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Sodium Fire Collaborative Study Progress–CNWG Fiscal Year 2022

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ABSTRACT

This report discusses the progress on the collaboration between Sandia National Laboratories (Sandia) and Japan Atomic Energy Agency (JAEA) on the sodium fire research in fiscal year (FY) 2022 and is a continuation of the FY2021 progress report. We only report the changes made to the current sodium pool fire model in MELCOR. We modified and corrected many control functions to enhance the fraction of oxygen consumed that reacts to form monoxide (FO2) parameter in the current model from the FY2021 report. This year's enhancements relate to better agreement of the suspended aerosol measurement from JAEA's F7 series tests. Staff from Sandia and JAEA conducted the validation studies of the sodium pool fire model in MELCOR. To validate this pool fire model with the latest enhancement, JAEA sodium pool fire experiments (F7-1 and F7-2) were used. The results of the calculation, including the code-to-code comparisons are discussed as well as suggestions for further model improvement. Finally, recommendations are made for new MELCOR simulations for FY2023.

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ACRONYMS AND DEFINITIONS

Abbreviation	Definition
1-D	One-dimensional
2-D	Two-dimensional
CF	Control function
CNWG	Civil Nuclear Energy Research and Development Working Group
CVH	Control volume hydrodynamics
CVHNAME	Control volume name
DAB	Oxygen diffusion coefficient model switch
FHEAT	Fraction of sensible heat from reactions added to pool
FNA2O	Fraction of Na_2O remaining in pool
FNA2O2	Fraction of Na_2O_2 remaining in pool
FNA2OX	A variable representing FNA2O and FNA2O2
FO2	Fraction of oxygen consumed that reacts to form monoxide
FY	Fiscal year
JAEA	Japan Atomic Energy Agency
NC	Table row index
NUM	Number of control volumes
RN	Radionuclide package
Sandia	Sandia National Laboratories
TOFF	Model deactivation time

SYMBOLS

Abbreviation	Definition
Δt	Timestep
g	Gravity, subscript for gas
H	Height of liquid
L	Pool diameter
m	Mass of phase i
μ	Viscosity Subscript: 0 for the temperature-dependent viscosity property
R	Liquid radius
ρ	Density
ε	Porosity

Abbreviation	Definition
r	Subscript r for pool surface
s	Subscript s for solid
T	Temperature Subscript: pool, pan, pan-1, pan-2, pool-pan, initial, respectively for the liquid pool, catch-pan, pan region under the pool, pan region outside the pool, pool to catch-pan, initial condition
T_{surf}	Oxide crust surface temperature
T_g	Ambient temperature
t	Time
ν	Kinematic viscosity

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1. INTRODUCTION

This report documents the progress on sodium fire research in fiscal year 2022 by Sandia National Laboratories (Sandia) and the Japan Atomic Energy Agency (JAEA) as a part of the Civil Nuclear Energy Research and Development Working Group (CNWG) between the United States and Japan. This progress report is a continuation of the progress report from fiscal year 2021; therefore, only pertinent information, data, and results of the research for this fiscal year are documented. Readers should consult the previous progress reports [Louie 2021, Louie 2021a], which focused on MELCOR sodium pool fire model validation. Sodium pool fires involve multiple interacting phenomena occurring from the reaction between oxygen in the air and sodium liquid/vapor on the surface of the sodium pool [Olivier 2010]. The extent of reaction can be limited by the degree to which oxygen can diffuse into contact and react with sodium. This diffusion can be limited by the buildup of oxide layers on the pool surface. The initial sodium pool fire model in MELCOR is a parametric model with greater limitations and accuracy. It has been extended and validated against the JAEA F7 experiments as part of collaborative research between JAEA and Sandia under the CNWG framework.

The following goals are established as a continuation of the collaboration research using JAEA's F7 experiments to validate MELCOR:

- Validate MELCOR thermal hydraulic modeling, focusing on evaluation of the pool, gas and catch-pan temperatures as described in this progress report.
- Enhance the validation basis for the MELCOR aerosol physics modeling, including the generation and behavior of aerosol species, Na_2O, Na_2O_2, and NaOH.
- Enhance the MELCOR pool fire model.

Section 2 of this progress report describes the initial parametric MELCOR pool fire model as well as the enhancement to this model. Section 3 presents the results of the MELCOR validation simulations against the experimental data. This also includes code-to-code comparisons. Based on the assessment of the F7 experiments, recommendations are made for further model improvements. In addition, the aerosol benchmark from the F7 experiments is assessed. Finally, the summary and conclusions are presented in Section 4.

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2. SODIUM POOL FIRE MODEL

The initial sodium pool fire model in MELCOR has been adapted from CONTAIN-LMR, which was originally based on the SOFIRE II code [Sandia 2018a]. The SOFIRE II model was developed from the results of earlier pool fire experiments. These tests concluded that the sodium burning rate was proportional to the oxygen concentration and was controlled by diffusion of oxygen to the pool surface through the convective boundary layer. This initial implementation of a MELCOR sodium pool fire model is a parametric model.

A mechanistic enhancement of the current model, to ensure broader applicability beyond the original testing basis of the parametric model, is an important motivation for this JAEA and Sandia collaboration under the CNWG framework. As observed in the sodium pool fire experiments conducted at Sandia [Olivier 2010], the progression of the sodium pool fire may depend on the oxide layers and other solidified materials at the pool surface. The inclusion of the rate-limiting oxide layer is a key model enhancement. In addition, the sodium pool fire experiments conducted at JAEA, such as the F-series tests, indicated that liquid sodium spreading impacts progression of sodium fires [Louie 2021]. The F-series tests conducted at JAEA also measured suspended aerosol, which would be influenced by the amount of sodium by-products residing in the pool.

