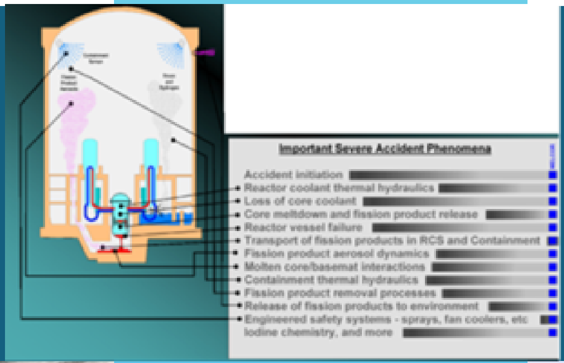
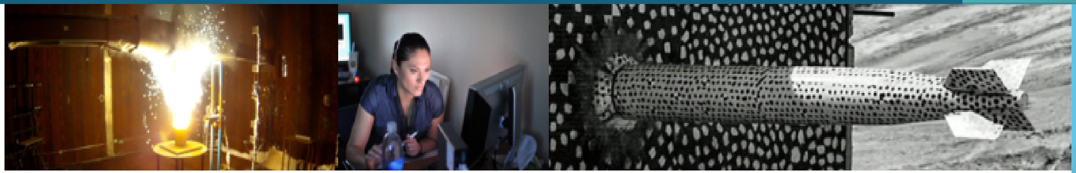
SAND2022-12478C

Sandia National Laboratories

US-Japan BLC-CNWG

MELCOR Validation Study of the Sodium Pool Fire Model with Comparison to SPHINCS





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Technical Meeting on State-of-the-art Thermal Hydraulics of Fast Reactors

Sep 26-30, 2022

The SNL work is supported by the DOE Work Package: RD-21SN040307

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Current Sodium Fire Models in

Under U.S. DOE Advanced Reactor Technologies – Fast Reactor Program

- Most sodium fire models from CONTAIN-LMR had been implemented:
  - Most input parameters for the models are constant
  - Original spray fire model enhanced to include an upward spray sub-model
  - Atmospheric chemistry model assumes the water vapor as an ideal gas
  - CF input approach improves the model flexibility and allows sensitivity studies
    - Added CF capability to input key fire model parameters.
- Previous validation works include benchmarks using ABCOVE AB5 and AB1 tests and comparison to CONTAIN-LMR results

