Validation of the Aerosol Model in the ISFRA Module for SFR Accident Analysis: Against the ABCOVE AB5 Tests

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1. Introduction

The Korea Atomic Energy Research Institute (KAERI) has developed the design and analysis technique of a pool-type sodium-cooled fast reactor as the prototype Gen-IV sodium-cooled fast reactor (PGSFR), since 1987.[1] Main advantage of the PGSFR is to reduce the radioactive nuclear waste amount from operating nuclear power reactors by transmutation. Other advantages of the PGSFR are the high safety level in the design and the efficient electric power generation.

In the safety analysis of the PGSFR, it is essential to predict the behavior of the radioactive fission product (FP) released from the core and estimate exactly the released amount to the environment under postulated nuclear power plant accidents. The Fauske & Associates, LLC (FAI) had developed the ISFRA (Integrated Sodium Fast Reactor Analysis) computer software under the contract with the KAERI by 2016. The ISFRA computer software is a best estimate computing tool used to simulate the consequences of beyond design basis accident transients and postulated severe accidents in the PGSFR. This computer program was designed to be a fast running simulation software used to accurately predict the initial transient and the subsequent release and transport of fission products.[2]

The ISFRA code tracks mass of FPs in three forms of the deposited, gas, and aerosol, as in LWR severe accident codes. Since aerosol FPs could be widely generated in the containment compartment during postulated PGSFR severe accidents due to the sudden pressure or temperature decreases when entering into the containment atmosphere, it becomes one of the main concerns in event consequence evaluation to predict the aerosol FP behavior inside the containment and the FP release rate to the environment. The purposes of this study are to evaluate the aerosol behavior models of the ISFRA code and to validate the aerosol models against available experimental data. The results of this study will be used as a basis for the improvement of the ISFRA aerosol models in the future.

2. Aerosol Model of the ISFRA

Since the number of fission product radionuclides in a real nuclear reactor core is over hundreds and it is impossible to track behavior of all the radionuclide species, FPs are modeled in 11 groups based on chemical and physical properties, and importance in health physics in the ISFRA as shown in Table 1. Compared to a typical LWR FP grouping such as the alternative source term (AST) from Regulatory Guide 1.183 (July 2000), the ISFRA FP grouping has additional FP groups of sodium iodide (NaI) and sodium (Na), because the PGSFR uses sodium as a coolant.

Figure 1 shows the radionuclide release passages and the containment nodalization for PGSFR source term evaluation in the ISFRA analyses for the PGSFR. The released FPs transport to the cover gas through evaporation and bubble movement, in the case of core damage accidents. The PGSFR containment is modeled with totally 5 control volumes, which consists of 4 containment compartments and 1 heat sink region for cooling of the reactor vessel outer surface.

The released FP aerosol particles in a compartment of the PGSFR containment coagulate with each other owing to Brownian motion, gravity, and turbulent flow motion. Coagulating aerosol particles deposit on a surface owing mainly to the action of gravity and the movement of the carrying gas stream.[3]

The kinetic equation of simultaneous coagulating and depositing particles being continuously supplied with particles and having a continuous particle size distribution is as follows:

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v K(\bar{v}, v-\bar{v}) n(\bar{v},t) n(v-\bar{v},t) d\bar{v} - \int_0^\infty K(\bar{v},v) n(\bar{v},t) n(v,t) d\bar{v} - \frac{n(v,t)u(v)}{h} + \dot{n}_p(v) \quad (1)$$

where v is the particle volume and t is time. $n(v, t)$ is particle size distribution function, so that $n(v, t)dv$ becomes the number concentration of particles in the particle volume range v to $v+dv$ at time t. $K(v, \tilde{v})$ is the Kernal representing the frequency of binary collisions between particles of volume v and $\tilde{v}$. $u(v)$ is a deposition or removal velocity for particles of volume v, and h is the effective height for deposition of the aerosol (= cloud volume/surface area). $\dot{n}_p(v)$ means the source rate of particles in the size range of v and $v+dv$.

