

Task 2-a

Development and V&V of multi-physics mechanistic numerical simulation methods

Akihiro Uchibori, Takashi Takata (JAEA)
David Louie (SNL)



Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Sector of Fast Reactor and Advanced Reactor Research and Development



Motivation for Collaboration

- Understanding and accurately characterizing sodium fires is extremely important:
 - Economics – Unexpected sodium fire behavior can lead to long shutdowns and low capacity factors.
 - Safety – Sodium fires are the primary drivers for radionuclide transport from the reactor to the public for low pressure sodium fast reactor (SFR) systems.
- The US has only recently attempted to regain its sodium fire modeling capability and this collaboration provides a mutually beneficial opportunity for improving sodium fire modeling capabilities in both countries.

Overview

- Influence of Forced convection on SNL P1 and P3 Experiment using SPHINCS code (JAEA)
- Multi-Dimensional Effect on SNL T3 Experiment with AQUA-SF code (JAEA)
- Benchmark Analysis of JAEA F7 Experiment using MELCOR code (SNL)
- New Pool Modeling in MELCOR code (SNL)
- Related Topics Exchange (JAEA and SNL)
- Technical Exchange and Outputs
- Summary and Future Collaborative Works

- Natural convection is applied in SPHINCS.

$$N_A = \left(\frac{Y_A}{1-Y_A} \right) \frac{C_A D_A}{L} \times Sh \quad Sh_j = 0.14 (Gr \cdot Sc_j)^{1/3} \quad [Nu = 0.14 Ra^{1/3}]$$

(Oxygen mass flux model to flame)

Fishenden, M., Saunders, O.A., 1950. Introduction to Heat Transfer. Clarendon Press, p. 180.

- SNL P-series experiments were performed outside.
Applicability of pool model on forced convection condition



Influence of forced convection has been investigated in a simple manner.
(by changing Nu and Sh number.)

Difference in Nu Number

- Range of Ra in SPHINCS Analyses in P1 and P3

Ra: $1.0 \times 10^8 - 1.0 \times 10^9$

- Turbulent heat transfer of horizontal plate

$$\overline{Nu} = 0.037 Pr^{1/3} Re^{4/5}$$
$$\left(\overline{Sh} = 0.037 Pr_m^{1/3} Re^{4/5} \right)$$

Johnson, H. A. and Rubesin, M. W., Trans ASME, 71-5 (1949), 447-456

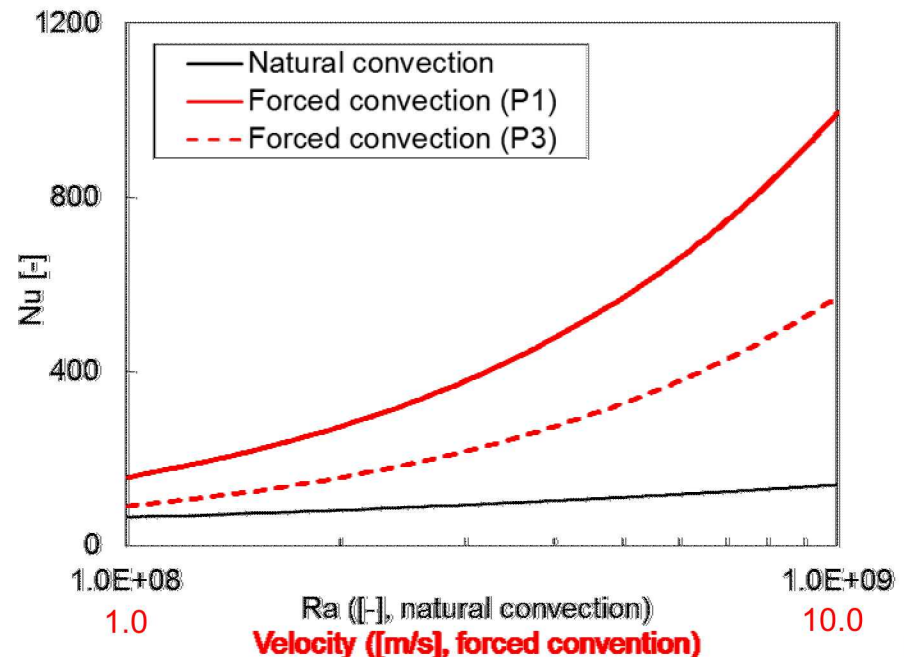
Velocity: 2.7m/s(P1)

1.4-7.8m/s(P3)