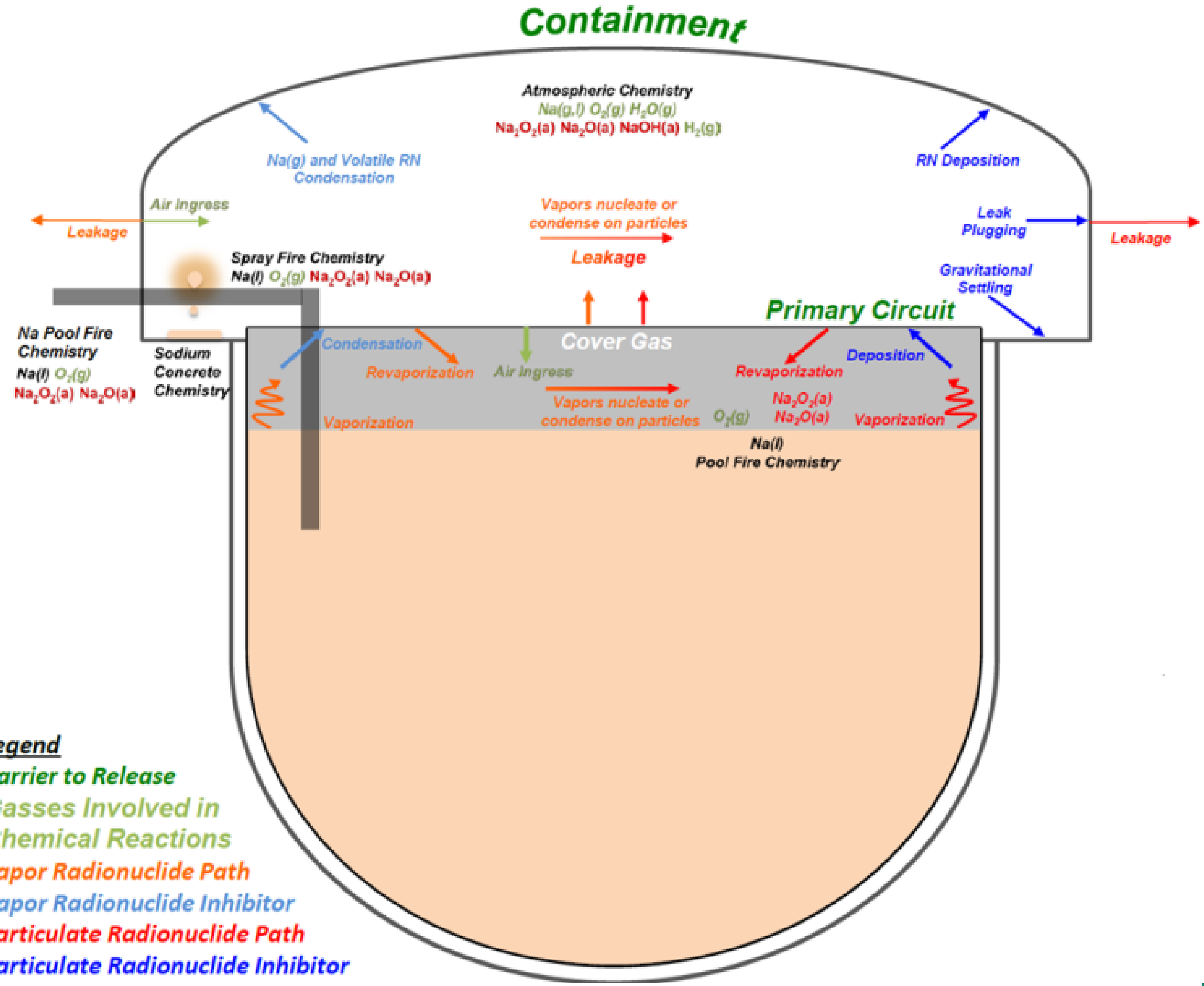


Figure adapted from ANL-ART-3

Sodium concrete chemistry (SLAM) has NOT yet been implemented into

Model improvements under Civil Nuclear Energy Research and Development Working Group Efforts between Sandia National Labs (SNL) and Japan Atomic Energy Agency (JAEA)

A Collaborated Research was identified to improve the MELCOR pool fire model using F series pool fire experiments from JAEA

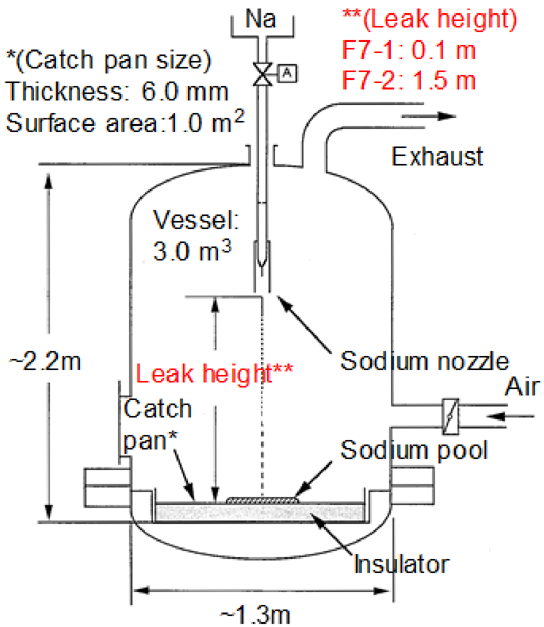
Current Sodium Pool Fire Model in MELCOR

Parameter	Description
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.
FHEAT	Fraction of the sensible heat from the reactions to be added to the pool. The balance will go to the atmosphere.
FNA2O	Fraction of the Na_2O remaining in the pool. The balance will be applied to the atmosphere as aerosols.
FNA2O2	Fraction of the Na_2O_2 remaining in the pool. The balance will be applied to the atmosphere as aerosols.
TOFF	Model deactivation time. This is useful for modeling experiments.
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.

