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ABC- INTG CODE FEATURES

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ABSTRACT

A computer code ABC-INTG has been developed to predict the Aerosol Behavior in Containment following a postulated accident of liquid metal fast breeder reactors. The code calculates such aerosol processes as coagulation, deposition, leakage and additional sources in a spatially homogeneous confined atmosphere. The equations to describe these aerosol processes are almost all the same as those of the former ABC versions. However, the numerical method is mostly revised by using the sectional representations by Gelbard, et al. The new code can reduce the required computing time extensively, compared with the former versions of ABC.

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1. Introduction

Postulated accidents in liquid metal fast breeder reactors (LMFBRs) often accompany the release of sodium oxide aerosol containing fission products and nuclear fuel. This aerosol is confined in the reactor containment system and partially leaks into the environment. The aerosol behavior within the container should be analyzed quantitatively to evaluate the environmental radioactivity release associated with LMFBR accidents.

Several aerosol behavior analysis codes, HAA-3[1)] and HAARM-3[2)] in the U.S., PARDISEKO-IIIb[3)] in Germany, AEROSIM in the U.K., AEROSOLS A1 and B1 in France, and ABC[4)] in Japan, have been developed. These codes are used to calculate the physical behavior of aerosol in a spatially homogeneous confined atmosphere. The physical models used in the codes are similar. However, the codes are roughly classified into two groups, due to the mathematical method for calculating the particle size distribution function. One group includes the so called Method of Moment[5)], which has been used in HAA-3 and HAARM-3. The method is used assuming the time dependent particle size distribution to be a log-normal distribution at any time. This assumption can reduce the computing time needed to solve the dynamic equations of aerosols extensively. However, the limit to its applicability is not yet clarified.

The other group includes the Sectioning Method, which expresses the distribution function by a finite set of discrete particle size classes. This is used in PARDISEKO-IIIb[3)] and former versions of ABC.[6)] This method has no limitation to the particle size distribution, and can be used to treat an arbitrary distribution. However, this method is accompanied with truncated errors due to the discretion and more particle size classes. Eventually, more computing time is needed to reduce the errors to a reasonably small amount.

Recently, more sophisticated sectional representations were reported by Gelbard, et al.[7)] These have been extended to deal with multi-component aerosol dynamics, and a computer code, MAEROS, has been developed.[8)] This MAEROS code has been incorporated in system code CONTAIN[9)] to analyze post-accident phenomenology within the containment.

In the present version of ABC, ABC-INTG, the numerical method is mostly revised by using the sectional representations by Gelbard, et al. The physical models to express the aerosol dynamics are essentially the same as the former versions of ABC.

2. Modeling Features

The ABC-INTG code calculates such aerosol processes as coagulation, deposition, leakage and additional sources in a spatially homogeneous confined atmosphere. The equations used to describe the aerosol behavior are almost all the same as those of the former ABC versions.[4) 6)] The physical models used in the code are summarized in order to understand the modeling differences from other aerosol behavior codes.

The dynamics of the spatially homogeneous particulate system are described by the following generalized equation.

$$\frac{\partial n(v,t)}{\partial t} = \frac{1}{2}\int_0^v K(v', v-v')n(v', t)n(v-v', t)dv'$$

$$-n(v, t)\int_0^\infty K(v, v')n(v', t)dv'$$

$$-R(v)n(v, t)$$

$$+S(v, t) \qquad \qquad (1)$$

n(v, t) is the size distribution density function, K(v, v') is the coagulation coefficient for particles of volume v and v', R(v) is the removal rate constant for particles of volume v and S(v, t) is the rate of addition of new particles into the system.

The dynamic equations for sphere particles are used to describe the particle motion. To extend the code applicability to real nuclear aerosol systems, two correction factors are used. These are dynamic shape factor χ, to correct the aerodynamic nature of non-sphere particles, and coagulation shape factor γ, to correct the coagulation coefficient for the particles. In addition, collision efficiency ε (v, v') is used as a correction factor for the gravitational coagulation and turbulent coagulation. Also, the Cunningham slip correction factor is included in the dynamic equations for small spheres. The equations and physical properties used in the code are described below.