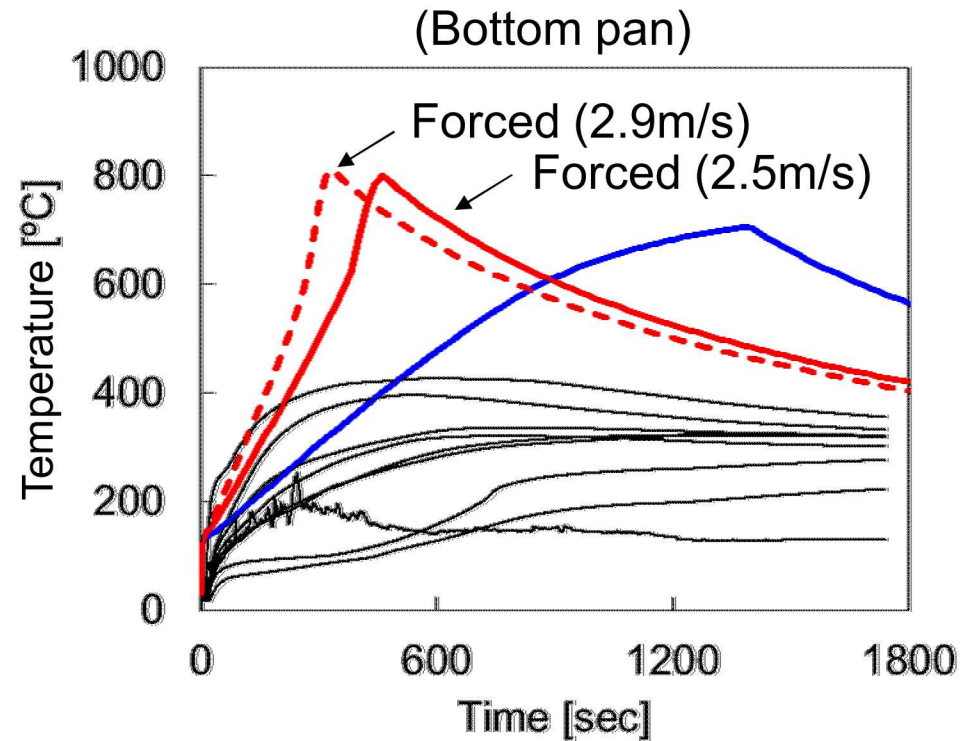
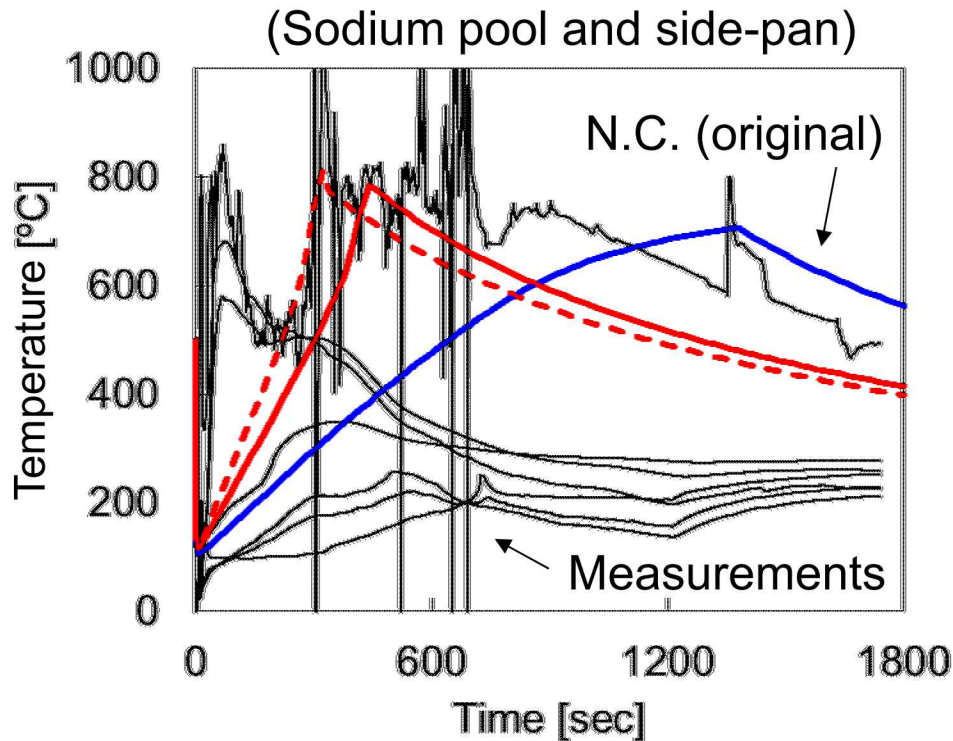
[from SNL data

at 10m height]