Using the Control Function input capability to enhance models with code modification for the proposed models:

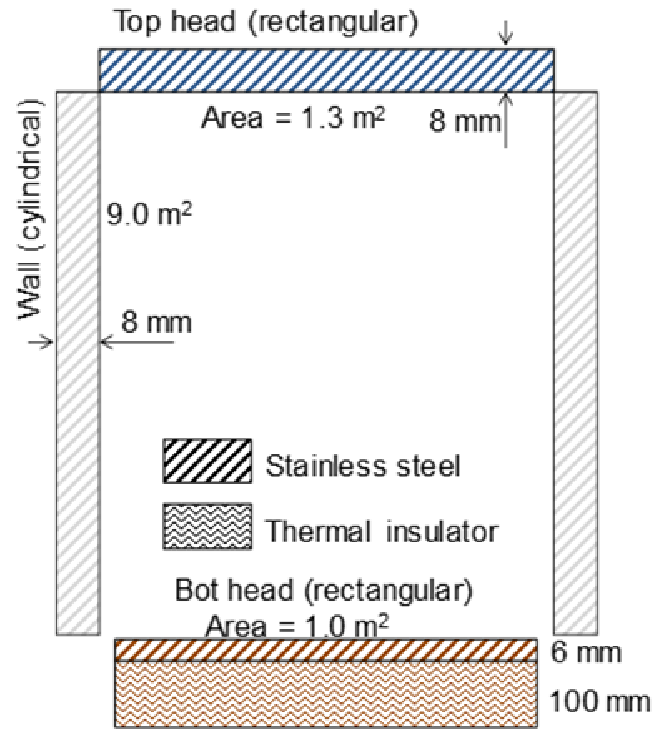
- Highlighted input parameters were enhanced last 2 years
  - DAB (FY2020)
    - Account the effect of oxide layer buildup
  - FNA2Ox (FY2021)
    - Allows better prediction of the suspended sodium aerosols
- FO2 is being enhanced in this year
- Other enhancement were made
  - Pool-Pan heat transfer – enhanced with pool radius functionality
  - Liquid sodium spreading
    - Viscosity dependent spreading

F7 pool fire experiments/MELCOR Model

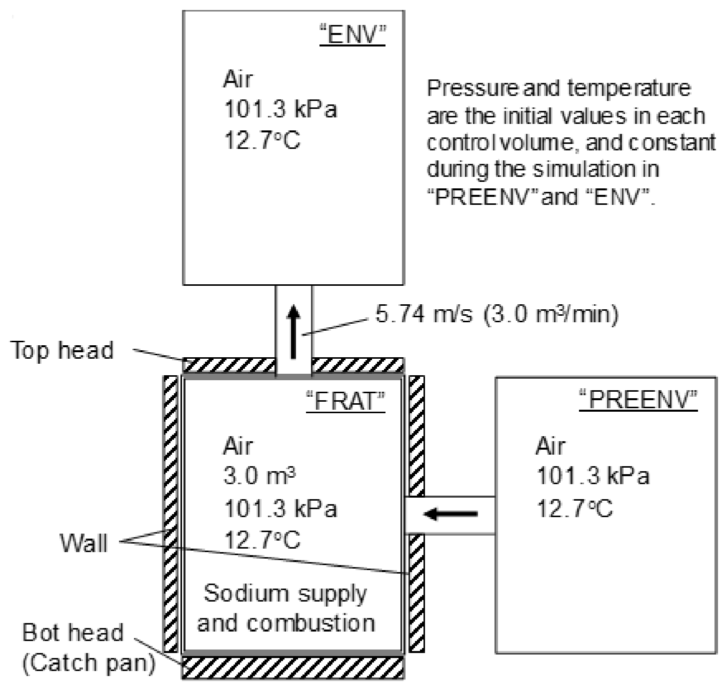


Test Conditions

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	



Measurements (representative)
- Temperature (gas, sodium pool, catch-pan, vessel wall)
- Concentration (oxygen, aerosol)



Pressure and temperature are the initial values in each control volume, and constant during the simulation in "PREENV" and "ENV".