2.1 Coagulation

Three coagulation mechanisms, Brownian coagulation, gravitational coagulation and turbulent coagulation are modeled in the code. The coagulation rate constants for each coagulation mechanism are expressed as $K_B(v, v')$, $K_G(v, v')$ and $K_T(v, v')$, respectively. The overall coagulation constant $K(v, v')$ is given from the sum of these three constants,

$$K(v, v') = K_B(v, v') + K_G(v, v') + K_T(v, v') \quad \text{.......................... (2)}$$

(1) Brownian Coagulation

Brownian coagulation results from the random motion of suspended particles. The rate constant for Brownian coagulation, K_B, is given by the following equation.

$$K_B = 4\pi (D_i + D_j)(r_i + r_j)\frac{\gamma}{\chi} \quad \text{.......................... (3)}$$

Where r_i is the particle i radius and D_i is the diffusion constant for particle i.

Diffusion constant D_i is given as follows.

$$D_i = \frac{koT}{6\pi\eta\ ri}\left(1 + \frac{Ai\,\lambda}{ri}\right) \quad \text{.......................... (4)}$$

ko = Boltzmann constant
T = Gas temperature (^oK)
η = Gas viscosity
Ai = Cunningham correction factor
λ = Mean free path

The gas viscosity, mean free path and Cunningham correction factor are given by the following equations.

Gas Viscosity

ABC uses the following linear formula.

$$\eta = \eta_0 \ \{1 + C(T - T_0)\} \quad \text{.......................... (5)}$$

$\eta_0 = 1.83 \times 10^{-5}\ kgm^{-1}s^{-1}$
$C = 2.64 \times 10^{-3}$
$T_0 = 296$ K

Mean Free Path

The formula used is

$$\lambda = \eta \cdot \frac{3}{\rho_g} \sqrt{\frac{\pi M_m}{8RT}} \quad \text{......................} \quad (6)$$

ρ_g = gas density

M_m = molar mean molecular weight (taken as 0.029 kg mol^{-1} for Air)

R = gas constant

Gas density ρ g is given by the following empirical formula:

$$\rho_g = \frac{1.293 \quad P}{1 + 0.00367t \cdot P_0} \quad \text{..........................} \quad (7)$$

t = temperature (°C)

p = gas pressure

P_0 = standard gas pressure

Equation (2) is derived from the Maxwell equation (1860) and the mean velocity. By using gas pressure P, it can be written as follows,

$$\lambda = \eta \sqrt{\frac{9\pi}{8P\rho_g}} \quad \text{...........................} \quad (8)$$

Cunningham Correction Factor

The Cunningham correction factor is expressed as,

$$A_i = 1.257 + 0.400 \exp\left(-\frac{1.10}{\lambda/r}\right) \quad \text{........................} \quad (9)$$

(2) Gravitational Coagulation

The rate constant for gravitational coagulation is given by the following equation,

$$K_G = \varepsilon\pi \quad (r_i + r_j)^2 \; |v_i - v_j| \; \frac{\gamma^2}{\chi} \quad \text{........................} \quad (10)$$

ε is gravitational collision efficiency and V_i is the terminal settling velocity for particle i.

Terminal settling velocity V is given as follows,

$$V_i = \frac{2\rho g r_i^2}{9\eta}\left(1 + \frac{A_i \lambda}{r_i}\right) \quad \text{.......................} \quad (11)$$

g is the gravitational constant.

Gravitational collision efficiency ε is based on the equation due to Fuchs[10] and expressed as follows,

$$\varepsilon = \left\{ 1 + \frac{r_j}{2(r_i + r_j)} \right\} \frac{r_i^2}{(r_i + r_j)^2}$$

$$r_i \leqq r_j \qquad \cdots\cdots (12)$$

For $r_i \ll r_j$, Eq. (12) can be simplified, as follows[11],

$$\varepsilon = \frac{3}{2} \left(\frac{r_i}{r_i + r_j} \right)^2 \qquad \cdots\cdots (13)$$

In addition to the above correction formulae, a constant ε value can be specified by input.

(3) Turbulent Coagulation

The collision frequency between particles suspended in a gaseous medium may be increased by induced turbulent motion in the gas due to the two independent mechanisms. One is collision, caused by particle motion resulting from the random turbulent motion of the air. The other is collision caused by particles' inertia.

The constant coagulation rate due to the first mechanism K_{T1}, is given as follows,

$$K_{T1} = \varepsilon \left(\frac{8\pi \rho_g}{15\eta} \varepsilon_T \right)^{1/2} (r_i + r_j)^3 \, \gamma^3 \qquad \cdots\cdots (14)$$

ε_T is the energy dissipation rate in the turbulent fluid. The same collision efficiency value ε , is used as the gravitational collision efficiency.

