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DEVELOPMENT AND VALIDATION OF ABC-INTG CODE

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ABSTRACT

A computer code, ABC-INTG, has been devloped to analyze the aerosol behavior within a containment following a postulated accident in a liquid metal fast breeder reactor.

ABC-INTG integrates digitally the coagulation probabilities of the particles due to Brownian motion, gravitational settling, and turbulent motion by using the sectional representations proposed by Gelbard, et al. By this method, the code extensively reduces the computing time compared with the former versions of ABC and conserves the aerosol mass almost perfectly.

The numerical validity of ABC-INTG in calculating the coagulation probabilities of the particles has been studied by comparing its numerical predictions with the analytical solutions calculated from the equations by Scott. Good agreement was obtained in this comparison. The code was validated also by comparing its numerical predictions with the test data from the LTV Test by Atomics International and the CSTF Test by Hanford Engineering Development Laboratory. Again, good agreement was obtained with the selected value of the gravitational collision efficiency in the code.

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INTRODUCTION

A postulated accident in a liquid metal fast breeder reactor (LMFBR) is often accompanied by the release of sodium oxide aerosols that contain fission products and nuclear fuels. Although most of these aerosols are confined in a reactor containment system, some leak out to the environment. From the viewpoint of reactor safety, therefore, the analysis of aerosol behavior within a containment is required for evaluating radiological consequence following an LMFBR accident.

To try to meet that requirement, the first version of ABC (Aerosol Behavior in Containment) [1] was developed in 1973. Since that time, the code has been successively improved and the ABC-2 [2], ABC-3B [3], and ABC-3C [4] versions were developed. Although these versions were respectively validated by test data, the experience in these codes showed that they had their own limitations, in particular, in computing time and in aerosol mass conservation.

To eliminate the limitations associated with the former versions, ABC-INTG has been developed by revising the numerical method. In the former verions of the code, the sectional method (the finite difference method) was adopted to discretize the particle size distribution. This method has an advantage in being able to treat an arbitrary distribution of the particle sizes, while the moment method is limited to the log-normal distribution. In ABC-INTG, the same sectional method is used to discretize the particle size distribution. Furthermore, the method to calculate the coagulation probabilities of the particles is revised by using the method of sectional representations proposed by Gelbard, et al [5][6].

In the present paper, the limitations of ABC-3B and ABC-3C that forced the development of ABC-INTG is explained at first. Then, the verification and the validation of the code are presented following the explanations on the numerical features of ABC-INTG.

I. NUMERICAL PROBLEMS WITH THE FORMER VERSIONS OF ABC

(1) Mass Conservation Problem in ABC-3B

The former ABC version, ABC-3B, solved the following integro-differential equation to describe the dynamics of aerosols that have a discrete particle size distribution.

$$\frac{dn_i}{dt} = \sum_{\alpha} K_{j,k} \cdot C^i_{j,k} \cdot n_j \cdot n_k - n_i \sum_{k=1}^{KL} K_{i,k} \cdot n_k + S_i - R_i \cdot n_i \qquad (1)$$

where n_i : number concentration in the i-th class particles,

$K_{i,k}$: coagulation probability between particles in the i-th and the k-th classes,

$C^i_{j,k}$: correction factor, $(= \frac{r_j^3 + r_k^3}{r_i^3})$,

S_i : source rate,
R_i : removal rate,
α : all possible combinations to produce the i-th class particles,
r_i : radius of i-th class particle,
KL : maximum particle size class.

Good agreement was obtained between the ABC-3B code predictions and the JAERI $1m^3$ test data for uranium oxide, sodium oxide, and their mixed aerosols [7]. But, during a run by ABC-3B to check its applicability to an extremely high concentration aerosols ($\simeq 8\times10^{-5}$ g/cm^3) in a large containment, a mass conservation problem was encountered. The calculation of Brownian agglomeration resulted in a gradual increase in the aerosol mass concentration even with no source term or no removal process. Moreover, the addition of gravitational agglomeration to the above calculation resulted in a marked decrease in the concentration. Figure 1 shows the changes in the aerosol mass concentration calculated where neither source term nor removal term was considered. These deviations became smaller at lower concentrations. Further, in a small containment, the deviations became negligibly small compared with the removal rate by gravitational settling.