Constant value of Nu and Sh are applied based on weather wind speed

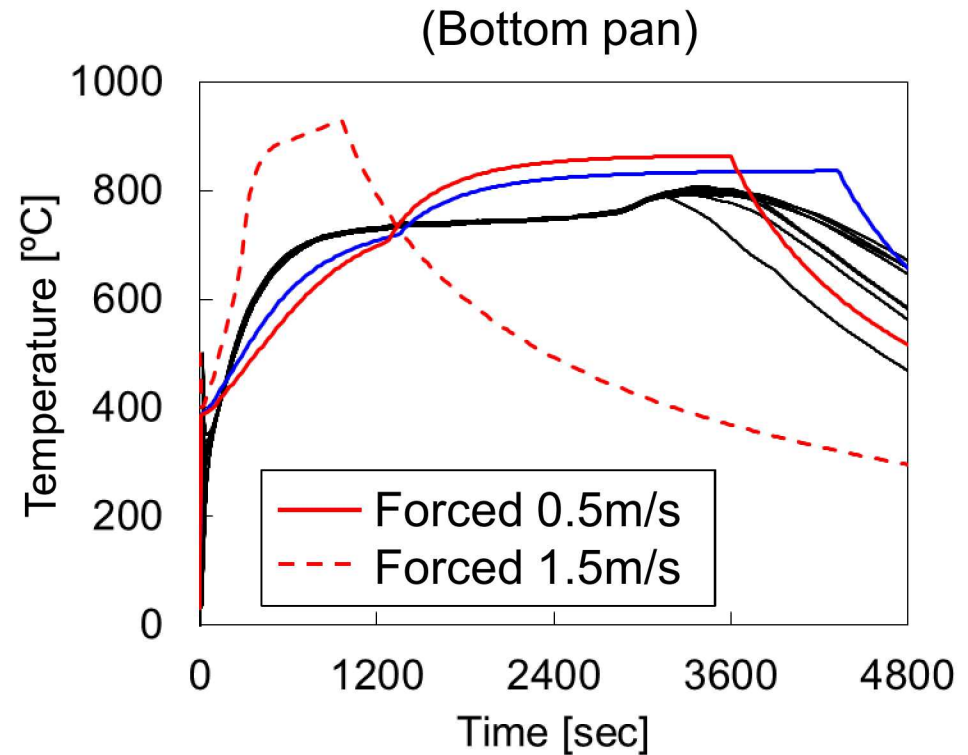
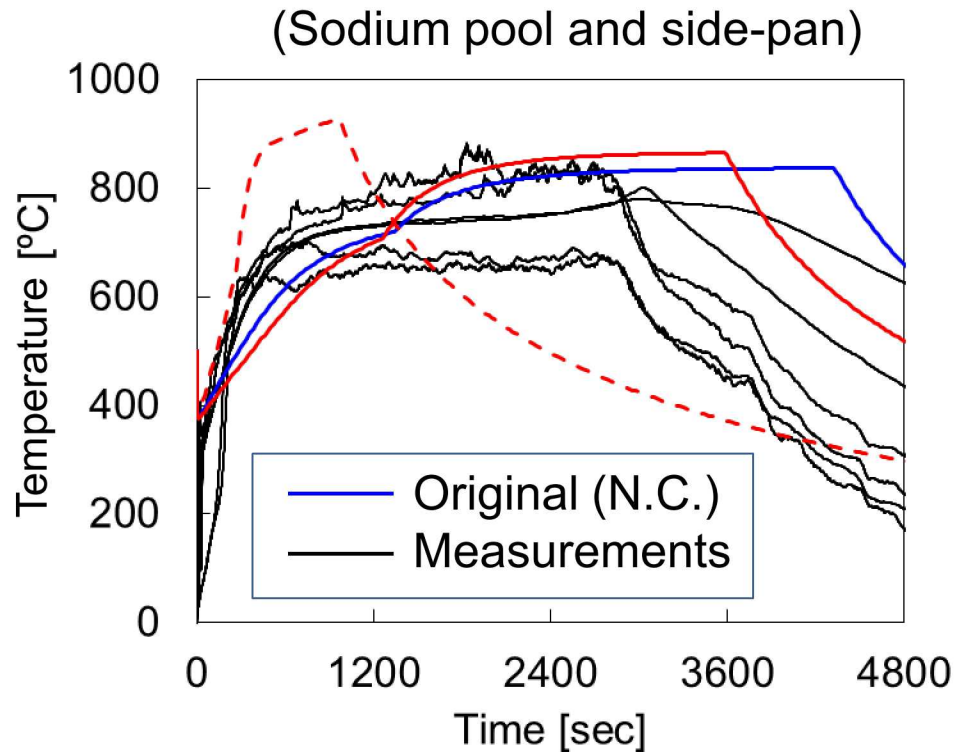


P1 Computation



- Burning rate changes dramatically.
- Maximum temperature increases slightly.

P3 Computation



- Lower contribution of forced convection in P3 experiment (Smaller area of pool and higher sidewall)

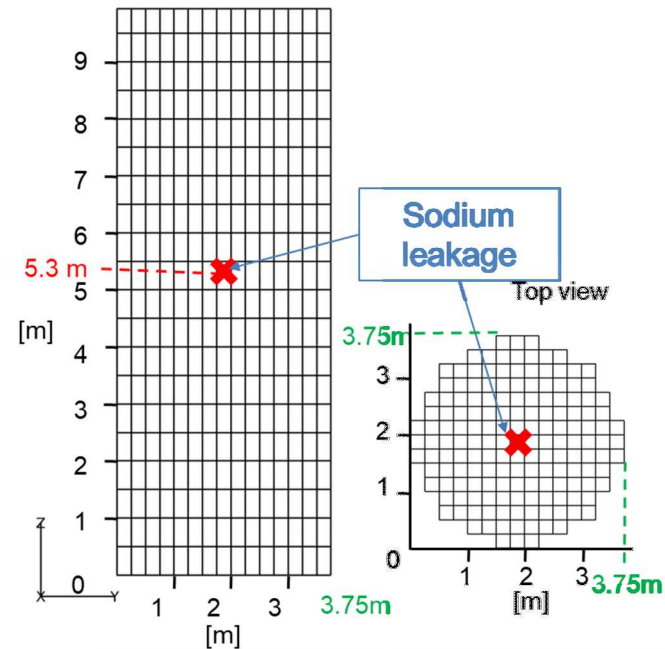
Multi-Dimensional Effect on SNL T3 Experiment

Spray burning rate seems to be underestimated slightly in the lumped-mass codes.

