently. This modelling equivalents to model an infinite thermal conductivity for the catch pan in the radial direction. As a result, the heat loss from the pool to the catch pan becomes excessive. We recommend improving the heat transfer model by considering the temperature distribution inside the catch pan to overcome this problem, such as subdividing the catch pan into multiple heat structures, and using the 2-dimensional heat structure model under development.

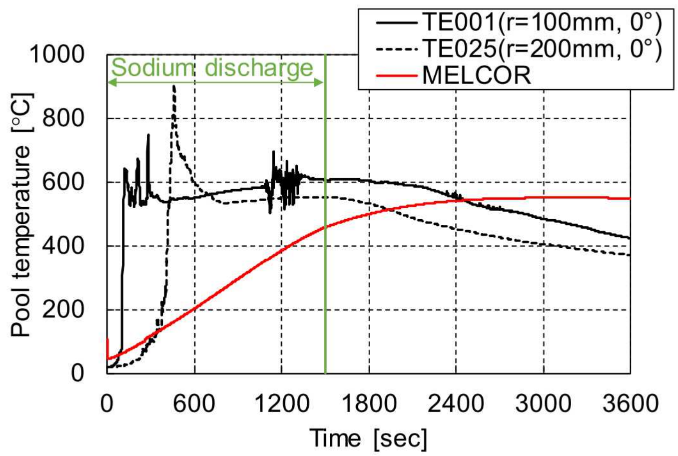

FIGURE 6: Pool temperature for the current MELCOR analysis and experimental data for thermocouple (TE) locations in radius measured from the center of the catch pan (r)

After the sodium discharge is stopped, the relation between the simulated pool temperature and the experimental data becomes opposite. This is mainly caused by the combustion rate, which remains high in the analysis as discussed in Section 3.1. The absence of heat capacity of the oxide layer in the model may overestimate the temperature increase during pool fire.

3.3 Catch Pan Temperature

FIGURE 7 compares catch pan (bot head) temperature predicted by the current MELCOR analysis to the experimental data. The average experimental data is obtained from accounting for the area ratio based on the distances among the TEs. If heat transfer to the catch pan was simulated correctly regardless of heat transfer inside the catch pan, the MELCOR temperature would agree with the experimental average. If the surface area of the catch pan was reduced to 0.28 m^2 in this analysis, it is appropriate to compare it with the experimental average for the same area. As shown in this figure, MELCOR predicts higher than the experimental averaged using a pool area of 1 m^2, but it is lower than the pool area of 0.28 m^2 as used in this current analysis.

As mentioned in the previous section, the predicted pool temperature by MELCOR is higher than the experimental data due to the need for segmenting the catch pan heat structural model, and the oxide layer effect. These observations are also applied to the catch pan temperature results.

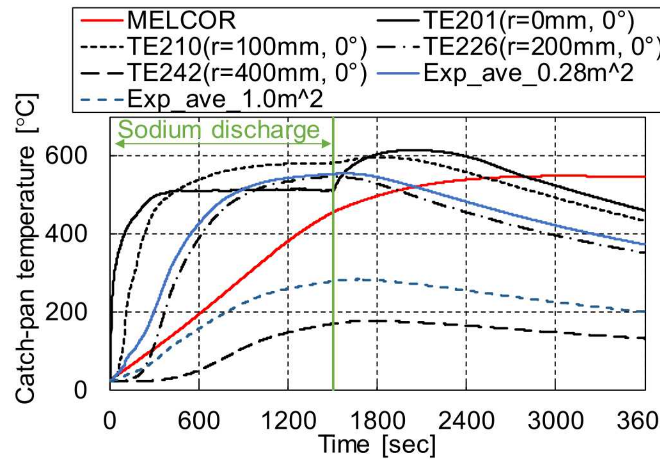

FIGURE 7: Catch-pan temperature for the current MELCOR analysis and experimental result (TEs and average)

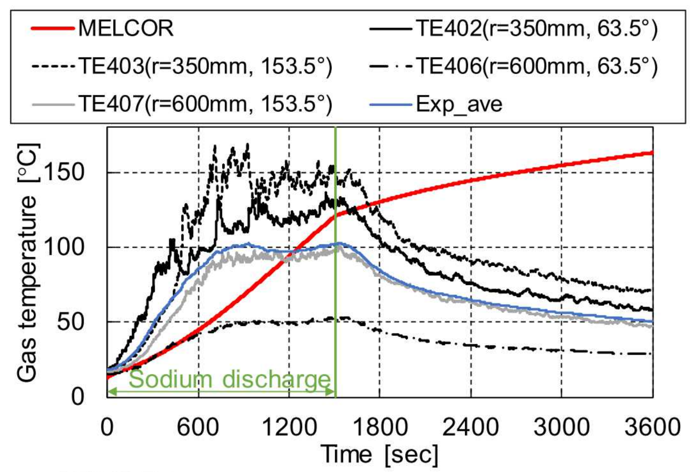

FIGURE 8: Gas temperature for the current MELCOR analysis and experimental result (TEs and average)

3.4 Gas Temperature

FIGURE 8 compares MELCOR gas temperature to the experimental data. An averaged experimental temperature was obtained based on the locations of TEs in the gas region of the test chamber. The relation between the analytical and experimental ones is very similar to that of combustion rate and the temperature results. We expect that a reasonable gas temperature can be possible when the pool combustion rate is improved through some modifications.