2.1. Current Sodium Pool Fire Model

The sodium pool fire model is described in greater detail, including model inputs, in [Louie 2021a]. A summary of the model inputs is provided below.

To provide flexibility in the testing of uncertain inputs of the current pool fire model, many of the input parameters can be implemented as control functions. This greatly extends the flexibility of the model, enabling exploration of parametric uncertainties and alternate modeling approaches [Sandia 2018b].

Sodium spreading on a surface can be explored within the framework of the control function infrastructure implemented to support the current pool fire model. The spreading of sodium will dynamically change the effective diameter of the pool on the spreading surface. In the current model, this is represented by the CV_PDIA record in the control volume hydrodynamics (CVH) package. Through control functions, this record can be dynamically adjusted throughout the course of a simulation to represent the spreading of the sodium pool (i.e., the change in its diameter) in the integral MELCOR simulation. How the pool diameter changes can be represented by control function inputs defined as part of a MELCOR simulation input file, as discussed further in [Louie 2021a].

Currently, these input parameters are entered as a constant throughout the entire calculation. A control function capability was added to each of these input parameters to easily permit the implementation of the model improvement. The improvement can be a correlation or equation. In FY2020 [Louie 2021], implementation of an enhancement to the oxygen diffusion coefficient model switch (DAB) parameter commenced. This parameter controls modeling of the oxygen diffusion to available sodium and thus enables a simulation to capture how reaction rates are altered due to the buildup of the oxide layers above the pool. In this progress report, effort is described that has supported further refinement of the oxygen diffusion correlation that can limit the rate of sodium consumption. In addition, as described in last year's progress report [Louie 2021a], the F-series experiments measured suspended aerosols. Aerosol formation and dynamics are influenced by many factors, including the amount of the sodium by-products arising from the pool fire. The updated input allows control functions to dynamically adjust the fractions of the sodium by-products such as

Na_2O and Na_2O_2 as FNA2O and FNA2O2, respectively. Table 2-1 lists the input parameters for the current sodium pool fire model in MELCOR with descriptions and the enhancement if any.

Table 2-1 Physics input parameters for the current sodium pool fire model in MELCOR

Parameter	Description	Enhancement
FO2	Fraction of the oxygen consumed that reacts to form monoxide. The value 1.0-FO2 is the remaining oxygen fraction for the reaction to form peroxide.	Modeled in this report
FHEAT	Fraction of the sensible heat from the reactions to be added to the pool. The balance will go to the atmosphere.	No model developed yet
FNA2O	Fraction of the Na_2O remaining in the pool. The balance will be applied to the atmosphere as aerosols.	Modeled in FY2021 [Louie 2021a] as FNA2OX
FNA2O2	Fraction of the Na_2O_2 remaining in the pool. The balance will be applied to the atmosphere as aerosols.	Modeled in FY2021 [Louie 2021a] as FNA2OX
TOFF	Model deactivation time. This is useful for modeling experiments.	Not used
DAB	Oxygen diffusion coefficient model switch. The default diffusion correlation will be used if a real value of greater than or equal to 0.0 is specified.	Modeled in FY2020 [Louie 2021] and improved in FY2021 [Louie 2021a]

2.2. Model Improvement

As previously described, the model improvement is a continuation of research during FY2021 [Louie 2021a]. A more detailed description of the model enhancement can be found in the FY2021 progress report [Louie 2021a]. In this section, only two topics are covered: (1) slight modification of the sodium spreading coefficients for the pool as shown in Section 2.2.1, and (2) a new model for FO2 as shown in Section 2.2.2.

2.2.1. Liquid Sodium Spreading

The spreading of the liquid sodium is an important phenomenon impacting the sodium fire intensity because the combustion rate is greatly dependent on the surface area of the reaction between the oxygen and liquid sodium. While extensive discussions of this 1-dimensional (1-D) radial spreading model (a pancake model) used in this research in the past couple years can be found in [Louie 2021 and Louie 2021a], only the coefficients in the equations used in the spreading model will be discussed here because these coefficients have been improved this year. The final radial spreading distance as implemented is shown below

$$R(t + \Delta t) = \sqrt[8]{R(t)^8 + C_1 \cdot \frac{g}{\mu\, \pi^3 \rho^2} m^3 \Delta t} \qquad \text{2-1}$$

where μ, ρ and C_1 in Equation 2-1 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 by

$$\mu = \mu_0 \cdot \exp\,(2.5\, C_2 \cdot \varepsilon) \qquad \text{2-2}$$

C_2 in Equation 2-2 is an empirical constant and ε is the solid fraction in the pool. As shown in these equations, both empirical constants can greatly influence the spreading; however, C_1 in Equation 2-1 controls the incremental spreading in a timestep, which is greater than on the effect by C_2 in Equation 2-2. In this study, we are adjusting these empirical constants to better represent the spreading and sodium combustion as observed in the experiments