Sodium Fire Models used
- Spray fire
- Pool fire

Enhancement to MELCOR Pool Fire Model

- Oxidation is limited by diffusion (DAB) through the oxide layer
  - Normal pool combustion

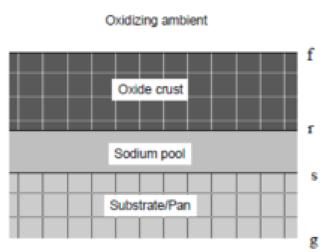
$$\dot{m}_{O2} = A_s H \rho_g Y_{O2} \qquad H = 0.14 D_{diff}\left(g S_c \frac{\beta}{\nu^2}\left|T_{surf} - T_g\right|\right)^{1/3} \qquad D_{diff} = \frac{6.4312\times 10^{-5}}{P_g}\left[\frac{\left(T_{surf}+T_g\right)}{2}\right]^{1.823}$$

=DAB: default

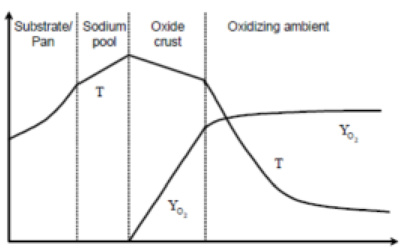
  - Oxygen diffusion through the oxide layer [Oliver 2010]

$$\dot{m}_{O2} = A_s\left[\left(\frac{Sh}{L}\right)\frac{D}{1+\delta/\Delta_1}\right]\rho_g Y_{O2,\infty} \qquad H^* = \left(\frac{Sh}{L}\right)\frac{D}{1+\delta/\Delta_1}$$

$$D_{diff} = \frac{\left(\frac{Sh}{L}\right)\frac{D}{1+\delta/\Delta_1}}{0.14\left(g S_c \frac{\beta}{\nu^2}\left|T_{surf} - T_g\right|\right)^{1/3}} \;\Rightarrow\; D_{diff} = \frac{D}{1+\delta/\Delta_l}$$



Schematic of the pool layers, temperature Profile (T), and Oxygen Fraction (YO2) [Olivier 2010]



The oxide layer thickness δ is given by the amount of oxide formed in the pool with an assumed porosity function.

[Olivier 2010] Olivier, T.J., et al., Metal Fires and Their Implications for Advanced Reactors Part 3: Experimental and Modeling Results, SAND2010-7113, Sandia National Laboratories, Albuquerque, NM, October 2010.

- Pool oxide fractions (FNA2Ox) – can influence the by-product sodium aerosol distribution

$$FNA2OX = a_1 \cdot \varepsilon^{a_2} + a_3 \cdot \varepsilon + a_4$$

Non-Sodium pool model enhancement

Liquid sodium spreading

- The spreading rate was improved using a viscosity dependent model adapted from the ex-vessel corium spreading model in MELCOR

Adapted corium spreading model:

$$\mu \frac{u}{H^2 R} \propto \rho g H \qquad \frac{dR}{dt} = C1 \frac{\rho g}{\mu \pi^3} \frac{V^3}{R^7}$$

$$R(t + \Delta t) = \sqrt[8]{R(t)^8 + C1 \cdot \frac{g}{\mu \pi^3 \rho^2} m^3 \Delta t}$$