Accounting for the heat capacity of large sodium aerosols in the gas region may improve the comparison to the experimental data. First, heat capacity of aerosol is not considered and hence increase in gas temperature is overestimated in the current analysis. In this analysis, 1.1 kg Na_2O and 0.5 kg Na_2O_2 aerosols are produced in total until 1,500 s and half of them transfer to atmosphere. This mass or heat capacity is not negligible as compared to initial air mass of 3.6 kg. The comparison of gas temperature becomes more appropriate after considering aerosol heat capacity. As for another aerosol effect, thermal radiation has important physics in sodium fire. The gray gas model in this analysis only considers the radiation transport to the gas and neglects radiation to and from aerosols does not consider the aerosol concentration. To include the effect of aerosols in the thermal radiation, the use of the new enclosure heat radiation model [8] will be considered in the future work.

4. CONCLUSION

The F7-1 pool fire experimental analysis is carried out using a NAC package in MELCOR to assess the models and provide a better enhancement for the pool fire model. The current MELCOR analysis yields lower values than the experimental data in pool combustion rate and pool, catch pan, and gas temperature until almost 1,000 s. The current treatment of heat transfer for the catch pan is the primary cause of the difference in the results from the experimental data. Excessive heat loss in a single heat structure representing the catch pan (bot head) affects combustion rate. After sodium discharge stopping, the pool combustion rate and temperature become higher than experimental data. This is caused by absence of a model for pool fire suppression due to the oxide layer buildup on the pool surface.

Recommendations for future works includes:

1) Heat transfer modification considering temperature distribution in the catch pan.
2) Implementation of the oxide layer model.
3) Modelling of heat capacity of the atmospheric aerosol and the pool surface oxide.
4) Using the enclosure radiation model for radiating to and from the aerosols.

ACKNOWLEDGEMENTS

This work was supported by Sandia, DOE, and JAEA staffs on the special assignment for Mitsuhiro Aoyagi and Akihiro Uchibori to Sandia in U.S. Sandia National Laboratories is managed and operated by National Technology and Engineering Solutions of Sandia, LLC under DOE NNSA contract DE-NA0003525. The authors express appreciation to the following Sandia staff: Dr. Larry Humphries for providing technical suggestions and peer review for this paper and Mr. John Reynolds for his support for MELCOR simulations.

REFERENCES

[1] Humphries, L., et al., "Non-LWR Model Development for the MELCOR Code," *Proceedings of the 26th International Conference on Nuclear Engineering (ICONE26)*, ICONE26-82415 (2018).

[2] Humphries, L., and Louie, D., "MELCOR/CONTAIN LMR Implementation Report– – FY16 Progress," *Sandia Report*, SAND2016-12101, Sandia National Laboratories, November (2016).

[3] Murata, K., et al., "User's Manual for CONTAIN 1.1, A Computer Code for Sever Nuclear Reactor Accident Containment Analysis," SAND87-2309 / NUREG/CR-5026 (1989).

[4] Morita, K., "Thermodynamic Properties and Equations of State for Fast Reactor Safety Analysis, Part II: Properties of Fast Reactor Materials," *Nuclear Engineering and Design*, 183, 193-211 (1998).

[5] Louie, D., and Uchibori, A., "Sodium Fire Collaborative Study Progress– – CNWG Fiscal Year 2019," *Sandia Report*, SAND2019-15043, Sandia National Laboratories, December (2019).

[6] Futagami, S., et al., "Sodium Pool Combustion Test Run-F7 (Interim Report)," *PNC Report*, PNC TN9410 98-074, Power Reactor and Nuclear Fuel Development Corporation, Oarai, Japan, August (1998) (in Japanese).

[7] Humphries, L., et al., NAC Package Users Guide in "MELCOR Computer Code Manuals, Vol. 1: Primer and Users' Guide, Version 2.2.14959," SAND 2019-12536 O, Sandia National Laboratories, October (2019).

[8] Humphries, L., et al., Heat Structure (HS) Package in "MELCOR Computer Code Manuals, Vol. 2: Reference Manual, Version 2.2.14959," SAND 2019-12537 O, Sandia National Laboratories, October (2019).