2.2.2. Monoxide Oxygen Fraction

As shown in Table 2-1, FO2 is the oxygen consumption fraction for the sodium monoxide formation. This fraction was given as the constant value in the current sodium pool fire model in MELCOR. Meanwhile, SPHINCS calculates this fraction by using a chemical equilibrium model for the Sodium-Oxygen-Hydrogen (Na-O-H) elements system in the named BISHOP code [Okano 1999]. In the case of the Na and O elements system, the formulation of chemical equilibrium can be simplified to the function of just two parameters: the Na and O_2 molar fraction before the reaction, and the reaction temperature. The following reactions are considered:

$$\mathrm{Na} + 0.25\ \mathrm{O_2} \rightarrow 0.5\ \mathrm{Na_2O}$$

$$\mathrm{Na} + 0.5\ \mathrm{O_2} \rightarrow 0.5\ \mathrm{Na_2O_2}$$

In the improvement of this pool model in MELCOR this year, FO2 is modeled to correspond to the SPHINCS/BISHOP model as described above. A table for FO2 with the Na/O_2 molar fraction and the reaction temperature has been developed based on the parametric calculation of BISHOP in SPHINCS. A model based on this table is developed for MELCOR for enhancing FO2, which is calculated by the ratio of Na/O_2 molar concentration and reaction temperature (see Table 2-2). The molar number of Na is given by the equation of state using the pool temperature. The molar number of O_2 is directly obtained by the calculated atmospheric gas composition. The pool temperature is substituted for the reaction temperature. This substitution is reasonably approximated for the reaction that took place in the pool. The functional plots from Table 2-2 are given in Figure 2-1 and Figure 2-2. As shown in Figure 2-1, FO2 remains at unity until the Na/O_2 molar fraction reaches 0.25. Above the Na/O_2 ratio of 0.25, the FO2 fraction decreases as a function of the reaction temperature until it reaches a plateau. This is better illustrated in Figure 2-2 when correlating FO2 with the reaction temperatures. As shown in this figure, only three distinct curves are shown for the Na/O_2 molar fractions.

Table 2-2. Tabular Values of FO2 from BISHOP

Reaction Temp (ºC)	O2 molar concentration/Na molar concentration							
	5.00E-03	1.00E-01	2.50E-01	4.00E-01	5.50E-01	7.00E-01	8.50E-01	1.00E+00
200	1.00E+00	1.00E+00	1.00E+00	4.00E-01	5.82E-07	5.82E-07	5.82E-07	5.82E-07
400	1.00E+00	1.00E+00	1.00E+00	4.00E-01	6.02E-04	6.02E-04	6.02E-04	6.02E-04
600	1.00E+00	1.00E+00	1.00E+00	4.00E-01	2.30E-02	2.30E-02	2.30E-02	2.30E-02
800	1.00E+00	1.00E+00	1.00E+00	4.00E-01	1.90E-01	1.90E-01	1.90E-01	1.90E-01
1000	1.00E+00	1.00E+00	1.00E+00	5.34E-01	5.34E-01	5.34E-01	5.34E-01	5.34E-01
1200	1.00E+00	1.00E+00	1.00E+00	7.68E-01	7.69E-01	7.69E-01	7.69E-01	7.69E-01
1400	1.00E+00	1.00E+00	1.00E+00	8.72E-01	8.71E-01	8.72E-01	8.72E-01	8.71E-01

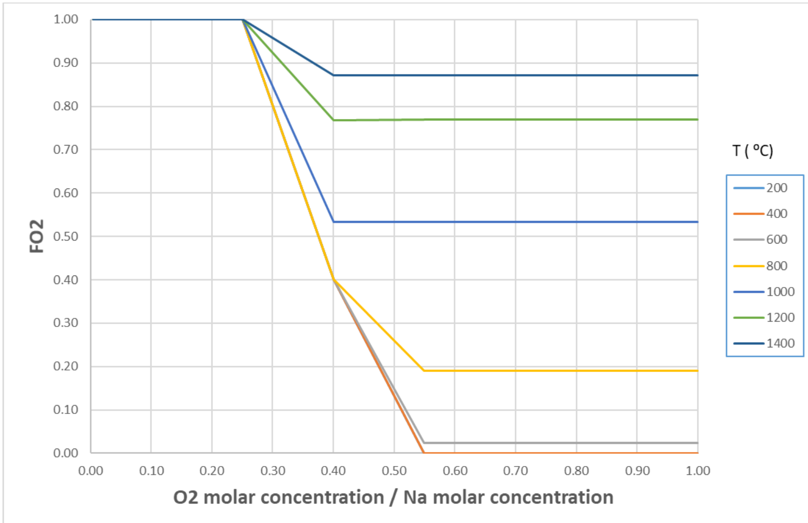

Figure 2-1. Plot of FO2 values as function of O2/Na molar concentration using BISHOP

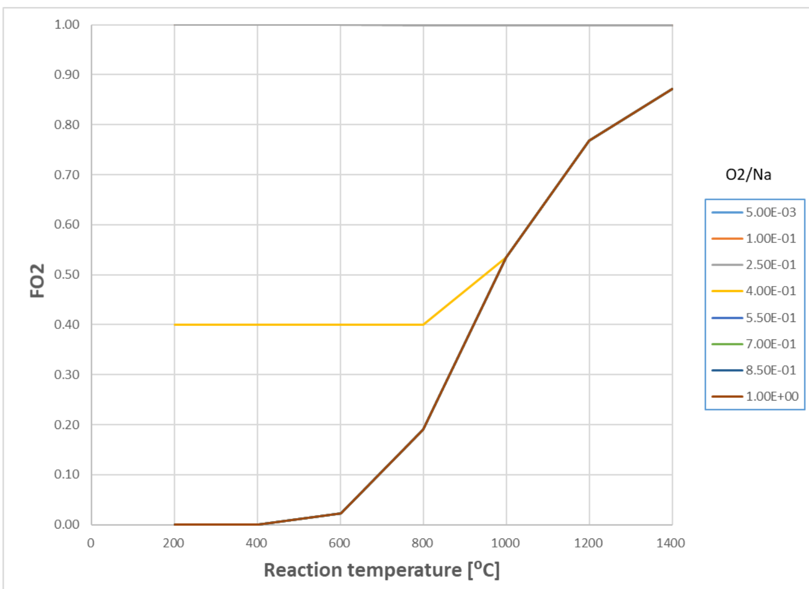

Figure 2-2 Plot of FO2 values as function of reaction temperature using BISHOP

2.3. Model Implementation Using Control Functions

One of main features of MELCOR is the ability to implement models explicitly via the control function (CF) package. The models can be tested and assessed before being added into MELCOR code.