Equation (1) becomes the ordinary differential equation for the density of the suspended mass, m:

$$\frac{dm(t)}{dt} = -\lambda(t) m(t) + \dot{m}_p \quad (2)$$

Here, m is the total mass concentration expressed as

$$m(t) = \rho \int_0^\infty v n(v,t) dv \cdot \quad (3)$$

$\dot{m}_p$ is the constant mass rate of production of aerosol particles per unit volume:

Table I: ISFRA Fission Product Grouping

Group	Fission Products
1	Noble gases (Xe, Kr)
2	Iodine (I_2)
3	Sodium Iodide (NaI)
4	Tellurium (Te_2)
5	Alkali metals (Cs, Rb)
6	Sodium (Na)
7	Refractory materials (Ru, Mo, Rh, Tc)
8	Barium (Ba)
9	Strontium (Sr)
10	Lanthanides (La, Pr, Nd, Sm, Y, …)
11	Cerium group (Ce, Np, Pu, U)

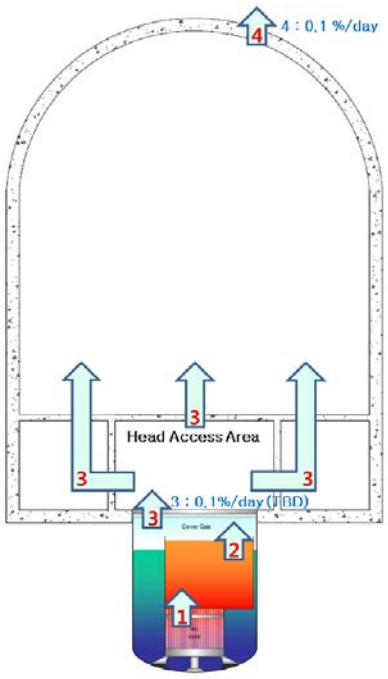

Fig. 1. Radionuclide release passage and containment nodalization for PGSFR source term evaluation.

$$\dot{m}_p(t) = \rho \int_0^\infty v \dot{n}_p(v,t)\, dv \tag{4}$$

And, λ is the aerosol removal rate constant defined as

$$\lambda(t) = \frac{\int_0^\infty v n(v,t) u(v)\, dv}{h \int_0^\infty v n(v,t)\, dv} \tag{5}$$

To avoid the complexity of the above governing equations, FAI transformed the aerosol equations to dimensionless forms which will readily reveal the nature of the similarities which exist among seemingly different aerosols. This 'similarity' means that as time increases the particle size distribution becomes independent of the initial distribution of sizes. For aging aerosols, $\dot{n}_p(v) = 0$. The governing equations are reduced to universal form, by introducing the dimensionless particle volume υ, dimensionless time τ, and dimensionless particle distribution function $N(\upsilon,\tau)$ as follows:

$n(v,t) = c_1 N(\upsilon,\tau)$, $\upsilon = c_2 v$, and $t = c_3 \tau$.

By solving the governing equations for c_1, c_2, and c_3, one can transform the quantities of m(t), λ(t), and $\dot{m}_p$ into the dimensionless total density of the suspended aerosol $M(\tau)$, dimensionless removal constant $\Lambda(\tau)$, and the dimensionless particle source strength $\dot{M}_p$. The derivation procedure and the expression for each variable are described in Reference [3]. To determine the functional relationships $\Lambda(M)$, FAI obtained empirical fitting equations based on many exact numerical solutions and experimental studies. The obtained algebraic fit equations are:

$$\Lambda_{SED}^{SS} = 0.266 M^{0.282} \left(1 + 0.189 M^{0.8}\right)^{0.695} \tag{6}$$

$$\Lambda_{SED}^{D} = 0.528 M^{0.235} \left(1 + 0.473 M^{0.754}\right)^{0.786} \tag{7}$$

Here, the superscript SS indicates when the removal rate constant refers to steady-state conditions, the superscript D denotes Λ for a decaying aerosol, and the subscript SED denotes particle removal by sedimentation.

3. ABCOVE AB5 Test

A program for aerosol behavior code validation and evaluation (ABCOVE) had been developed in accordance with the LMFBR Safety Program Plan.[4] The ABCOVE program was a cooperative effort between the U.S. Department of Energy, the U.S. Nuclear Regulatory Commission, and their contractors. A series of large-scale confirmatory tests were performed in the Containment Systems Test Facility (CSTF) vessel in the Hanford Engineering Development Laboratory (HEDL), covering a range of aerosol source release rates, source duration times, and complexity of aerosol composition. The test cases are summarized as follows:

1) AB1: Sodium pool fire test (1979) in the "dry" condition
2) AB2: Sodium pool fire test (1979) in the "wet" condition
3) AB5: Single-species aerosol test (1982) by spraying sodium at high rate into an air atmosphere.
4) AB6: NaI aerosol release test (1983) in the presence of a sodium spray fire.
5) AB7: NaI aerosol release test (1984) after the end of a small sodium pool fire.