- Local effects of temperature and oxygen concentration are investigated using AQUA-SF code



Surtsey facility



- Mesh configuration
X : 0.25m × 15
Y : 0.25m × 15
Z : 0.5m × 18 + 0.41m × 2

Mesh configuration

Experimental and Numerical Conditions (Best Estimate)

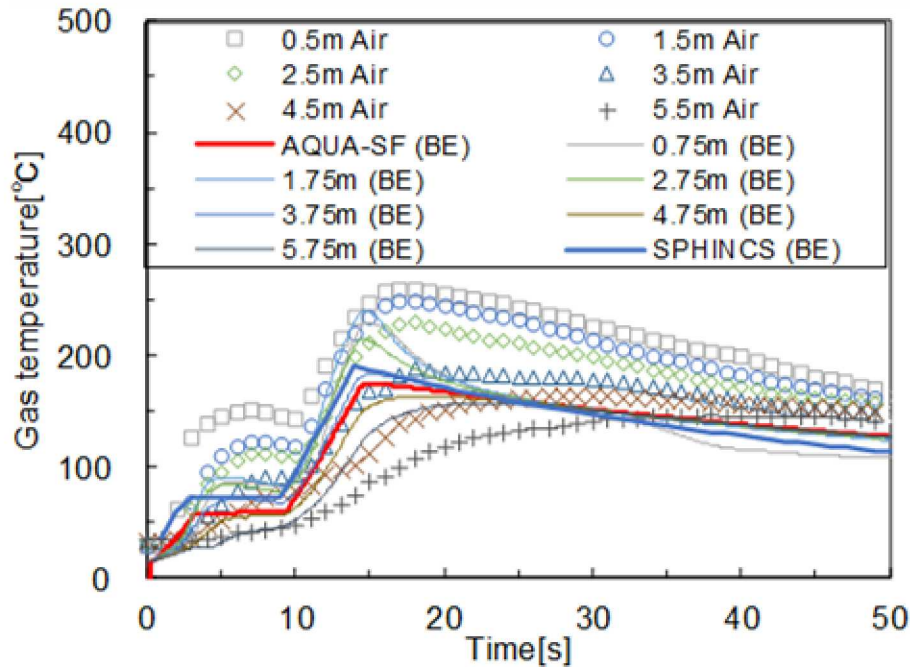
Terms	Experiment	SPHINCS	AQUA-SF
Volume	99m ³	←	←
Spray height	5.3m	←	←
Sodium leakage rate	1.0kg/s	1.429kg/s	←
Duration	20s	0-3, 9-14s	←
Initial Sodium temperature	200°C	←	←
Initial gas temperature	15°C	←	←
Initial gas pressure	101.3kPa A	←	←
Sodium outlet velocity	-	13.34m/s	←
Mean droplet diameter	-	2.00mm	2.50mm
Wall emissivity	-	0.9 [-]	←
Oxygen concentration	-	0.21 [-]	←
Pool height	-	Auto	6.88mm

Underestimation of burning rate in lumped-mass model. (discuss later)

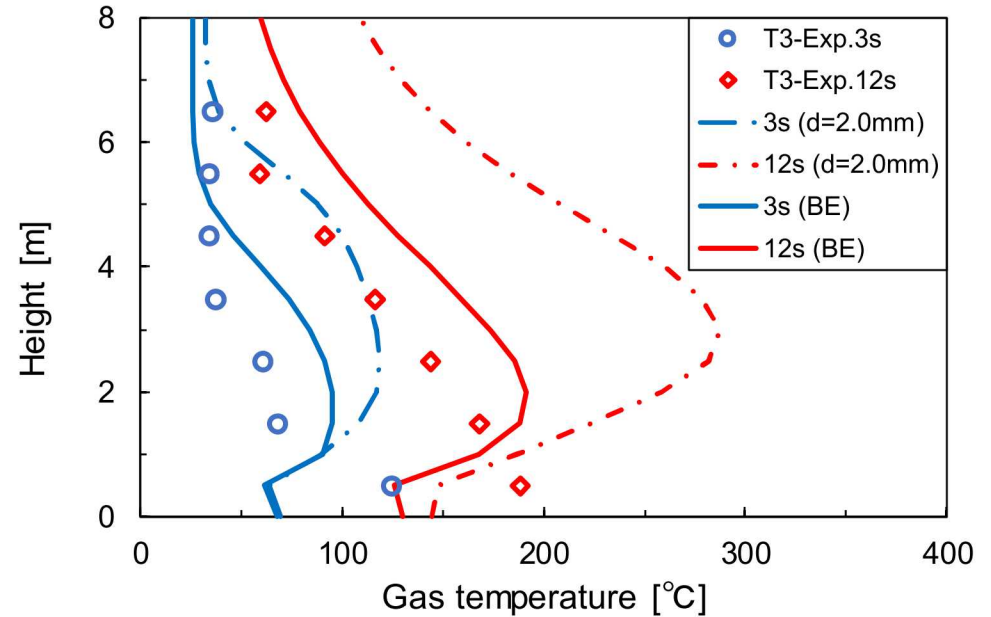


(Consistency)