In this report, we attempt to model FO2 using CFs and keep other model parameters as previously reported in FY2021 [Louie 2021a]. The reader is encouraged to consult our FY2021 progress report for the modeling details, including their CF modeling for the other model parameters as shown in Table 2-1.

One additional modeling adjustment was required. Because an additional parameter for the pool fire model is adjusted, it affects other parameters. The liquid sodium spreading rate was slightly modified to ensure that it closely represents the trend of the sodium combustion. Thus, Section

2.2.1 presents the important coefficients (see the empirical constants in Equations 2-1 and 2-2) for the sodium spreading model that were modified for this study.

As mentioned in Section 2.2.2, the monoxide oxygen fraction (FO2) is modeled more realistically to represent the oxygen fraction reacting with the liquid sodium to form sodium monoxide and the remaining oxygen available for the sodium peroxide formation. The lookup of Table 2-2 information was implemented for FO2.

The implementation of the CF models mentioned here are described in Section 3.2.

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3. MELCOR VALIDATION STUDY

This section describes the validation of the pool fire model in MELCOR using the JAEA F7 series sodium pool fire experiments (F7-1 and F7-2) [Futagami 1998]. Section 3.1 only briefly describes the JAEA F7 experiments because the details of these experiments are included in our FY2021 progress report [Louie 2021a]. Section 3.2 describes the MELCOR input model of the F7 experiments. The MELCOR model described in Section 3.2 was adapted from a previous input model [Louie 2021]. In addition, Sections 3.2.1-3.2.4 describe MELCOR CFs corresponding to the improved models described in Section 2.2 . Section 3.3 discusses the MELCOR results for the F7 tests. Section 3.3.1 shows the comparison of the model improvement in FY2022 and FY2021 for the F7-1 test. Then, Section 3.3.2 explores the impact of the improved models and their comparison to the JAEA code results for the F7-2 test. Finally, Section 3.4 provides recommendations for future validation work.

3.1. F7 Test Descriptions

The test apparatus, shown in Figure 3-1, consists of the stainless-steel vessel named FRAT-1, 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 m^2, 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 m^2 for F7-1 and 0.30 m^2 for F7-2, respectively. The air in the vessel is ventilated with a steady flow of approximately 3.0 m^3/min. The test conditions are summarized in Table 3-1.

The experimental temperature measurements of the vessel surface, the atmosphere, the pool, the bottom surface of the catch pan, and the surface between the two-thermal insulation layers were monitored with multiple thermocouples. The concentrations of oxygen, hydrogen, and aerosolized material were also measured in this test. The measured values used for comparison with the computational results were obtained from [Futagami 1998]. The reader is encouraged to review our FY2021 progress report for the details of the experimental data collected in the F7 series tests [Louie 2021a].