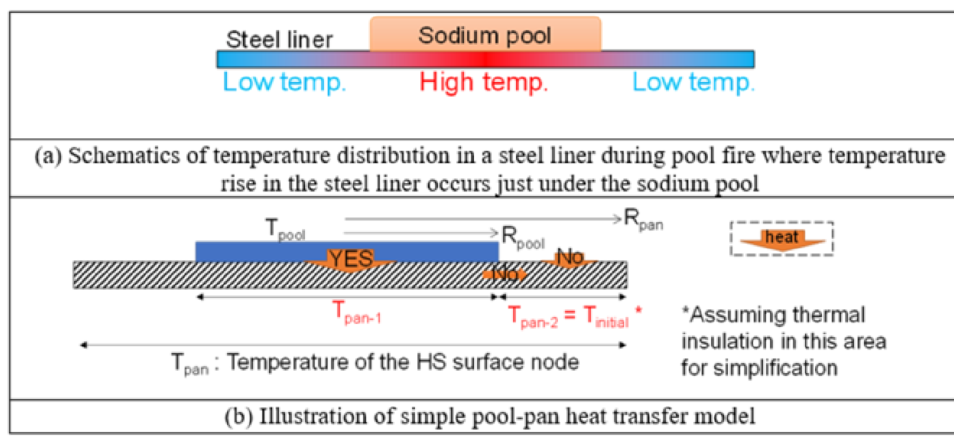
Ramacciotti correlation:

$$\mu = \mu_0 \cdot \exp(2.5 \cdot C \cdot \varepsilon)$$

Solid fraction $\varepsilon = \frac{\Sigma \frac{m_j}{\rho_j}}{\Sigma \frac{m_i}{\rho_i}}$

Pool-to-pan heat transfer

- Addressing the limitation of 1-dimensional heat structure model in MELCOR
  - A quasi 2-dimensional heat transfer model developed



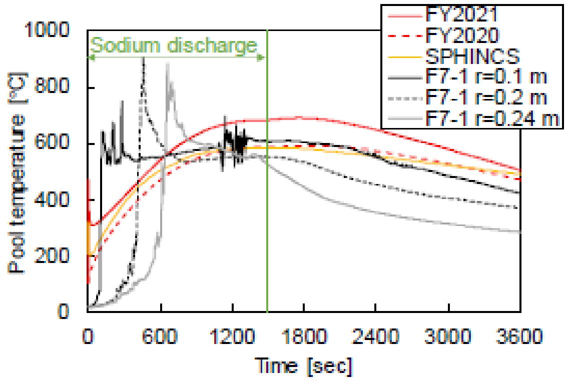
(a) Schematics of temperature distribution in a steel liner during pool fire where temperature rise in the steel liner occurs just under the sodium pool

(b) Illustration of simple pool-pan heat transfer model

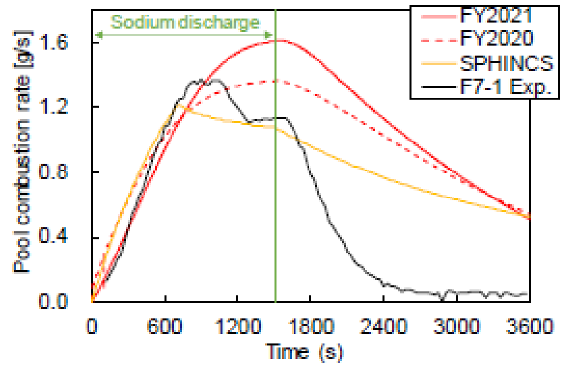
SPHINCS Sodium Pool Fire Model

- SPHINCS is developed by JAEA
  - Sodium fire analysis code – lumped mass model for control volumes with 1-dimensional flow model network (similar to MELCOR)
    - Flame sheet model employed for pool combustion - between
      - pool and flame sheet
      - atmosphere and flame sheet
    - Accounts for the oxide layer effect on pool combustion
    - Liquid pool spreading is modeled by surface tension and gravitational forces
    - SPHINCS has a 2-dimensional heat transfer model between pool and substrate

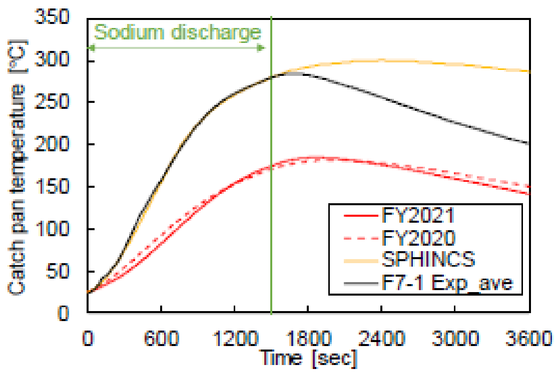
MELCOR – SPHINCS Comparison on F7-1 Test