(2) Numerical Truncation Problem in ABC-3C

To solve the mass conservation problems described with ABC-3B, the numerical scheme to solve the integro-differential equation was rechecked and was revised as follows to strictly conserve the aerosol mass. The code thus revised was named ABC-3C:

$$\frac{d(n_i m_i)}{dt} = \sum_{\alpha} K_{j,k} \cdot n_j \cdot n_k (m_j + m_k) - \sum_{k=1}^{KL} K_{i,k} \cdot n_k \cdot n_i \cdot m_i + S_i - R_i \cdot n_i \cdot m_i \quad (2)$$

where m_i : mass of particles in the i-th class.

With ABC-3C, the aerosol mass was conserved almost perfectly during agglomeration calculations. But its computing time strongly depended on the number of particle classes. The larger the number, the longer the computing time, as shown in Table 2. Although the computing time can be reduced remarkably by reducing the number of particle classes, this results in an increase in the truncation errors. Therefore, the number cannot be reduced below a limited value. The reasonably accurate results were obtained only with the particle size classes larger than 80 as shown in Figure 2, where KL indicates the number of particle size classes. But, such large number is not practicable for most of the cases where calculations are required for long hours, namely several hundred hours.

II. DEVELOPMENT OF ABC-INTG

(1) Numerical Scheme

To further solve the numerical problems associated with ABC-3C and also to make computing time reasonably short, the ABC-INTG code has been developed. In the code, the numerical method has been revised by using the sectional representations by Gelbard and Seinfeld [5][6], which feature as follows:

1) volume concentrations (instead of number concentrations) of particles are calculated as unknown quantities,

2) the coagulation probabilities of particles are numerically integrated.

In the numerical scheme of ABC-INTG, an entire particle size domain is divided into m classes. An integral quantity of volume concentration Q_i in the i-th class is defined by Eq.(3).

$$Q_i(t) = \int_{v_{i-1}}^{v_i} v\, n(v,t)dv \qquad (3)$$

where, $i = 1,2 \ldots\ldots m$,
v is volume of a particle,
$n(v,t)$ is a number concentration.

The integro-differential equation that describes aerosol dynamics is expressed in terms of $Q_i(t)$ ($i=1,2, \ldots m$, where v_{i+1} must be larger than $2v_i$) as follows:

$$\frac{dQ_i}{dt} = \frac{1}{2}\sum_{j=1}^{i-1}\sum_{k=1}^{i-1} {}^{1}\overline{\beta}_{j,k,i} \cdot Q_j \cdot Q_k - Q_i \sum_{j=1}^{i-1} {}^{2}\overline{\beta}_{j,i} \cdot Q_j$$
$$- \frac{1}{2}\, {}^{3}\overline{\beta}_{i,i} \cdot Q_i^2 - Q_i \sum_{k=i+1}^{m} {}^{4}\overline{\beta}_{k,i} \cdot Q_i$$
$$+ \overline{S}_i(t) - \overline{R}_i(t) \cdot Q_i \qquad (4)$$

where, β: coagulation coefficients.