Computational Results



Gas temperature transient



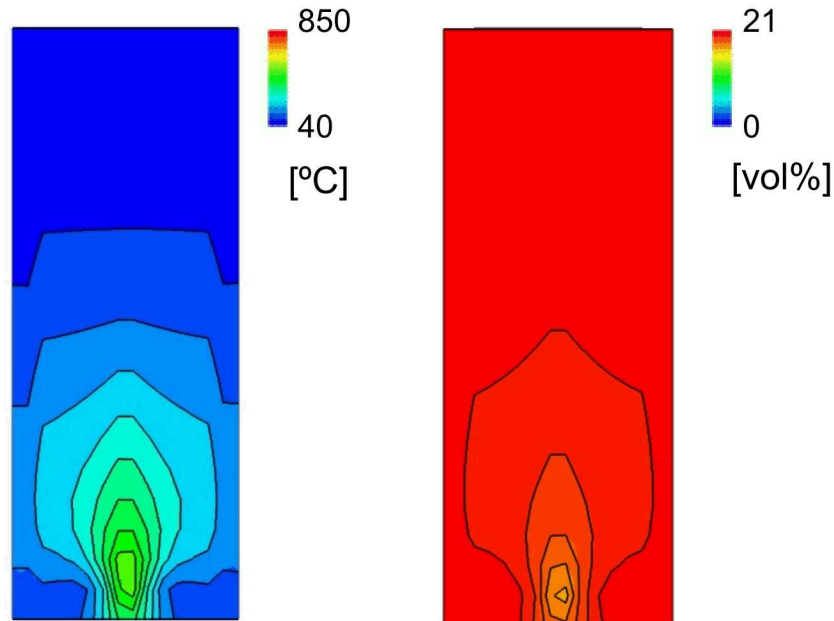
Vertical distribution of gas temperature

- A comparatively good agreement is identified in AQUA-SF with larger diameter of 2.5mm (SPHINCS: 2.0mm).

Multi-Dimensional Effect on Burning Rate

Influence of spray burning rate:

- ✓ Increase due to local increase of gas temperature.
(droplet temperature increase)
- ✓ Decrease due to local decrease of oxygen concentration.



(Gas temperature) (Oxygen concentration)

Local distributions at 12s

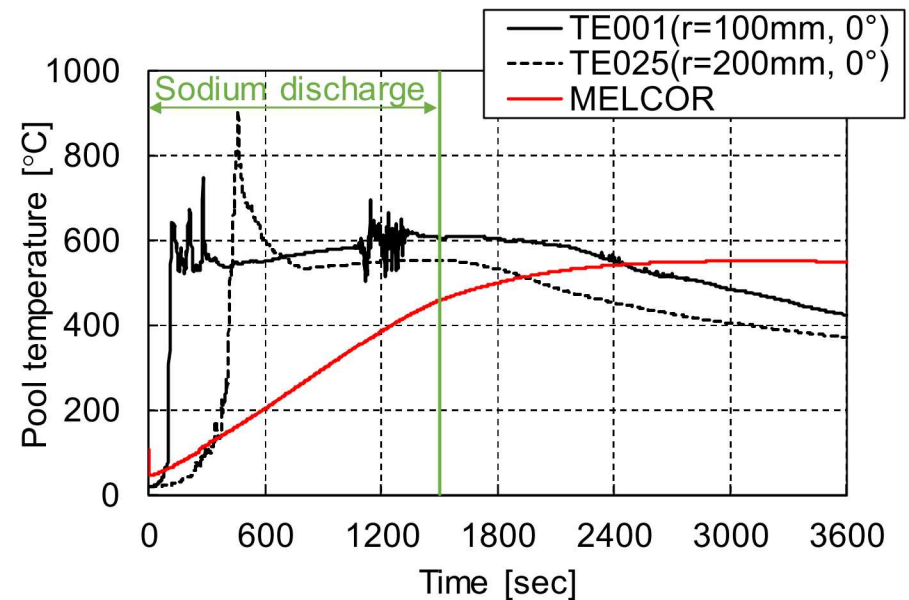
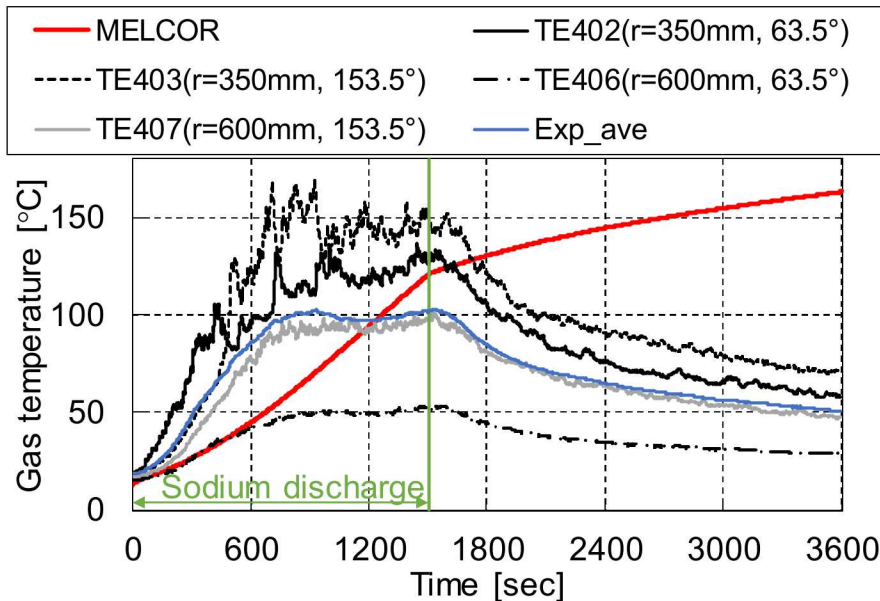
➤ In T3 experiment, local temperature increase affects the burning rate strongly.