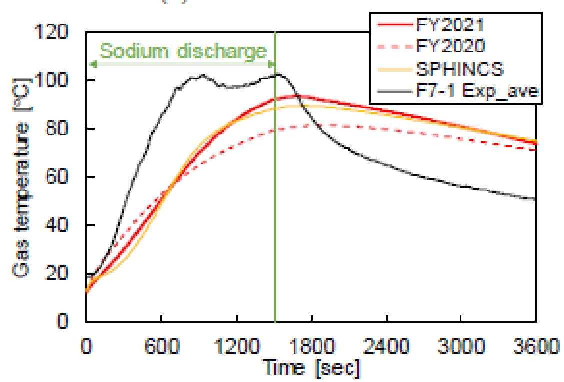
(a) Pool temperature



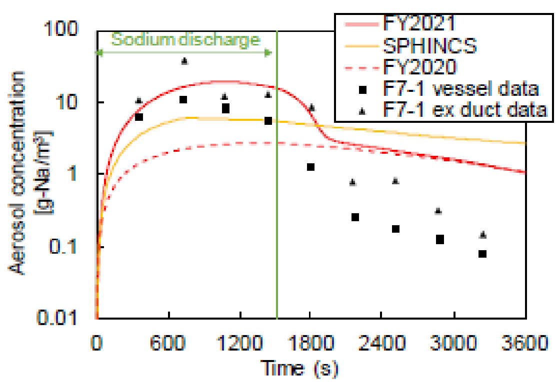
(b) Combustion rate



(c) Catch pan temperature



(d) Gas temperature

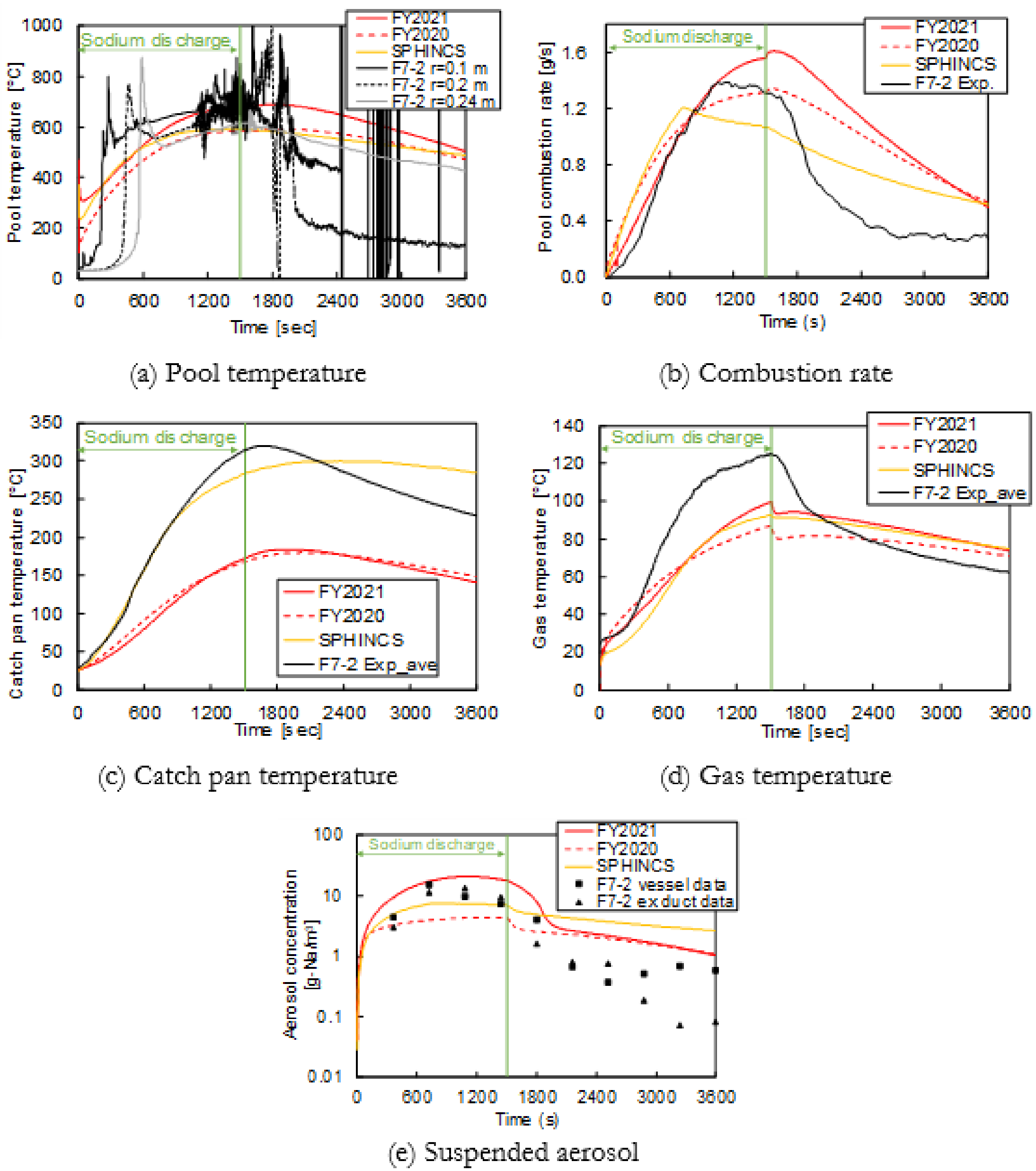


(e) Suspended aerosol

- Results indicate:
  - Similar predictions on pool combustion rate up to 600s
  - Pool temperatures are similar
  - MELCOR underpredicts the catch pan temperature*
  - MELCOR generally predicted better aerosol concentration

*The catch pan temperature modeling in MELCOR was not updated from FY2021 to FY2022

MELCOR – SPHINCS Comparison on F7-2 Test



- Results indicate:
  - Similar predictions on pool combustion rate up to 1200s
  - Pool temperatures are similar
  - MELCOR underpredicts the catch pan temperature*
  - MELCOR generally predicted better aerosol concentration

*The catch pan temperature modeling in MELCOR was not updated from FY2021 to FY2022

Summary and Conclusion

- This paper presents the progress on sodium fire collaboration between SNL and JAEA
- Validation study including for code-to-code comparison was possible using the JAEA's F7 experimental results