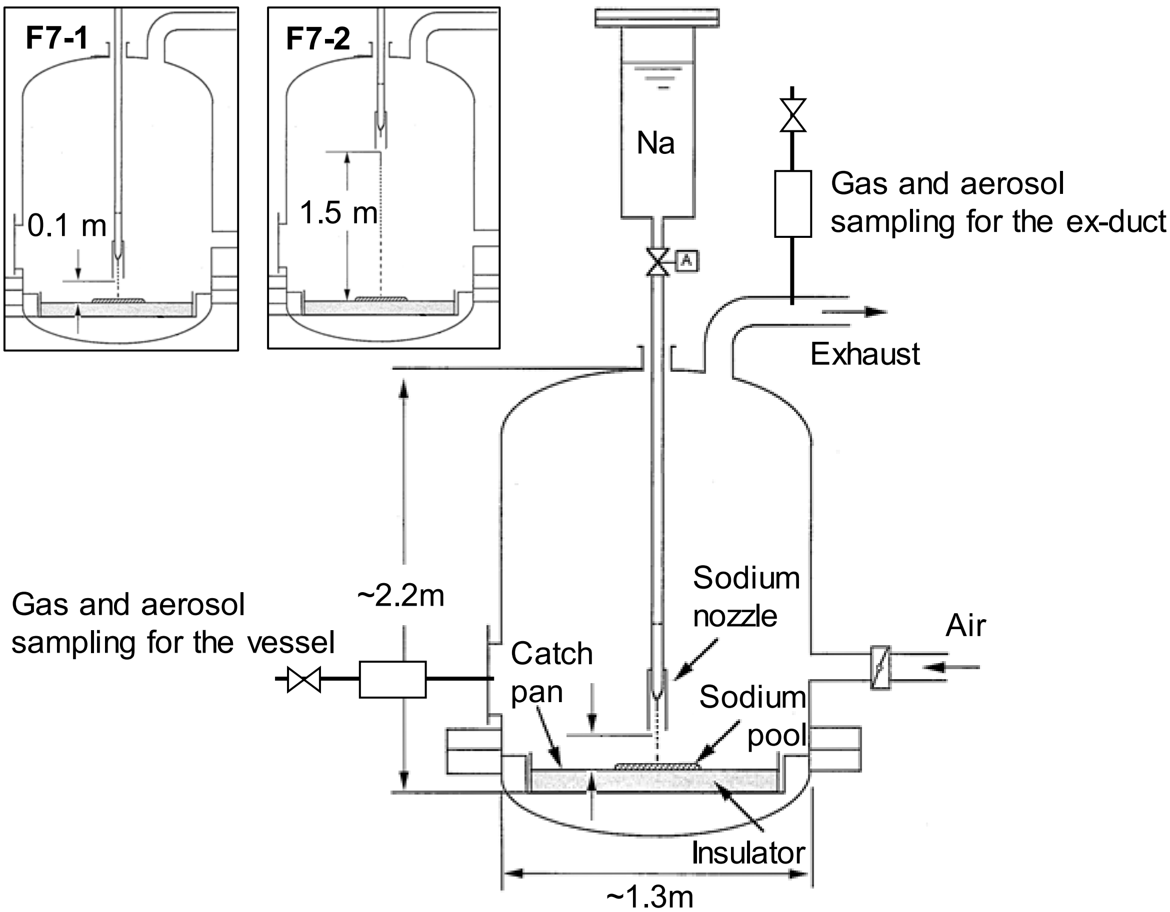


Figure 3-1. Test apparatus

Table 3-1. Test conditions

Parameter	F7-1	F7-2
Sodium temperature	505°C	
Sodium leak form	Column	
Sodium leak height from catch pan	0.1 m	1.5 m
Sodium leak duration	Approximately 1,500 s	
Average sodium leak rate	3.3 g/s	
Total leak quantity of sodium	4.94 kg	
Oxygen concentration (initial)	20.8%	20.7%
Atmosphere temperature (initial)	12.7°C	19.6°C
Atmosphere relative humidity	49.2%	71.5%
Ventilation flow rate	Approximately 3.0 m^3/min	

3.2. MELCOR Model

Like the previously developed MELCOR model [Louie 2021a], the current MELCOR model uses three control volumes and the two flow paths as shown in Figure 3-2. The spray and pool fire occur in the control volume "FRAT," which corresponds to the vessel of the F7 tests. "PREENV" and "ENV" correspond to the environment as shown in Figure 3-2. The sodium fire computation is summarized in Table 3-2. As shown in Table 3-2, a sodium spray fire model was activated for both tests, which may not reflect the column formation observed in the experiments. In addition, FY2021 MELCOR simulations did not include FO2 control function models. The control functions for the enhancement described in Section 2.2 are given in Sections 3.2.1 and 3.2.2

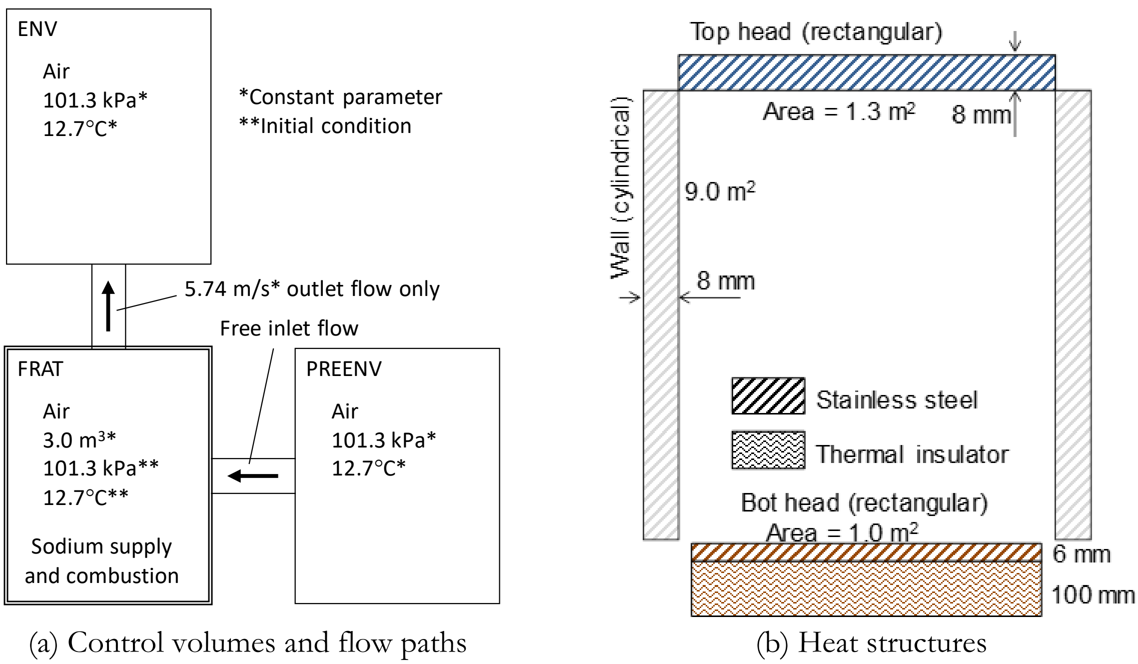


Figure 3-2. MELCOR model setup. Note both ENV and PREENV are modeled as time independent volumes.

Table 3-2. Computational conditions of sodium spray and pool fire

Spray fire	Height	0.1 m for F7-1, 1.5 m for F7-2
	Droplet diameter	0.0045 m
	FNA2O2	1.0
	Time step	Terminal velocity model
Pool fire	FO2	Function (see 2.2.2 and 3.2.2)
	FHEAT	0.6
	FNA2O	See FY2021 report [Louie 2021a]
	FNA2O2	See FY2021 report [Louie 2021a]
	TOFF	3600.0 s
	DAB	See FY2021 report [Louie 2021a]

3.2.1. Liquid Sodium Spreading

To implement the sodium spreading model as described in Section 2.2.1, a series of CFs are used. Only the coefficients in Equations 2-1 and 2-2 were adjusted for this report. Other CFs related to the sodium spreading were not affected and are documented in our FY2021 progress report [Louie 2021a].