Benchmark Analysis of JAEA F7 Experiment

- As a collaborative effort, JAEA F7-1 test is used to validate MELCOR
 - ✓ Primary goal is to validate the thermal-hydraulic modeling in MELCOR, such pool, gas and catch-pan temperatures (described here)
 - ✓ Secondary goal is to enhance the validation basis for the aerosol physics model in MELCOR, including the aerosol species, Na_2O , Na_2O_2 and NaOH .
 - ✓ Improvement of pool fire model in MELCOR by the newly developed enhancement.
 - This improvement is not only for MELCOR, but for JAEA codes as well
 - Using a control function approach for model development, no code modification is involved in MELCOR, providing a flexible way to test new models.

Status of MELCOR Validation – JAEA F7-1 Test

➤ Assess the thermal hydraulic models in MELCOR



- ~1200 s: MELCOR estimated gas temperature is lower due to lower pool temperature resulting in smaller pool burning rate
- 1200 s~: MELCOR estimated gas temperature is higher due to no treatment for the oxide crust on the pool
- Recommendation: Models improvement for pool-floor heat transfer and pool surface phenomenology

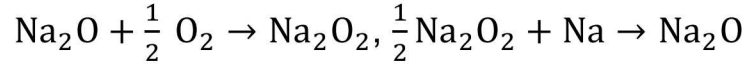
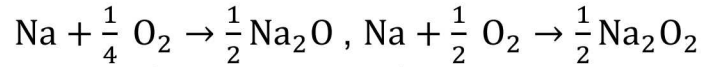
New Pool Modeling in MELCOR code*

- Current sodium pool fire model in MELCOR does not treat effect of oxide crust on pool upper surface. Relevant to:
 - ✓ Release of aerosols from pool
 - ✓ Air ingress and diffusion of oxidant (e.g., air) to the pool surface/flame zone
- Modeling these effects is important for several reasons:
 - ✓ Formation of oxide crust can affect evolution of reactions and aerosol generation
 - ✓ Characterization of oxygen diffusion to sodium



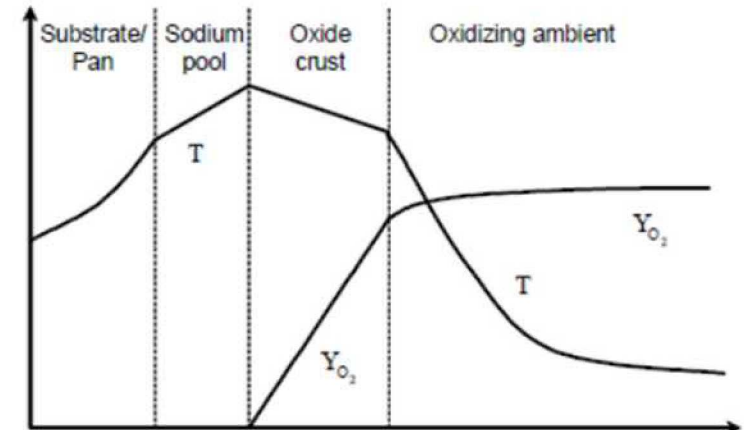
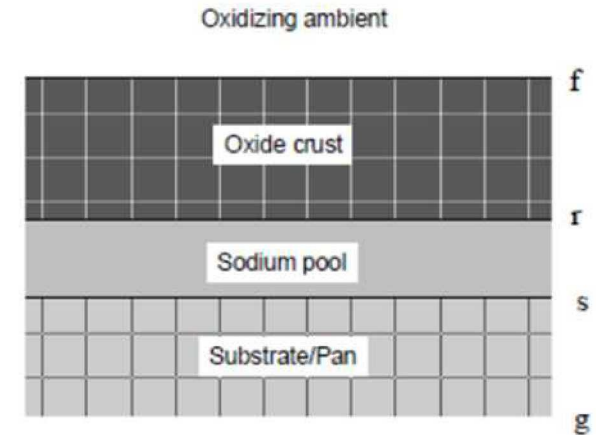
1-D View of Sodium Pool Fire*

Oxidation Reactions*:



4-layer geometry from SAND2010-7113:

- Oxidizing ambient – provide oxygen for fire
- Oxide crust – a layer between liquid Na and air
 - Na_2O formation – adequate oxygen
 - Na_2O layer – reacts with $\text{O}_2 \rightarrow \text{Na}_2\text{O}_2$
 - Melt at 1132°C
 - Na_2O_2 formation – inadequate oxygen
 - Na_2O_2 layer – reacts with $\text{Na} \rightarrow \text{Na}_2\text{O}$
 - Melt at 675°C
 - Oxide-sinking period
 - Oxide-crust period
 - Oxide crust characteristics
 - Oxygen mass rate for reactions
- Implement the model as control function without code modification
 - Re-run model for F7-1 test

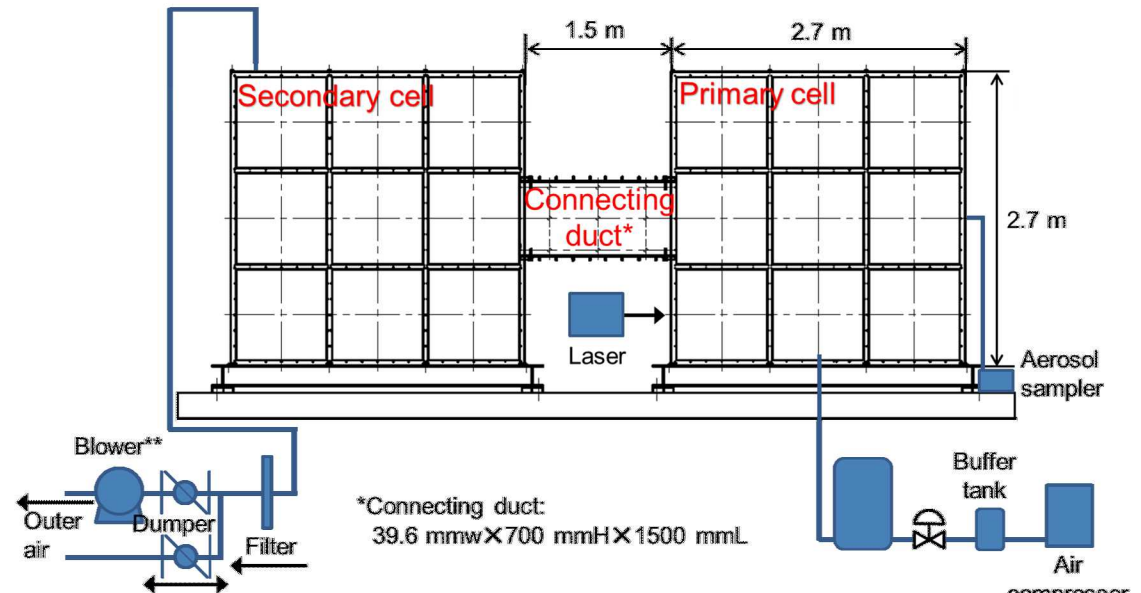


Related Topics Exchange (1/2)

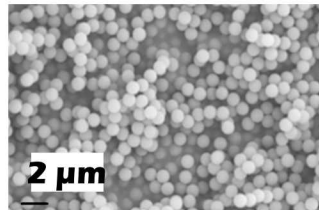
➤ Aerosol transfer experiment through opening (JAEA)



Overview



Test set up for horizontal cells



Simulant aerosol
(SiO₂)

Related Topics Exchange (2/2)

- SNL will study the behavior of aerosol in F7-1 test
- Current spray and pool fire models only consider oxygen reactions. No water vapor reaction is modeled.
- F7-1 and other sodium fire tests indicate significant amount of NaOH exist, particularly in the humid areas where tests were conducted
- SNL will exercise the atmosphere chemistry (AMTC) model in MELCOR to model the water vapor reactions with Na and its oxides
- ✓ Only limited capability of AMTC model is available at this time
- ✓ Treating water vapor as an ideal gas

Technical Exchange and Outputs

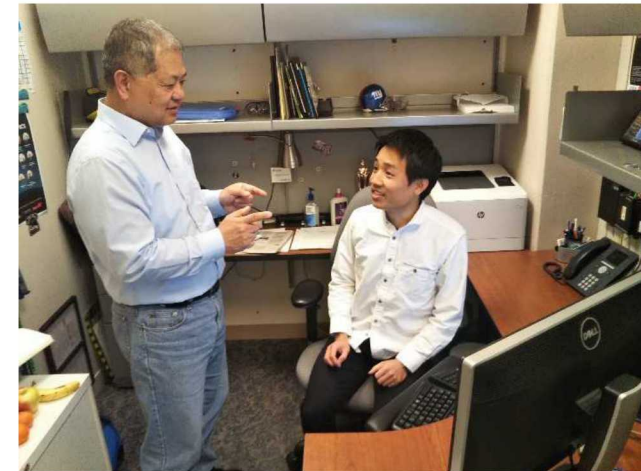
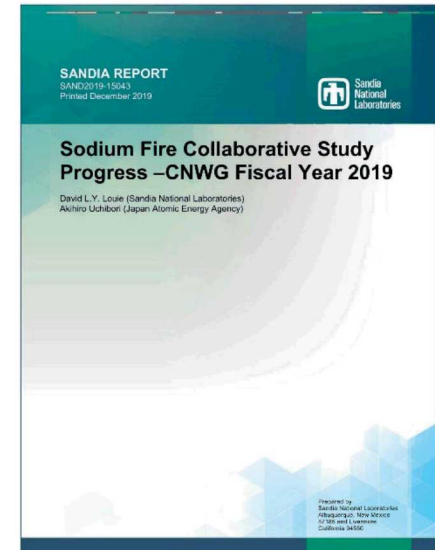
➤ Technical exchange

