Implementation and Validation of the MAEROS Aerosol Model in ISFRA SFR Severe Accident Analysis Program

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1. Introduction

KAERI has been developing a design and analysis technique for a pool-type sodium-cooled fast reactor called Prototype Gen-IV Sodium-cooled Fast Reactor (PGSFR) since 1987 [1]. To this end, KAERI and Fauske & Associates, LLC (FAI) jointly developed the ISFRA (Integrated SFR Analysis Program for PSA) computer program to simulate the response of the PGSFR with metal fuel during a severe accident [2]. The ISFRA computer program adopts the aerosol correlation technique of Epstein et al. [3,4,5,6] to predict behavior of non-volatile fission product (FP) aerosols, tracking the suspended and deposited aerosol masses.

The ISFRA aerosol model, which is based on the aerosol correlation technique, provides fast and stable calculations and is based on rigorous analysis. The governing equations for simultaneously coagulating and settling aerosols are transformed into non-dimensional equations based on aerosol similitude, where the particle size distribution reaches a log-normal distribution independent of the initial size distribution after a sufficiently long time. Actually, aerosol coagulation and deposition depend on particle sizes. Therefore, if there is strong source or sink of specific aerosol size, the aerosol similitude would not be maintained, and the aerosol correlation technique may not work well.

To overcome the above mentioned limitation of ISFRA's aerosol correlation technique, the sectional method aerosol program, MAEROS, has been implemented into ISFRA program as an optional model for aerosol analysis in this study. The implemented sectional method was validated against the ABCOVE AB5 experiment [7]. It was revealed that the total suspended aerosol masses calculated by using the aerosol correlation technique and by using the sectional method show good agreements with the experimental data, and that the sectional method however provided more information on the aerosol particle size distribution.

2. Methods and Results

The FAI aerosol model is a ISFRA default model based on the aerosol correlation technique, and the MAEROS aerosol model is the newly installed aerosol model based on the sectional method.

2.1 FAI Aerosol Model

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

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

Here, the functional form for the collision kernel $K(v, \tilde{v})$ that appears in Eq. (1) depends on the coagulation mechanisms being assumed to govern aerosol behaviors. Detailed expressions for $K(v, \tilde{v})$ are found in Epstein et al. [3].

Taking the first moment of Eq. (1) to temporarily avoid the many complications, the total aerosol mass concentration is expressed as

$$m(t) = \rho\int_0^\infty v n(v,t) dv \; . \quad (2)$$

Then, Eq. (1) becomes the ordinary differential equation:

$$\frac{dm(t)}{dt} = -\lambda(t) m(t) + \dot{m}_p \quad (3)$$

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

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

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 variables as follows:

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

By solving the governing equations for c_1, c_2, and c_3 by using similarity analysis [3, 8], quantities of m(t), λ(t), and $\dot{m}_p$ can be transformed into the dimensionless parameters of $M(\tau)$, $\Lambda(\tau)$, and $\dot{M}_p$.

In steady-state aerosols, the particle size distribution of an aerosol continually reinforced by the introduction

Table 1: Dimensionless major variables for aerosols undergoing Brownian and gravitational coagulation and settling

Time, τ	Particle volume, ν	Particle number density, N
$\left(\frac{\alpha g \rho K_0}{\chi^2 \gamma \mu h^2}\right)^{1/2} \cdot t$	$\left(\frac{\gamma g \rho}{\alpha^{1/3} \mu K_0}\right)^{\frac{3}{4}} \cdot v$	$\left(\frac{\gamma^3 K_0^{\,5} \mu^5 h^4}{\alpha g^5 \rho^5}\right)^{1/4} \cdot n$
Mass density, M	**Decay constant, Λ**	**Particle production rate, $\dot{N}_p$**
$\left(\frac{\gamma^9 g h^4}{\alpha^3 K_0 \mu \rho^3}\right)^{\frac{1}{4}} \cdot m$	$\left(\frac{\gamma \chi^2 \mu h^2}{\alpha K_0 g \rho}\right)^{1/2} \cdot \lambda$	$\left(\frac{\gamma^5 \chi^4 K_0^{\,3} \mu^7 h^8}{\alpha^3 g^7 \rho^7}\right)^{\frac{1}{4}} \cdot \dot{n}_p$

of particles at a steady rate and losing particles by sedimentation will ultimately achieve an equilibrium condition in which $\partial n(v,t)/\partial t = 0$. Here, time does not enter into the coagulation equation but of course the source term $\dot{n}_p(v)$ must be retained. Similar transformations can be derived by introducing the dimensionless parameters ν, τ, $N(\nu,\tau)$, and an additional dimensionless particle source rate $\dot{N}_p(\nu)$. Table 1 summarizes the dimensionless major variables for aerosols undergoing Brownian and gravitational coagulation and settling.