- The code-to-code comparison between MELCOR and SPHINCS demonstrated significant improvement on the agreement on many key parameters

THANK YOU

Backups

DAB in Control Functions

- To model DAB, a control function variable is added to NAC input section

```
!!
! //// add NAC models
!             iactv
NAC_INPUT
!             NaCL1     NaCL2       NaCL3         NaCL4         NaCL5
NAC_RNCLASS   H2OA      NA          NAOH          NA2O2         NA2O
!
NAC_SPRAY 1
          !n  CVHNAME    HITE  DME     FNA2O2  SPRDT SOU-TYPE  MASS-NAME   THERM-NAME
           1  'FRAT'  0.1   0.0045     1.0     -1.     TF         'NA-M'    'NA-T'
!
NAC_PFIRE 1
          !n  CVHNAME  FO2    FHEA   FNA2O   FNA2O2  TOFF    DAB
           1  'FRAT'   0.60   0.6    0.9     0.9     3600.0  'DABOX' !Pool oxide
                                                                     ! layer model
!        change FNA2O and FNA2O2 from 0.5 to 0.9
!   FO2 = Fraction of O2 that reacts to form monoxide.
! FHEAT = Fraction of heat from rxn added to pool. Balance goes to atmosphere.
! FNA2O = Fraction of monoxide that remains in the pool. Balance goes to atmosphere.
! FNA2O2= Fraction of peroxide that remains in the pool. Balance goes to atmosphere.
```