✓ Researcher assignment from JAEA to SNL

- Akihiro Uchibori (Nov. 5, 2018 – Nov. 4, 2019)
Joint SNL report, SAND2019-15043
- Mitsuhiro Aoyagi (Oct. 28, 2019 – Oct. 27, 2020)
MELCOR, ADAPT, DAKOTA, Fire modeling

➤ Publication

- M. Sonehara, et al., ICONE-27, 2019.
- M. Sonehara, et al., ICONE-28, 2020.
- M. Aoyagi, et al., ICONE-28, 2020.



Summary and Future Collaborative Works

➤ Summary

Joint benchmark activities and discussion of sodium fire modeling have been continued fruitfully in Task 2-a.

In addition, significant research exchanges have occurred.

➤ Future collaborative works

In 2020, to address the need for characterization and understanding of sodium fires, SNL and JAEA continue evaluations of sodium fires and their consequences in terms of containment response and source term analyses.

A third one-year visiting researcher from JAEA is also being planned.

Thank you for you kind attention!!

Computational Conditions

➤ Pool configuration (P1, P3)

Test Number	Diameter of Pan (m)	Height of Pan (m)	Mass of Sodium (kg)	Base Steel Thickness (mm)	Melt Generator Pressure at System Dump Time (psi)	Average Peak Temperature at Bottom of Pan (deg C)	Thickness Ratio (liquid sodium/stainless steel)
Pool 1	0.6	0.0508	2.6	15.875	2.6	320	0.7
Pool 2	0.6	0.0508	2.6	15.875	2.2	320	0.7
Pool 3	0.3	0.127	4.4	6.35	2.4	800	11.5
Pool 4	0.2	0.1778	1.0	6.35	2.5	780	5.9

➤ Nu and Sh numbers ($Nu = Sh, Pr = Sc = 0.7$)

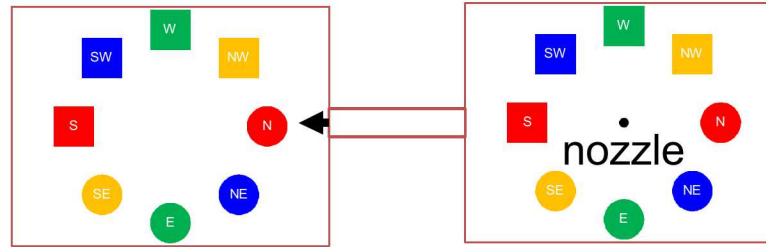
P1		P3	
Nu, Sh	Velocity	Nu, Sh	Velocity
275	2.0m/s	52	0.5m/s
380	2.9m/s	125	1.5m/s

(Nu in natural convection : approximately 100)

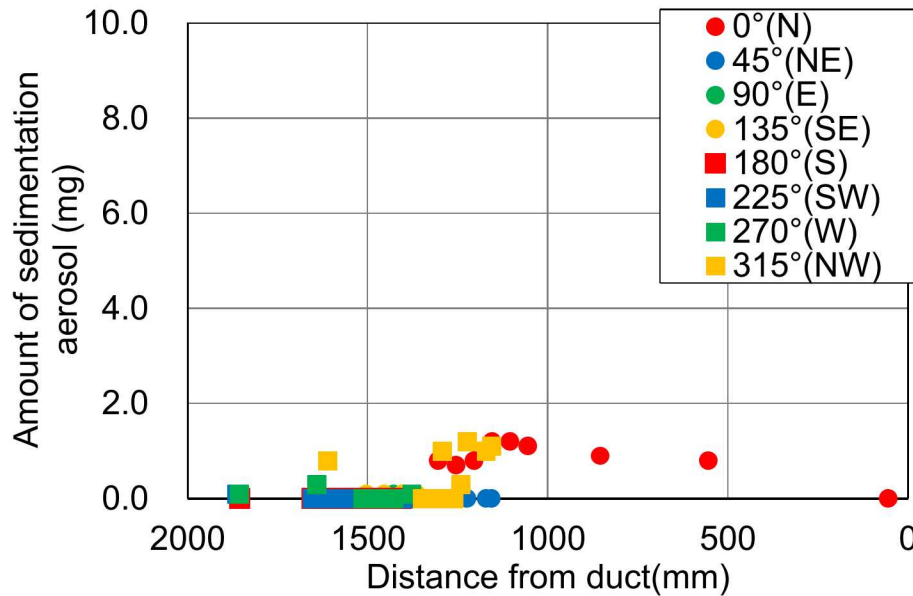
Characteristics length: 0.6m (P1), 0.3m(P3)
(Diameter of Pan)

Related Topics Exchange

➤ Preliminary test result



Secondary cell



Primary cell