To determine the functional relationships of Λ(M), FAI obtained empirical fitting equations based on many exact numerical solutions and experimental studies. Numerical solutions are obtained by running a sectional analysis tool, the MAEROS code, which was developed by Gelbard et al. [9,10]. Figure 1 shows the dimensionless removal rate constant as a function of dimensionless suspended aerosol mass concentration, from the ABCOVE experiments and several numerical experiments using the MAEROS code. The lower dashed curve corresponds to aerosols continually supplied with particles, under steady-state conditions. The upper dotted curve is the dimensionless removal rate versus dimensionless mass relation for decaying aerosols in the absence of a source.

Written in dimensionless form, steady-state and decaying conditions are expressed as follows:

$$\frac{dM}{d\tau} = -\Lambda_{SED}^{SS}(M) \cdot M + \dot{M}_p = 0 \tag{6}$$

$$\frac{dM}{d\tau} = -\Lambda_{SED}^{D}(M) \cdot M \tag{7}$$

2.2 MAEROS Aerosol Model

Aerosol dynamics for assessing health consequences account for two important parameters, particle size and chemical species. Assuming that coagulation and condensation occurs in series and that any two mechanisms cannot occur simultaneously, the general aerosol kinetic equation is transformed into the governing equation (8) for aerosol dynamics with sectional subscripts l and component identifier k [11].

$$\begin{aligned}\frac{dQ_{l,k}}{dt} &= \frac{1}{2}\sum_{i=1}^{l-1}\sum_{j=1}^{l-1}\left[{}^{1a}\bar{\beta}_{i,j,l}Q_{j,k}Q_i + {}^{1b}\bar{\beta}_{i,j,l}Q_{i,k}Q_j\right] \\ &-\sum_{i=1}^{l-1}\left[{}^{2a}\bar{\beta}_{i,l}Q_lQ_{i,k} - {}^{2b}\bar{\beta}_{i,l}Q_iQ_{l,k}\right] - \frac{1}{2}\,{}^{3}\bar{\beta}_{l,l}Q_lQ_{l,k} \\ &-Q_{l,k}\sum_{i=l+1}^{m}{}^{4}\bar{\beta}_{i,l}Q_i + \bar{F}_{l,k}Q_l + {}^{1}\bar{G}_{l,k}Q_l \\ &-\sum_{i=1}^{s}\left[{}^{2}\bar{G}_{l,i}Q_{l,k} - {}^{2}\bar{G}_{l-1,i}Q_{l-1,k}\right] + {}^{3}\bar{G}_{l-1,k}Q_{l-1} + \bar{S}_{l,k} - \bar{R}_{l,k}\end{aligned} \tag{8}$$

with $Q_l(t) = \sum_{k=1}^{s} Q_{l,k}(t) = \int_{v_{l-1}}^{v_l} vn(v,t)dv$.

Here, $Q_{l,k}$(t) is the total mass concentration of aerosol component k per unit volume of fluid in section l at time t, s is the total number of components, $\bar{\beta}$'s are sectional coagulation coefficients, $\bar{F}$ is sectional coefficient for intra-particle chemical reaction, $\bar{G}$'s are sectional growth coefficients due to gas-to-particle conversion, $\bar{S}$ is a source and $\bar{R}$ is a removal rate.

The detailed expressions of the coagulation coefficients and the deposition coefficients for each mechanism are found in MAEROS user manual [10]. The growth coefficients are calculated from an isothermal condensation correlation. For sectional coefficients, the obtained coefficients are integrated over sections by the two-point Gauss-Legendre quadrature formula. By this point, every terms of eq. (8) are composed to form an ordinary differential equation, which will be now solved

SYMBOL	h [m]	$\dot{m}_p$ [kg/m³/s]	ρ [kg/m³]	γ	χ	σ	r_0 [μm]
□	3.1017	9.1549E-7	2450	2.25	1.5	2.0	0.125
△	10.0	8.2160E-6	4000	2.5	1.0	1.55	0.136
○	3.1017	5.9038E-6	2130	2.25	1.5	2.0	0.25
◇	5.0	2.3122E-4	5000	1.0	1.0	1.55	0.27
▽	3.1017	1.1737E-4	3670	2.25	1.5	2.0	0.5
X	2.0	2.9343E-5	2000	1.0	1.0	2.5	1.0
⬡	1.0	1.1737E-4	1000	1.0	1.0	1.5	0.5