The coagulation coefficients in Eq.(4) are expressed in Eq.(5) through Eq.(9) as follows:

$${}^{1}\overline{\beta}_{j,k,i} = \int_{x_{j-1}}^{x_j}\int_{x_{k-1}}^{x_k} \frac{\theta(v_{i-1}<u+v<v_i)(u+v)K(u,v)}{uv(x_j-x_{j-1})(x_k-x_{k-1})}\, dydx \qquad (5)$$

where, $2 \leq i \leq m,\ 1 \leq j < i,\ 1 \leq k < i,\ {}^{1}\overline{\beta}_{j,k,i} = {}^{1}\overline{\beta}_{k,j,i}$

$${}^{2}\overline{\beta}_{j,i} = \int_{x_{j-1}}^{x_j}\int_{x_{i-1}}^{x_i} \frac{[\theta(u+v>v_i)u - \theta(u+v<v_i)v]K(u,v)}{uv(x_j-x_{j-1})(x_i-x_{i-1})}\, dydx \qquad (6)$$

where, $2 \leq i \leq m,\ j < i,\ {}^{2}\overline{\beta}_{j,i} \neq {}^{2}\overline{\beta}_{i,j}$

$$^{3}\overline{\beta}_{i,i} = \int_{x_{i-1}}^{x_i}\int_{x_{i-1}}^{x_i} \frac{\theta(u+v>v_i)(u+v)K(u,v)}{uv(x_i-x_{i-1})^2}\,dydx \tag{7}$$

where, $1 \leq i \leq m$

$$^{4}\overline{\beta}_{j,i} = \int_{x_{j-1}}^{x_j}\int_{x_{i-1}}^{x_i} \frac{uK(u,v)}{uv(x_j-x_{j-1})(x_i-x_{i-1})}\,dydx \tag{8}$$

where, $1 < i < m,\ j > i,\ {}^{4}\overline{\beta}_{j,i} \neq {}^{4}\overline{\beta}_{i,j}$

$$x_i = f(v_i),\ u = f^{-1}(y),\ v = f^{-1}(x) \tag{9}$$

In Eqs.(5) through (7), the function θ is equal to one if the specified condition is satisfied; and zero, if not.

The source term $\overline{S}_i(t)$ in Eq.(4) for the i-th class is expressed as follows:

$$\overline{S}_i(t) = \int_{v_{i-1}}^{v_i} v \cdot S(v,\ t)\,dv \tag{10}$$

The removal rate $\overline{R}_i(t)$ in Eq.(4) for the i-th class is given by Eq.(11).

$$\overline{R}_i(t) = \int_{x_{i-1}}^{x_i} \frac{R(v)}{(x_i-x_{i-1})}\,dx \tag{11}$$

Since the size distribution of aerosol particles is usually expressed in terms of logarithms of the particle diameter, Eq.(12) can be used as a variable for the numerical integration of the integro-differential equation.

$$\begin{aligned} x = f(v) &= \log_{10}(6v/\pi)^{1/3} \\ &= \log_{10}(2r) \end{aligned} \tag{12}$$

(2) Addition of Turbulent Coagulation Term

The turbulent coagulation term of particles had not been considered in the former versions of ABC, therefore, this term was added to ABC-INTG. The collision frequency between the particles suspended in a gaseous medium increases with the increase in turbulent motion. Such collision is due to the following two independent processes [8]: one is the collision of particles by random motion of the gaseous medium, and another is the collision of particles by the particle inertia itself. To consider these collision processes, the two coefficients are added to the coagulation coefficients i.e., Brownian and gravitational.

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

$$K_{T1} = \varepsilon\left(\frac{8\pi\rho_g}{15\eta}\varepsilon_T\right)^{1/2}(r_i+r_j)^3\gamma^3 \tag{13}$$

where, ε_T : the energy dissipation rate in the turbulent fluid,
ε : gravitational collision efficiency,
γ : coagulation shape factor,
ρ_g : density of carrier gas,
η : viscosity of carrier gas.

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

$$K_{T2} = \varepsilon \, (r_i + r_j)^2 \, |v_i - v_j| \frac{\gamma^2}{\chi} \tag{14}$$

where, χ : dynamic shape factor,
v_i is particle velocity and is given by Eq.(15)

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

where, ρ : density of aerosol,
A_i : Cunningham slip correction factor,
λ : molecular mean free path of carrier gas.