- Equation 2-1 in Section 2.2.1 uses a C_1 value of 4.0E-5 to closely match the spreading observed in the F7 tests during the injection phase:

```
cf_id   'SpreadR' 45 formula
!
cf_formula   13   (R^e8+c1*g/(mu*pi^e3*rho^e2)*mass^e3*dt^e4)^e5
!     N   ARG NAME   VALUE
      1   R          cf-valu(SpreadR)          ! previous value
      2   e8         8.0                       ! constant
      3   c1         4.0E-5                    ! guess constant
      4   g          9.8                       ! gravity
      5   mu         cf-valu('Na_mu')          ! viscosity sodium
      6   pi         3.14156                   ! pi
      7   e3         3.0                       ! constant
      8   rho        cvh-rho('FRAT',POOL)      ! liquid density
      9   e2         2.0                       ! constant
     10   mass       cvh-mass('FRAT',POOL)     ! unburned na mass
     11   e4         1.0                       ! constant
     12   dt         exec-dt                   ! timestep
     13   e5         0.125                     ! constant
```

- Ramacciotti correlation, Equation 2-2 in Section 2.2.1, with C=5 times C_2 =42, for closely matching the spreading rate observed in the F7-1 test. Fsolid CF is for the solid fraction as shown in Equation 2-2 (see [Louie 2021a] for this control function listing).

```
!
cf_id   'Na_mu'  43 formula
cf_formula  3  mu0*exp(C*fs)
!     N   ARG NAME   VALUE
      1   mu0        cf-valu('Na_mu0')   ! pure sodium viscosity
      2   C          42.0                ! constant, assumed
      3   fs         cf-valu('Fsolid')   ! solid fraction
```

3.2.2. Monoxide Oxygen Fraction

The FO2 model as described in Section 2.2.2 is based on a correlated table of FO2 values as functions of the reaction temperatures and the ratio of Na and O_2 molar concentration from the BISHOP results in SPHINCS. To implement this table as lookup values using CFs, Figure 2-1 and Figure 2-2 in Section 2.2.2 were examined to create a number of CFs for the FO2 value to be input to the pool fire model. To obtain the molar concentration of oxygen and sodium, the following CFs were used according to the ideal gas law.

- Molar concentration of Na

```
CF_ID  'M_Na'  1001  FORMULA
!           NUM OF ARGS    FORMULA TEXT
CF_FORMULA      4          l-a-ifte(Tp>zero,Pg/(R*Tp),zero)
!     N   ARG NAME   VALUE
      1   Tp         CVH-TLIQ('FRAT')      ! Pool temperature, K
      2   Pg         CVH-P('FRAT')         ! gas pressure, Pa
      3   R          8.31446               ! Gas constant, M2-Pa/K-mol
      4   zero       0.0                   ! zero

!
```

- Molar concentration of O_2

```
CF_ID  'M_O2'  1002  FORMULA
!           NUM OF ARGS    FORMULA TEXT
```

```
CF_FORMULA      5          1-a-ifte(Tg>zero,Pg/(R*Tg)*Yo2,zero)
!     N   ARG NAME   VALUE
      1   Tg         CVH-TVAP('FRAT')      ! Gas temperature, K
      2   Pg         CVH-P('FRAT')         ! gas pressure, Pa
      3   R          8.31446               ! Gas constant, M2-Pa/K-mol
      4   zero       0.0                   ! zero
      5   Yo2        CVH-x('FRAT','O2')    ! mole fraction of O2
```

- Ratio of O_2 to Na molar concentration

```
!
CF_ID  'R_O2NA'  1003  FORMULA
!          NUM OF ARGS    FORMULA TEXT
CF_FORMULA      3          1-a-ifte(M_Na>zero,M_O2/M_Na,zero)
!     N   ARG NAME   VALUE
      1   M_NA       cf-valu('M_Na')
      2   M_O2       cf-valu('M_O2')
      3   zero       0.0                  ! zero
```

Once this ratio is determined, a number of CFs were used to interpret the corresponding ratio column in Table 2-2 and the corresponding reaction temperature. In this case, we use the pool temperature.

3.3. Simulation Results and Discussions

This section describes the MELCOR simulations using the model described in Section 3.2. MELCOR 2.2 Version 15254 was used to perform these MELCOR simulations. Section 3.3.2 describes the comparison of MELCOR results of F7-1 between the modeling in FY2021 and FY2022 as well as the comparison with the JAEA code results. In Section 3.3.3, the FY2022 MELCOR results are applied to F7-2.

3.3.1. Modeling Improvement in FY2022

Modeling improvements in FY2022 from FY2021 are summarized as:

- Sodium spreading model: Modification of model parameter (C_1 and C_2 values in Equations 2-1 and 2-2) are in Section 2.2.1 and the corresponding CFs are given in Section 3.2.1.
- Monoxide oxygen fraction model (FO2): Implementation of the function for the fraction of the sodium monoxide or peroxide formation are in Section 2.2.2 and the corresponding CFs are given in Section 3.2.2

This report discusses the MELCOR result in the FY2022 model, which includes all these improvements over the modeling as described in the FY2021 report [Louie 2021a].

3.3.2. Code Simulations Results for F7-1 Test

Figure 3-3 shows comparison of the results of MELCOR-FY2021, -FY2022, SPHINCS, and the F7-1 test data. The FY2022 result shows better agreement with the test data and the SPHINCS result than the FY2021 result for the pool temperature and combustion rate. As shown in Figure 3-3 (f), the monoxide oxygen fraction (FO2) for FY2022 changes during calculation. This result matches reasonably with the SPHINCS result. The difference from SPHINCS is mainly caused by the definition of the reaction temperature. Because SPHINCS employs the flame sheet model for pool combustion, the flame temperature can be obtained and used as the reaction temperature. MELCOR simulates the variation of the monoxide oxygen fraction by substituting the pool temperature for the reaction temperature. The concentration of suspended aerosol shown in Figure 3-3 (e) also agrees well with the test data in the FY2022 modeling, which had been improved in FY2021.