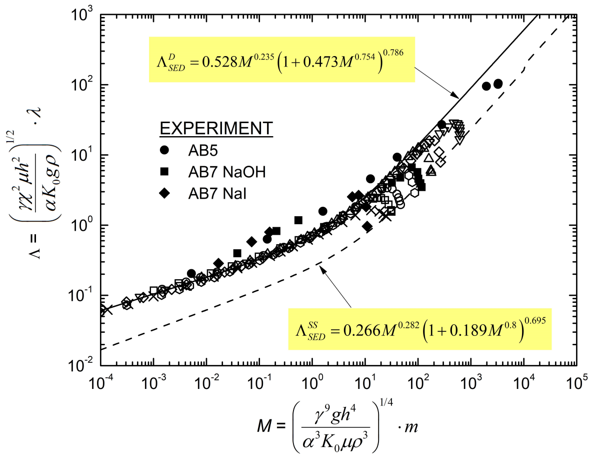

Fig. 1. Dimensionless aerosol removal rate constant for sedimentation as a function of dimensionless suspended mass concentration; steady-state and aging aerosol curves and experimental data. (Reproduction of Figure 1 in [5])

by the Runge-Kutta-Fehlberg Method. Before printing the output, the value of $Q_{l,k}$(t) is linearly interpolated in temperature and pressure.

3. Implementation of MAEROS Model and its Validation

3.1 Implementation of MAEROS Model into ISFRA

As an integrated reactor analysis program developed specifically for PGSFR, the ISFRA consists of thermal-hydraulics module, reactor kinetics module and various component modules covering a core, a vessel, heat exchangers, containments, et al. Since aerosol behavior combining with FPs is important and analyzed in the primary coolant circuit and the containment under severe accident conditions, the aerosol FP source term analysis module is called from the reactor vessel analysis and the reactor containment analysis modules.

The MAEROS model is implemented as an optional aerosol analysis model for users to select one proper aerosol model considering required level of uncertainty and computing cost. However, the MAEROS model is a zero-dimensional aerosol analysis model which solves macroscopic lumped aerosol behavior inside a single compartment. Therefore, to make the implemented MAEROS model work in ISFRA properly, following modification procedures should be completed:

(1) implementation of the original MAEROS model,

(2) modification of the FP component treatment from MAEROS's 8-grouping to the 11-grouping, to match with the ISFRA grouping method,

(3) implementation of the interaction model between different aerosol components,

(4) implementation of the aerosol transport model between compartments, and

(5) registering the new variables into ISFRA I/O data structure system and modification of ISFRA I/O module.

Among above four additional steps, the procedure (1) has been completed so far.

3.2 Validation against ABCOVE AB5 Test

The Aerosol Behavior Code Validation and Evaluation (ABCOVE) experiments were conducted under the LMFBR (Liquid-Metal Fast Breeder Reactor) Safety Program Plan [9]. 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 CSTF vessel is a cylindrical steel tank (7.6 m diameter, 20.3 m high) of about 852 m^3, which is furnished with instrumentation to monitor both thermal-hydraulics and aerosol behavior. Test AB5 is a single-species aerosol test that involves spraying sodium at a high rate into an air atmosphere, while AB6 and AB7 are experiments for the case of a two-component aerosol simulating the release of a fission product (FP) in the presence of a sodium fire.

According to the implementing procedures in Section 3.1, following V&V will be performed:

(1) validation of the implemented MAEROS model against AB5 experiment,

(2) validation of the interaction model between aerosol components against AB6 and AB7 experiments,

(3) verification of the aerosol transport model against a conceptual problem, and

(4) validation of the complete MAEROS model installed in ISFRA for PGSFR severe accident analyses.

Since the implementation of the original MAEROS model has been completed so far, validation of the implemented MAEROS model against AB5 experiment is performed and presented in this study.

For the aerosol analyses of the AB5 test using ISFRA, the CSTF vessel was modeled as a single control volume containing atmospheric air and aerosols. During a sodium spray fire, the measured CSTF shell and atmosphere temperatures were provided as input to ISFRA as functions of time. The addition of aerosol mass induced by the sodium spray fire for initial 872 s was modeled as a constant aerosol mass source rate of 0.445 kg/s. The aerosol source due to the sodium spray fire was modelled to have a log-normal distribution with the mass mean diameter (MMD) of 0.5 μm and the geometric standard deviation (GSD) of 1.5. Figure 2(a) shows the total airborne aerosol masses obtained by the ISFRA calculations with MAEROS model and with FAI's correlation-based model, compared with AB5 experimental data. The calculated aerosol masses using ISFRA with MAEROS model is in good agreement with the experimental data as well as with the results of the original ISFRA. Figure 2 (b)~(e) give the aerosol particle size distributions at 5, 100, 872, and 10000 s, respectively. After 872 s at which the aerosol source is terminated, portion of larger particles are increased and smaller particles become depleted due to aerosol coagulation.