(3) Code Verification

The code verification has been carried out by comparing the ABC-INTG predictions with the analytical solutions that were calculated from the equation proposed by Scott [9]. In this event, changes in the particle number concentration at a constant coagulation probability with no source term or no removal term were calculated.

In case of no source term or no removal term, Scott defined the non-dimensional distribution density that is expressed by Eq.(17). He also derived the total number of particles as expressed by Eq.(16).

$$N(t) = \frac{2 N_0}{\tau + 2} \tag{16}$$

where, $N(t)$: total number of particles,
N_0 : initial total number of particles,
τ : nondimensional time, $= CN_0t$,
C : constant coagulation rate,
t : time (sec).

$$\phi(x, \tau) = \frac{8 e^{-2x} \sinh \{ 2x \, (\frac{\tau}{\tau + 2})^{1/2} \}}{\tau^{1/2} (\tau + 2)^{3/2}} \tag{17}$$

where, $\phi(x, \tau)$: nondimensional number distribution density,
x : nondimensional volume,

$$x = v/v_0$$

v : particle volume,
v_0 : initial averaged volume of particles.

By using Eqs. (16) and (17), the analytical solutions were calculated. On the other hand, the corresponding numerical predictions were calculated by ABC-INTG. Table 1 summarizes the initial conditions for obtaining the analytical solutions and also for the ABC-INTG calculations. The results are given in Figures 3 and 4. The code predictions agree fairly well with the analytical solutions in regard to both the mass concentration and the number concentration.

Table 1 Initial Conditions for Obtaining the Analytical Solutions and the ABC-INTG Calculations

initial number concentration	238.732	(number/cm^3)
initial mass concentration	10^{-6}	(g/cm^3)
geometric count mean radius	10^{-4}	(cm)
minimum radius of particle	10^{-5}	(cm)
maximum radius of particle	3.0×10^{-4}	(cm)
aerosol density	1.0	(g/cm^3)
constant coagulation rate	1.80×10^{-4}	(cm^3/sec)
time step	1.0	(sec)

(4) Code Validation

In the first phase, the code validation was carried out by comparing the ABC-INTG numerical prediction with that by the former version, ABC-3C. Since fairly good mass conservation was obtained by ABC-3C with KL, the number of particle size classes, larger than 80, as explained, the calculation by ABC-3C was carried out with KL equal to 120. On the other hand, the calculation by ABC-INTG was carried out with KL equal to 20. With this KL value, ABC-INTG generated a smaller truncation error than that by ABC-3C with KL equal to 120. Figure 5 shows the ABC-INTG prediction with that by ABC-3C. The ABC-INTG prediction agrees with that by ABC-3C. Table 2 summarizes the relationship between the number of particle classes and the computing times by ABC-INTG and ABC-3C. For ABC-3C, the results at KL equal to 20, 40, and 80 are also presented for the comparison. Table 2 shows that the computing time (CPU time) saving by ABC-INTG is considerable, that is, CPU time by ABC-INTG is 6.66 sec., while that by ABC-3C with KL equal to 120 is 419.12sec.. The mass conservation with ABC-INTG was excellent.

In the second phase, the code validation was carried out by comparing the code predictions with the data from the LTV test by Atomics International [10] and the CSTF test by Hanford Engineering Laboratory [11]. Table 3 summarizes the input data for the ABC-INTG calculation to analyze these tests. The aerosol mass concentration predicted by the code are presented in Figures 6 and 7 with various collision efficiencies, together with the test data. The numerical predictions indicated by "Fuchs" in these figures are those calculated with the Fuchs' definition [12],[13] for the gravitational collision efficiency. These figures indicate that the decay curve of the numerical mass concentration changes according to the change in gravitational collison efficiency, ε, and the numerical prediction at ε equal to 0.3 agrees well with the test data.