Figure 2 shows the CSTF vessel arrangement for the AB5 test, against which this first validation was performed. The CSTF containment vessel is a 852 m^3 carbon steel vessel installed in a concrete pit. Aerosols were generated by a sodium spray fire. 223 kg of sodium was sprayed over a period of 872 s, with all the sodium converted to a 60% Na_2O and 40% NaOH

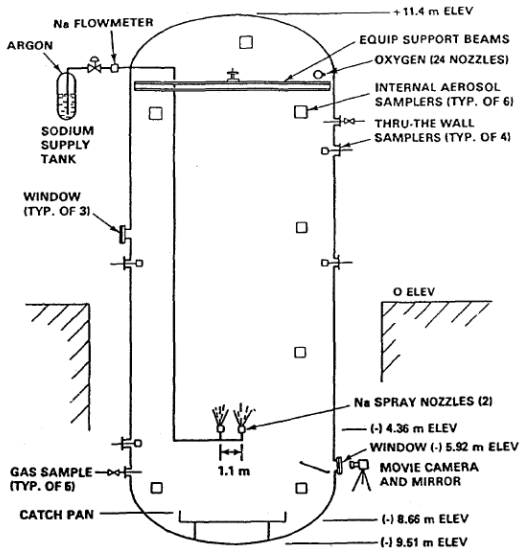

Fig. 2. CSTF Vessel Arrangement: Test AB5.

aerosols. Compressed air (23.3% O_2) was injected at several times in the test to make up for sampling losses and to prevent the containment pressure from going negative. The containment vessel was kept sealed for $5.136X10^5$ s (5.94 days). The maximum containment pressure and mean atmospheric temperature attained were 214 kPa and 553 K. The maximum suspended mass concentration measured was 170 g/m^3, which was attained 383 s after the initiation of sodium spray. The suspended concentration then decreased to a steady-state value of 110±17 g/m^3 for the duration of the spray period.

4. Validation of the FAI Aerosol Model

In this study only the decaying aerosol models have been tested, because any chemical reaction model to represent the sodium fire was not included yet. Since the ISFRA module was developed for the PGSFR accident analysis, it is impossible to treat an arbitrary geometry such as the ABCOVE test section (CSTF vessel) and test conditions. The subroutines that are related to aerosol models are extracted the ISFRA sources and manipulated to compose an independent Fortran program capable of handling the inputs containing arbitrary geometries and conditions.

Input parameters used for the AB5 test simulation by using the ISFRA aerosol models are summarized in Table II. During the sodium spray fire, the gas temperature increases and reaches the maximum temperature of 533 K at the test time 872 s. After then, the gas temperature decreases without any sodium fire as shown in Fig. 3. The measured CSTF shell and atmosphere temperatures are used in the ISFRA input values as functions of time, since the containment thermal-fluidic subroutines were not included in this validation. The measured CSTF atmosphere pressures

Table II: Input Data for ISFRA Test AB5: After 872 s

Description	Value
CSTF TEST PARAMETER	
CSTF Total Height	20.3 m
CSTF Cylinder Diameter	7.62 m
CSTF Vessel Volume	852 m^3
Sedimentation Area	274.7 m^2
Impaction Area	0.0 m^2
CSTF Shell Temperature	See Fig. 3
GAS PARAMETER	
Ar Mole Fraction	0.01
Na Mole Fraction	0.0
N_2 Mole Fraction	0.8
H_2 Mole Fraction	0.0
O_2 Mole Fraction	0.19
Gas Viscosity	Air Property
Gas Thermal Diffusivity	Air Property
Gas Temperature	See Fig. 3
CSTF Atm. Pressure	See Fig. 3
AEROSOL CONSTANT	
Dynamic Shape Factor	1.5
Agglomeration Shape Factor	2.25
Slip Coefficient	1.37
Sticking Coefficient	1.0
Aerosol Particle Density	2500 kg/m^3
Aerosol Source Rate	0.0 kg/s

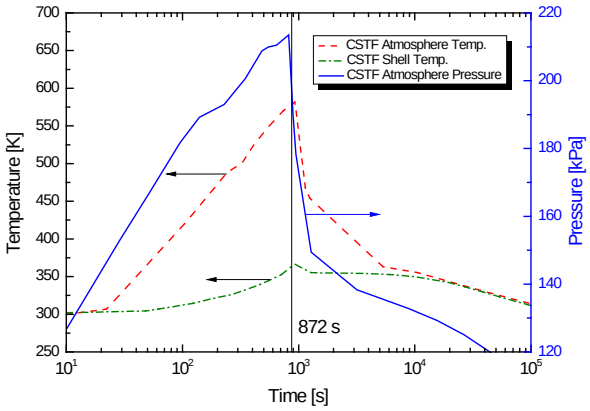

Fig. 3. Measured CSTF Atmosphere Temperature, Shell Temperature, and Atmosphere Pressure of the Test AB5.

as shown in Fig. 3 were also applied in the ISFRA input.