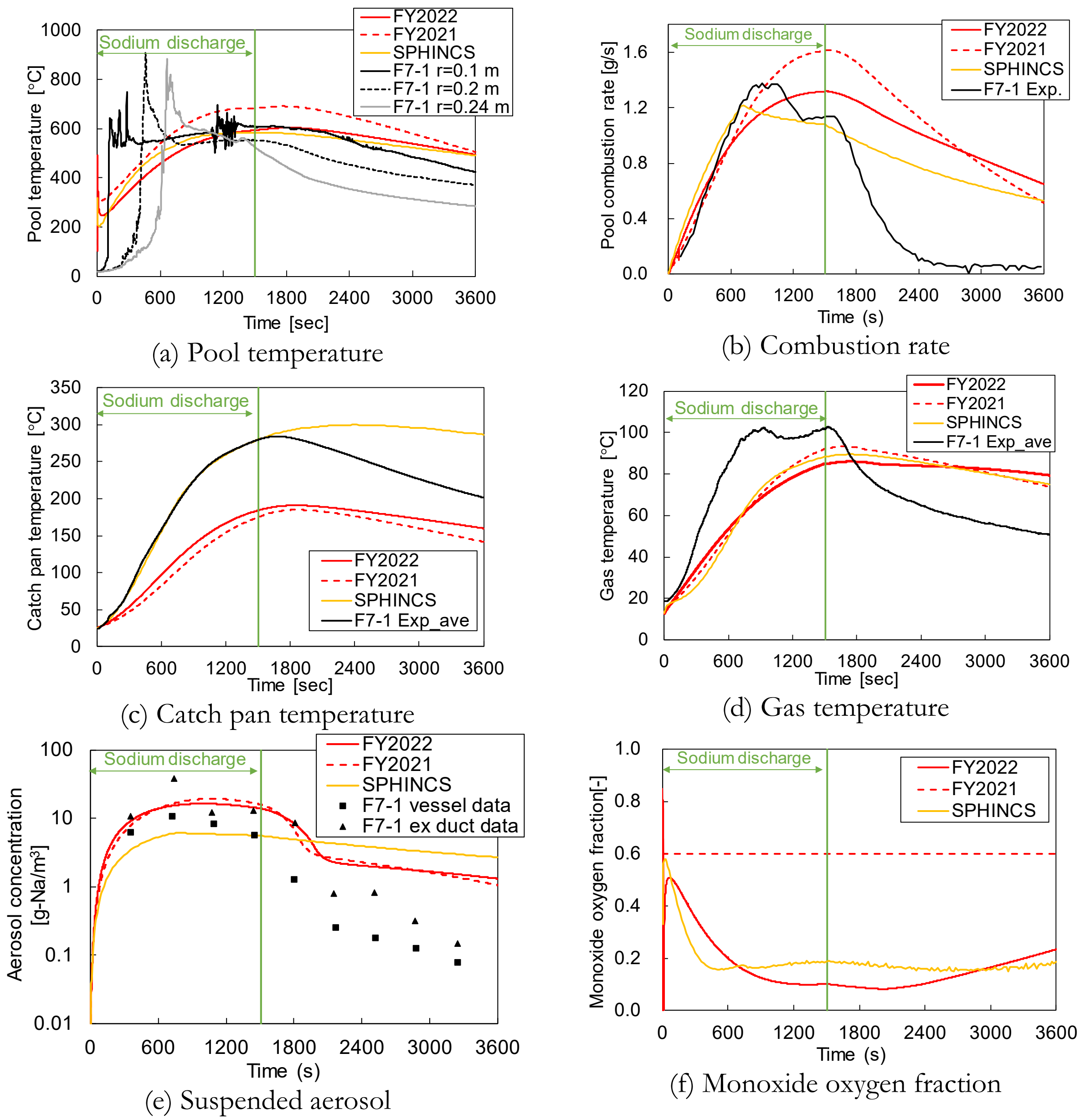
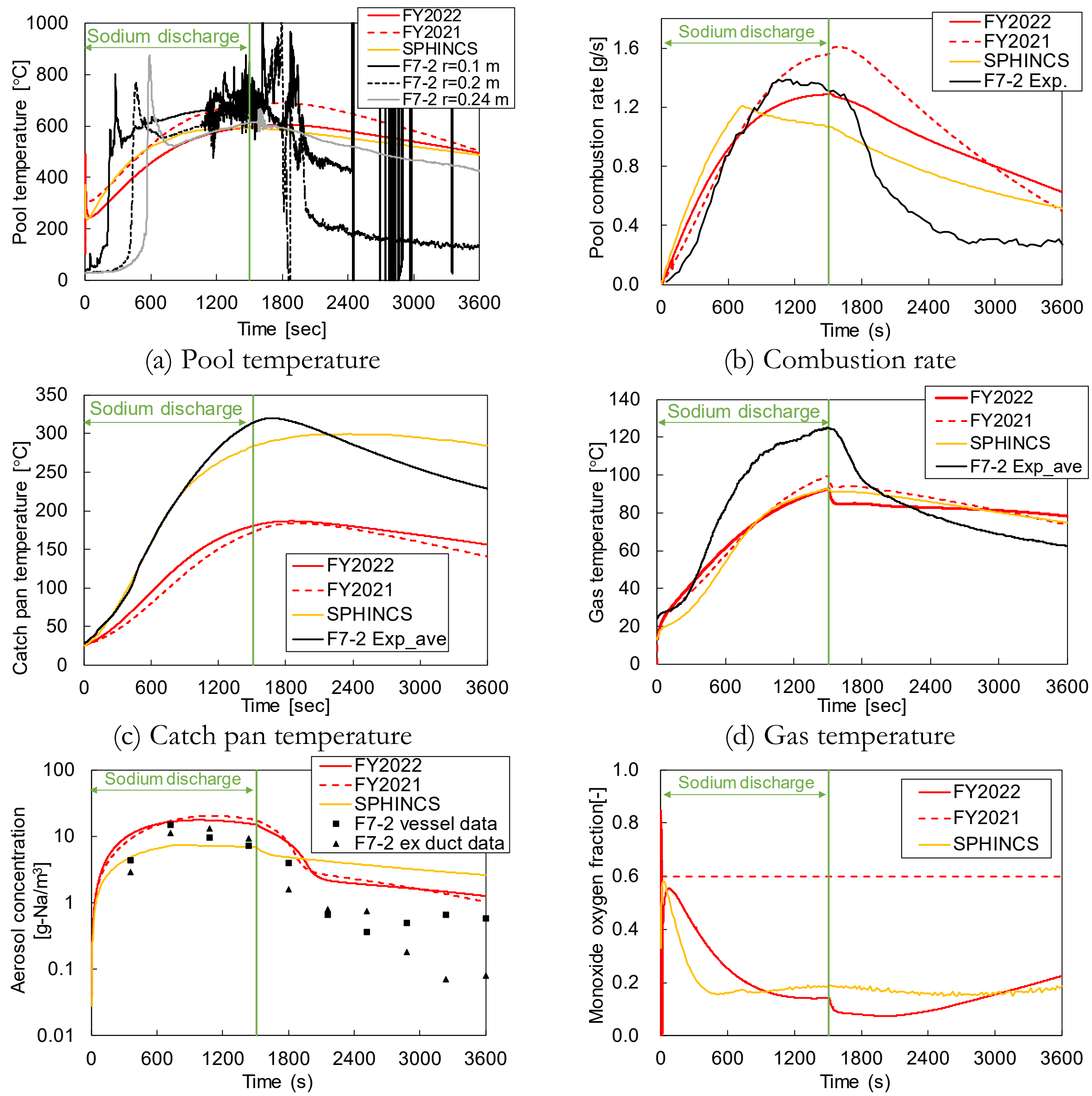