The constant coagulation rate due to the second mechanism K_{T2}, is given as follows.

$$K_{T2} = \varepsilon \quad (r_i + r_j)^2 \, | v_i - v_j | \, \frac{\gamma^2}{\chi} \qquad \cdots\cdots (15)$$

v_i is particle velocity.

Particle velocity v_i is given as follows,

$$v_i = \left[\frac{4\rho \sqrt{2\pi}}{9\eta} \right] \left[\frac{1.69 \, \varepsilon_T^3 \, \rho_g}{15\eta} \right]^{1/4} r_i^2 \left(1 + \frac{A_i \lambda}{r_i}\right) \qquad \cdots\cdots (16)$$

2.2 Removal Rates

Suspended aerosols are removed from the atmosphere by deposition and leakage. Three kinds of deposition mechanism, diffusion, gravitational settling and thermophoresis, are modeled. Removal rate constant R(v) in Eq. (1) is the sum of the above three deposition rates and the leakage rate.

(1) Deposition due to diffusion

The removal rate constant due to Brownian diffusion, R_D, is expressed as follows,

$$R_D = D_i \frac{Aw}{V \cdot \delta_d} \frac{1}{\chi} \quad \text{.................. (17)}$$

Aw = deposition area

v = vessel volume

δ_d = Brownian boundary layer thickness

(2) Deposition due to gravitational settling

The deposition rate constant due to gravitational settling, R_G, is expressed as follows,

$$R_G = V_i \cdot \frac{Af}{V} \cdot \frac{1}{\chi} \quad \text{...................... (18)}$$

Af = floor area

(3) Deposition due to thermophoresis

The deposition rate constant due to thermophoresis, R_T, is expressed as follows,

$$R_T = \frac{3\eta(1 + A_i \lambda /r_i)}{2\rho g \cdot T} \cdot \frac{Aw \cdot V_T \cdot K_T}{V} \cdot \frac{1}{\chi} \quad \text{................. (19)}$$

V_T = temperature gradient between gas and wall

K_T = a constant that depends on particle and gas properties

Factor K_T is based on Brock's theory and expressed as follows[12],

$$K_T = \frac{1}{1 + 3C_m \lambda /r_i} \left\{ \frac{k_f/k_s + C_t \lambda /r_i}{1 + 2(k_f/k_s + C_t \lambda /r_i)} \right\} \quad \text{.............. (20)}$$

k_f = thermal conductivity of gas

k_s = thermal conductivity of aerosol

C_t = a constant associated with the temperature pump (= 3.32)

C_m = a constant associated with the velocity slip (= 1.00)

(4) Leakage

Leakage rate L (1/sec) is specified by input. Total removal rate R(v) is given by the following equation,

$$R(v) = R_D(v) + R_G(v) + R_T(v) + L \qquad (21)$$

2.3 Source Term

Instantaneous and continuous aerosol sources are modeled. Both the sources are assumed to be log-normal distribution. Distribution function f(r) is expressed as follows,

$$f(r) = \frac{1}{\sqrt{2\pi}\ln\sigma_g} \exp\left(-\frac{\ln^2 r/r_g}{2\ln^2\sigma_g}\right) \cdot \frac{1}{r} \qquad (22)$$

r_g = geometric number mean radius

σ_g = geometric standard deviation

For an instantaneous source, particle size distribution n(r) is given as follows,

$$n(r) = \frac{C_o}{\frac{4}{3}\pi r_g{}^3 \rho \exp(4.5 \ln^2\sigma_g)} \cdot f(r) \qquad (23)$$

C_0 = initial mass concentration

For a continuous source, source rate distribution s(r, t) is given as follows,

$$S(r, t) = \frac{S_o(t)}{\frac{4}{3}\pi r_g{}^3 \rho \exp(4.5 \ln^2\sigma_g)} \cdot f(r) \qquad (24)$$

So(t) = aerosol source rate

For the time dependent source, a stepwise source rate function is used.

3. Numerical Features

The numerical method, which is used in the ABC-INTG code to solve the dynamic equation for aerosol, is based on the sectional representations by Gelbard, et al. Hereafter, the numerical features are explained briefly.