4. Conclusions

In this first step of the studies for improving the uncertainty level of the SFR severe accident analysis tool, ISFRA computer program, MAEROS model using the sectional method has been implemented into ISFRA as an additional aerosol model option. From the validation of the implemented MAEROS model against ABCOVE AB5 experiment, it is concluded that ISFRA calculation with the newly implemented MAEROS model provides the similar suspended total aerosol mass as the original ISFRA and experimental data and additional information of aerosol size distributions. The rest steps of implementation and validation described in Section 3 will be performed in the future researches, for the improvement of the ISFRA aerosol models.

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NOMENCLATURE

g	gravitational constant [m/s^2]
h	effective height for aerosol deposition [m]
$K(v, \tilde{v})$	kernel representing the frequency of binary collisions between particles of volume v and $\tilde{v}$
K_0	normalized Brownian collision coefficient
m	total mass concentration of the suspended aerosols [kg/m^3]
$\dot{m}_p$	aerosol mass production rate [kg/m^3/s]
M	dimensionless total suspended aerosol mass
$\dot{M}_p$	dimensionless source rate
n	particle size distribution function [m^{-3}]
$\dot{n}_p$	source rate of particles [m^{-3}s^{-1}]
$N(\nu,\tau)$	dimensionless particle distribution function
v	particle volume [m^3]
t	time [s]
u	particle deposition or removal velocity [m/s]
α	density correction factor [-]
χ	particle settling shape factor [-]
γ	collision shape factor [-]
λ	aerosol removal rate constant [s^{-1}]
Λ	dimensionless decay constant
μ	viscosity of the carrier gas [kg/m/s]
ν	dimensionless particle volume
ρ	density of the aerosol material [kg/m^3]
τ	dimensionless time

Superscripts

D	decaying aerosol
SS	steady-state

Subscripts

B	Brownian (coagulation)
g	gravitational (coagulation)
SED	sedimentation

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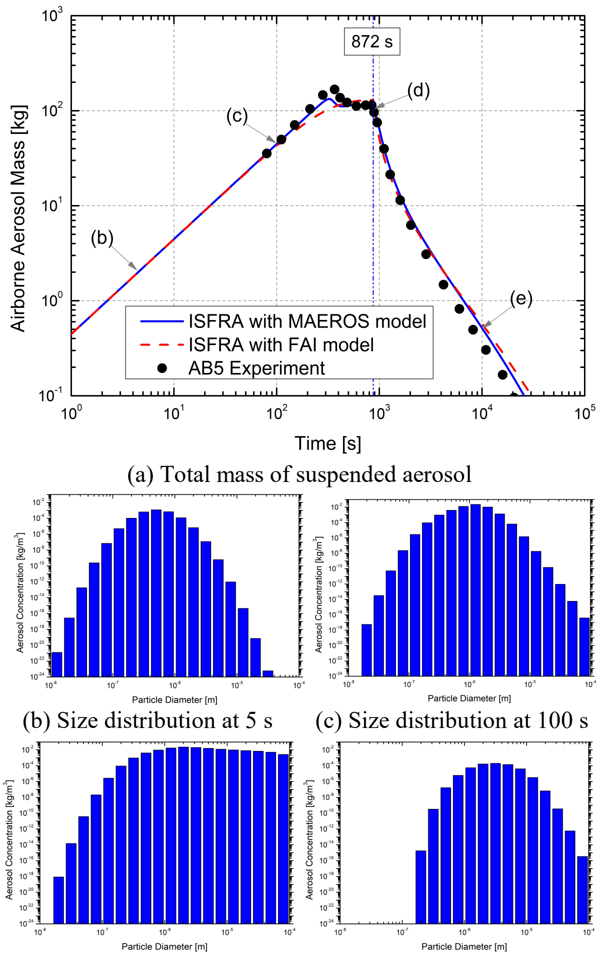

(a) Total mass of suspended aerosol

(b) Size distribution at 5 s (c) Size distribution at 100 s

(d) Size distribution at 872 s (e) Size distribution at 10000 s

Fig. 2. Validation of the implemented MAEROS aerosol model against ABCOVE AB5 experiment and aerosol size distributions at selected times.