DAB in Control Functions (continue)

```
!DAB considering oxide layer
CF_ID  'DABOX'  93  FORMULA
!            NUM OF ARGS    FORMULA TEXT
CF_FORMULA       3          MIN(DAB0,AAA/BBB)
!      N   ARG NAME   VALUE
       1   DAB0       CF-VALU(DAB0)      ! Ddiff for no oxide layer
       2   AAA        CF-VALU(AAA)       !
       3   BBB        CF-VALU(BBB)       !
CF_ID  'DAB0'  81  FORMULA !Gas diffusion coefficient (Ddiff for no oxide layer)
!            NUM OF ARGS    FORMULA TEXT
CF_FORMULA       6          A/P*((TPL+TGS)/TWO)^B
!      N   ARG NAME   VALUE
       1   A          6.4312E-05         ! CONSTANT
       2   P          CVH-P('FRAT')      ! Gas pressure
       3   TPL        CVH-TLIQ('FRAT')   ! Pool temperature
       4   TGS        CVH-TVAP('FRAT')   ! Gas temperature
       5   TWO        2.0                ! CONSTANT
       6   B          1.823              ! CONSTANT
CF_ID  'AAA'  89  FORMULA   !DAB_ox-layer = AAA/BBB
!            NUM OF ARGS    FORMULA TEXT
CF_FORMULA       6          (SH/L)*(DAB0/(ONE+DELT/DELL))
!      N   ARG NAME   VALUE
       1   SH         CF-VALU(SH)        ! Sherwood number
       2   L          CF-VALU(DIAM)      ! Pool diameter
       3   DAB0       CF-VALU(DAB0)      ! Ddiff for no oxide layer
       4   ONE        1.0                ! CONSTANT
       5   DELT       CF-VALU(THICKOX)   ! Oxide layer thickness
       6   DELL       CF-VALU(DELL)      ! Characteristic length scale
```

DAB in Control Functions (concluded)

```
CF_ID  'BBB'  92  FORMULA   !DAB_ox-layer = AAA/BBB
!            NUM OF ARGS    FORMULA TEXT
CF_FORMULA       8          A*(G*SC*BET/(NYU*NYU)*ABS(TPL-TGS))^B
!      N    ARG NAME    VALUE
       1    A           0.14               ! CONSTANT
       2    G           9.8                ! Gravity
       3    SC          CF-VALU(SC)        ! Schmidt number,
       4    BET         CF-VALU(BET)       ! Gas expansion,
       5    NYU         CF-VALU(NYU)       ! Kinematic viscosity
       6    TPL         CVH-TLIQ('FRAT')   ! Pool temperature
       7    TGS         CVH-TVAP('FRAT')   ! Gas temperature
       8    B           0.3333333          ! CONSTANT
CF_ID  'THICKOX' 71  FORMULA
CF_FORMULA      7             (X1/D1+X2/D2)/((one-P)*A)
        1    X1        RN1-AML('FRAT',NA2O,TOT)   ! aerosol na2o in pool
        2    D1        2280.0                     ! density of na2o
        3    X2        RN1-AML('FRAT',NA2O2,TOT)  ! aerosol na2o2 in pool
        4    D2        2800.0                     ! density of na2o2
        5    P         cf-valu('porosity')        ! porosity
        6    one       1.0
        7    A         CF-VALU(PAREA)             ! pool area
cf_id   'porosity'   70   formula
CF_ULB 3  0.0   0.95
cf_formula    2  P*x
        1    P        cf-valu('FSOLID')           ! solid fraction
        2    x        1.5                         ! multiplier
cf_id   'Fsolid'     42  formula
cf_formula   4  min(vmax,s/(s+nal/rho))
!       N    ARG NAME   VALUE
        1    s         cf-valu('Na_Ox_V')    ! total oxide volume
        2    nal       cvh-mass('FRAT',POOL) ! pool mass
        3    rho       cvh-rho('FRAT',POOL)  ! pool density
        4    vmax      0.98                  ! max solid fraction allowed
```

$$0.14\left(g\,S_c\frac{\beta}{\nu^2}\left|T_{surf}-T_g\right|\right)^{\frac{1}{3}}$$