3.1 Sectional Representations

The entire particle size domain is divided into m sections. An integral quantity of aerosol Q_ℓ is defined in section ℓ as follows,

$$Q_\ell(t) = \int_{v_{\ell-1}}^{v_\ell} v.n\,(v, t)\,dv \qquad \text{................... (25)}$$

$$\ell = 1, 2, \text{............} m$$

It is assumed that only binary collisions occur. The rate of coagulation between particles in volume ranges $[u, u + du]$ and $[v, v + dv]$ is given by $K(u, v)\,n\,(u, t)\,n\,(v, t)\,du\,dv$.

The Eq. (1) can be rewritten as follows, using $Q_\ell(t)$.

$$\frac{dQ_\ell(t)}{dt} = \frac{1}{2}\int_{V_0}^{V_{\ell-1}}\int_{V_0}^{V_{\ell-1}} \theta(v_{\ell-1}<u+v<v_\ell)(u+v)K(u,v)n(u,t)n(v,t)\,dudv$$

$$-\int_{V_0}^{V_{\ell-1}}\int_{V_{\ell-1}}^{V_0}\left\{\theta(u+v>v_\ell)u - \theta(u+v<v_\ell)v\right\}K(u,v)n(u,t)n(v,t)\,dudv$$

$$-\frac{1}{2}\int_{V_{\ell-1}}^{V_\ell}\int_{V_{\ell-1}}^{V_\ell}\theta(u+v>v_\ell)(u+v)K(u,v)n(n,t)n(v,t)\,dudv$$

$$-\int_{V_\ell}^{V_m}\int_{V_{\ell-1}}^{V_\ell} uK(u,v)n(u,t)n(v,t)\,dudv$$

$$-\int_{V_{\ell-1}}^{V_\ell} R(v)vn(v,t)\,dv$$

$$+\int_{V_{\ell-1}}^{V_\ell} S(u,t)\,dv \qquad \text{........................ (26)}$$

where the function θ is equal to one if the specified condition is satisfied, and is equal to zero if it is not satisfied.

To express dQ_ℓ/dt in terms of Q_i, $i=1, 2 \ldots m$, a size variable $x=f(v)$ is chosen. The following is assumed within each section ℓ,

$$vn(v, t) = \bar{q}_\ell(t)\, f'(v) \qquad \ldots\ldots\ldots\ldots (27)$$

where $f'(v)=df/dv$ and $\bar{q}_\ell(t)$ is a constant in each section. Then, the size distribution density function is expressed as follows for $v_{\ell-1}<v<v_\ell$,

$$n(v, t) = \frac{Q_\ell(t)\, f'(v)}{v[f(v_\ell) - f(v_{\ell-1})]} \qquad \ldots\ldots\ldots\ldots (28)$$

The equation (26) is expressed as follows in terms of $Q_\ell(t)$ ($\ell=1, 2 \ldots m$)

$$\frac{dQ_\ell}{dt} = \frac{1}{2}\sum_{i=1}^{\ell-1}\sum_{j=1}^{\ell-1} {}^{1}\bar{\beta}_{i,j,\ell}\, Q_i Q_j - Q_\ell \sum_{i=1}^{\ell-1} {}^{2}\bar{\beta}_{i\ell}\, Q_i$$

$$- \frac{1}{2}\, {}^{3}\bar{\beta}_{\ell,\ell}\, Q_\ell^2 - Q_\ell \sum_{i=\ell+1}^{m} {}^{4}\bar{\beta}_{i,\ell}\, Q_i$$

$$- \bar{R}_\ell(t) Q_\ell + S_\ell(t) \qquad \ldots\ldots\ldots\ldots (29)$$

Coagulation coefficients are given as follows.

$${}^{1}\bar{\beta}_{i,j,\ell} = \int_{x_{i-1}}^{x_i} \int_{x_{j-1}}^{x_j} \frac{\theta(v_{\ell-1} < u+v < v_\ell)(u+v)K(u,v)}{uv(x_i - x_{i-1})(x_j - x_{j-1})}\, dy\,dx$$

$2 \leq \ell \leq m$, $1 \leq i < \ell$, $1 \leq j < \ell$,

$${}^{1}\bar{\beta}_{i,j,\ell} = {}^{1}\bar{\beta}_{j,i,\ell} \qquad \ldots\ldots\ldots\ldots (30)$$

$$ {}^{2}\bar{\beta}_{i,\ell} = \int_{x_{i-1}}^{x_i} \int_{x_{\ell-1}}^{x_\ell} \frac{\left[\theta(u+v>v_\ell)u-\theta(u,v)<v_\ell)v\right] K(u,v)}{uv(x_i - x_{i-1})(x_\ell - x_{\ell-1})} dydx $$