The simulation calculation was performed for the Test AB5 after 872 s, when the aerosol source rate became zero. The total suspended aerosol mass at 872 s was calculated to be (110 g/m^3 X 852 m^3 =) 93.72 kg and used as a given aerosol mass at that time in the simulation. Figure 4 shows comparison of the measured and the simulated suspended aerosol masses, both of which show very similar trends of the decaying suspended aerosol mass. As a result, it is concluded that the ISFRA aerosol models predict the decaying sodium aerosol quite reasonably.

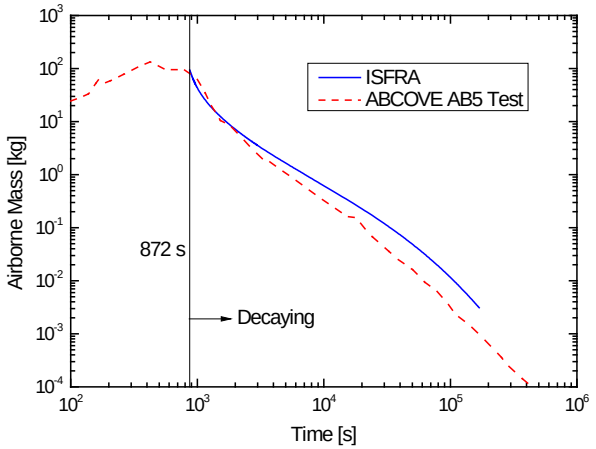

Fig. 4. Predicted and Measured Suspended Decaying (without Source) Aerosol Mass inside the CSTF for Test AB5.

Table III compares the predicted and the measured suspended aerosol masses at three selected transient times. The ISFRA aerosol model slightly underestimates the suspended aerosol mass at 1,020 second, while it overestimates the suspended aerosol masses at the later stage (11,000 or 104,000 second). An overestimation of the suspended aerosol mass implies conservative evaluation, because the larger suspended aerosol mass would result in the larger source rates into the environment. The underestimation of suspended aerosol mass by the ISFRA aerosol model only appears in the early stage of the simulation, which is for 872 ~ 1,100 s. During this early stage of the simulation, the atmospheric pressure and the shell and atmospheric temperature differences changed abruptly with transient time, which might affect the aerosol behavior through thermophoresis or diffusion mechanisms. However, the more investigation on the reasons of these over- and under-estimation of the suspended aerosol mass will be continued in the succeeding studies. This series of studies are aimed at improvement of the existing ISFRA aerosol models by using advanced solving methods and recently developed correlations, so that the abilities and limitations of the ISFRA aerosol models were identified without claiming any superiority of the software.

5. Conclusions

In this study, the ISFRA aerosol models were identified and validated against the ABCOVE AB5 experimental data. Since the aerosol generation model during a sodium spray fire and the steady-state aerosol models with a source rate were not fully prepared for the validation, the validation was performed only for the test data after the 872 s when the sodium spray was terminated. As a result of the validation, it was proven that the ISFRA aerosol models predict the suspended decaying aerosol masses in a compartment reasonably well.

The future works concerning the validation of the ISFRA aerosol models are listed as follows:

- Validation of the steady-state aerosol model against experimental data,
- Sensitivity study of the transition model between the steady-state and the decaying aerosol models for simulating the initial stage of the transient test, and
- Estimation of the inter-node aerosol treatment through aerosol leakage model.

ACKNOWLEDGMENTS

This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT) (No. NRF-2012M2A8A2025624)

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Table III: Comparison between the Predicted and the Measured Suspended Aerosol Masses

Time [s]	Measured in AB5 Test		Predicted by ISFRA
	Aerosol Conc. ± Standard Error [g Aerosol/m^3] (a)	Suspended Aerosol Mass ± Error [kg]	Suspended Aerosol Mass [kg]
1,020	69.8 ± 11	59.33 ± 9.35	38.30
11,000	0.322 ± 0.048	0.2737 ± 0.0408	0.4337
104,000	0.00308 ± 0.00046	0.00262 ± 0.000391	0.008493

(a) Average suspended concentration in 850 m^3 containment atmosphere, at containment T, P conditions. [4]