Figure 3-3. Comparison between FY2021 and FY2022 models for F7-1 Test

3.3.3. Code Simulation Results for F7-2 Test

Figure 3-4 shows the F7-2 results in the MELCOR FY2021 and FY2022 models comparing with the SPHINCS result and the F7-2 test data. The FY2022 MELCOR results are in better agreement with the SPHINCS result and the test data for the pool temperature and the pool combustion rate. The monoxide oxygen fraction (FO2) also shows reasonable agreement with the SPHINCS calculation as shown in Figure 3-4 (f). The rapid decrease in FO2 at 1,500 s may be related to the oxygen concentration in atmosphere. The gas temperature also decreases at this moment. Because the F7-2 test has larger spray height (1.5 m) than the F7-1 test (0.1 m), the spray combustion is much more significant. When the sodium discharge stops at 1,500 s, the oxygen consumption due to the spray combustion is also terminated. Then, the fraction of the monoxide formation decreases because of an increase in the oxygen concentration.



(a) Pool temperature (b) Combustion rate

(c) Catch pan temperature (d) Gas temperature

(e) Suspended aerosol (f) Monoxide oxygen fraction

Figure 3-4. Comparison between FY2021 and FY2022 models for F7-2 Test

3.4. Recommended Future Studies

The previous two sections described the progress of the MELCOR validation study in FY2022. The studies of the thermodynamic issues, and gas radiation modeling should be continued. From the viewpoint of mass transport, the moisture reaction with NaOH aerosols is an important phenomenon to be considered.

This year, we did not implement a better model for FHEAT, which represents the fraction of the sensible heat from the reactions to the pool that could influence the energy balance between the pool and the atmosphere. With this fraction enhanced, the calculational results should be matched closer to the experiments such as the F7 series tests. Therefore, we recommend FHEAT should be enhanced.

4. SUMMARY AND CONCLUSION

This progress report documents the current work during FY2022 between Sandia and JAEA on the validation of the MELCOR sodium pool fire model. The collaboration enables Sandia and JAEA to improve the sodium fire models in their respective severe accident codes. Descriptions of the current sodium fire model and suggestions for improved physics model were provided in the report.

The sodium fire tests F7-1 and F7-2 were calculated by the MELCOR code to investigate capability of the current pool fire model. The MELCOR code had a better prediction of the increase of pool and atmosphere temperatures and the suspended sodium aerosol due to pool fire. By enhancing the monoxide oxygen consumption fraction using the results from BISHOP of SPHINCS, the comparison between MELCOR and SPHINCS shows better agreement than without this oxygen fraction model.

The agreement with the experimental data is improved by using exploratory control function models to simulate or improve the following:

- heat transfer between the sodium pool and the catch pan,
- inclusion of the pool oxide layer in the combustion rate model,
- a viscosity-based pool spreading rate,
- an aerosol fraction to pool model to improve the actual aerosol release from the pool fire, and
- improvement and corrections of some model parameters.

The improved MELCOR result also shows better agreement with the result from JAEA's SPHINCS code.

In conclusion, the validation study on MELCOR's sodium pool fire model has progressed. Additional MELCOR input deck refinement is recommended to better capture the spatial effects observed in the F7-1 and F7-2 experiments. Some recommendations were made for model improvements as shown in Section 3.4

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