$2 \leq \ell \leq m,\ i < \ell,\ {}^{2}\bar{\beta}_{i,\ell} \neq {}^{2}\bar{\beta}_{\ell,i}$ .... (31)

$$ {}^{3}\beta_{\ell,\ell} = \int_{x_{\ell-1}}^{x_\ell} \int_{x_{\ell-1}}^{x_\ell} \frac{\theta(u+v>v_\ell)(u+v)K(u,v)}{uv(x_\ell - x_{\ell-1})^2} dy\,dx $$

$1 \leq \ell \leq m$ .... (32)

$$ {}^{4}\beta_{i,\ell} = \int_{x_{i-1}}^{x_i} \int_{x_{\ell-1}}^{x_\ell} \frac{uK(u,v)}{uv(x_i - x_{i-1})(x_\ell - x_{\ell-1})} dydx $$

$1 < \ell < m,\ i > \ell,\ {}^{4}\bar{\beta}_{i,\ell} \neq {}^{4}\bar{\beta}_{\ell,i}$ .... (33)

$X_i = f(v_i),\ u = f^{-1}(y),\ v = f^{-1}(x)$

The removal constant rate for section ℓ, R_ℓ, is given as follows,

$$ \bar{R}_\ell = \int_{x_{\ell-1}}^{x_\ell} \frac{R(v)}{(x_\ell - x_{\ell-1})} dx \qquad (34) $$

The source term for section ℓ, $S_\ell(t)$, is given as follows,

$$ \bar{S}_\ell(t) = \int_{V_{\ell-1}}^{V_\ell} v.S(v,t)\,dv \qquad (35) $$

Because the size distribution for aerosol particles is usually expressed in terms of particle diameter logarithms, the following equation is used as a size which is variable in the numerical integration of the above equations.

$$ \begin{aligned} x = f(v) &= \log_{10}(6v/\pi)^{1/3} \\ &= \log_{10} 2r \end{aligned} \qquad (36) $$

3.2 Aerosol Data Calculation

The time dependent variables to be solved in the ABC-INTG code are $Q_\ell(t)$, $\ell = 1, 2 \ldots m$. Other aerosol data are calculated as follows, using Q_ℓ values,

(1) Suspended mass concentration, C(t)

$$C(t) = \rho \sum_{\ell=1}^{m} Q_\ell \quad \text{.................... (37)}$$

(2) Geometric mass mean radius, R50

$$R50 = \exp\left\{ \frac{\sum_{\ell=1}^{m} (\ln \bar{r}_\ell) Q_\ell}{\sum_{\ell=1}^{m} Q_\ell} \right\} \quad \text{.................... (38)}$$

where r_ℓ: average radius in section ℓ

$$= \sqrt[3]{\frac{3}{4\pi} \bar{v}_\ell} \quad \text{.................... (39)}$$

$\bar{v}_\ell$: average volume in section ℓ

$$\bar{v}_\ell = \int_{v_{\ell-1}}^{v_\ell} v . dv \,/\, (v_\ell - v_{\ell-1}) \quad \text{.................... (40)}$$

(3) Geometric standard deviation, σg

$$\sigma g = \exp\left\{ \frac{\sum_{\ell=1}^{m} (\ln \bar{r} - \ln R50)^2 Q_\ell}{\sum_{\ell=1}^{m} Q_\ell} \right\} 1/2 \quad \text{.................... (41)}$$

(4) Particle size distribution, dM/d ln r

$$\frac{dM}{d\ln r} = m(r_\ell) = \rho Q_\ell \frac{\bar{r}_\ell}{r_\ell - r_{\ell-1}}, \ \ell = 1, 2 \ldots m,$$

$$\text{.................... (42)}$$

4. Concluding Remarks

ABC-INTG predictions were compared with those for ABC-3C for various particle size class numbers. The ABC-INTG code gives results nearly equal to those for ABC-3C at 120 particle classes, by using only 20 particle size sections. This reduces the required computing time extensively. The ABC-INTG Code numerical validity in solving the coagulation dynamics has been studied by comparing it with the analytical solution for constant coagulation rate published by Scott[13].

The code is now extended to a three-cell model to deal with the conainment system used in Japanese fast breeder reactors.

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