Table 2 Number of Particle Classes and Computing Time (Computer : FACOM M-380)

	number of particle classes	computing time (sec)	simulation time (sec)
ABC-3C	20	2.75	60000
	40	15.63	60000
	80	105.84	60000
	120	419.12	60000
ABC-INTG	20	6.66	60000

Table 3 Input Data for the Analyses of the U.S. Experimental Data

	TEST-3 in LTV/AI	AB-1 in CSTF/HEDL
initial mass conc. (g/cm^3)	1.505×10^{-7}	2.25×10^{-8}
geometric count mean radius (cm)	5.0×10^{-4}	5.0×10^{-4}
geometric standard deviation	1.7	1.7
aerosol density (g/cm^3)	0.3	0.3
vessel height (cm)	9.00×10^{2}	2.03×10^{3}
vessel volume (cm^3)	6.00×10^{7}	8.50×10^{8}
inner surface aera (cm^2)	7.70×10^{5}	5.20×10^{6}
floor area (cm^2)	6.60×10^{4}	4.23×10^{5}

III. DISCUSSIONS AND CONCLUSIONS

The aerosol codes so far developed and now used in many countries adopt the one of the following methods to represent the particle size distribution: one is the moment method and another is the sectioning method (finite difference method). The former method has an advantage in making computation very short. But this method is restricted only for the log-normal particle size distribution. Therefore, the particle size distribution of a realistic form cannot be treated. In contrast, the latter method has an advantage in treating arbitrary particle size distributions but has a disadvantage of larger truncation errors with a smaller number of particle classes. The former versions of ABC used this sectioning method, therefore, they showed large truncation errors, unless a longer computing time is spent.

In ABC-INTG, although the method of the discretization is essentially the same as those in the former versions, the numerical method is completely revised by introducing the sectional representations of Gelabrd et al. With the aid of this representations, ABC-INTG can not only perfectly conserve the aerosol mass almost but also greatly reduce the computing time, i.e., almost 1/70 of the former version of ABC. Furthermore, the verification and the validation of ABC-INTG showed good results, indicating that the disadvantage associated with the sectioning method has been eliminated. These advantages of ABC-INTG have also been made clear in the aerosol codes comparison study [14] conducted in the framework of the Commission of European Communities in 1982 and 1983. PARDISEKO-IIIB, AEROSIM, AEROSOLS-A2, and AEROSOLS-B1 joined this comparison study together with ABC-INTG. The essence of the study is that the code predictions by ABC-INTG gave good agreement with those by the other codes whose discretization method is the sectioning. On the other hand, the code with the moment method gave poor results, which indicated the limitation of this method.

In conclusion, the newly developed ABC-INTG code has enough reliability in its application to the analyses of the aerosol behavior within a containment.

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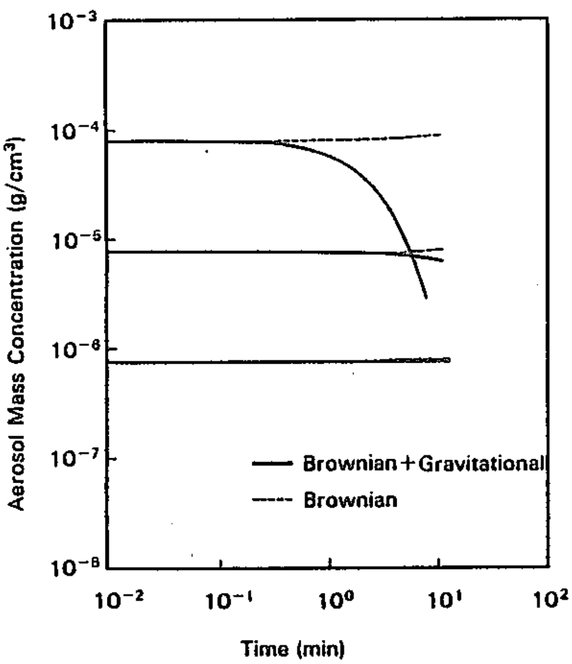

Fig.1 Changes in Mass Concentration in Agglomeration Calculation by ABC-3B

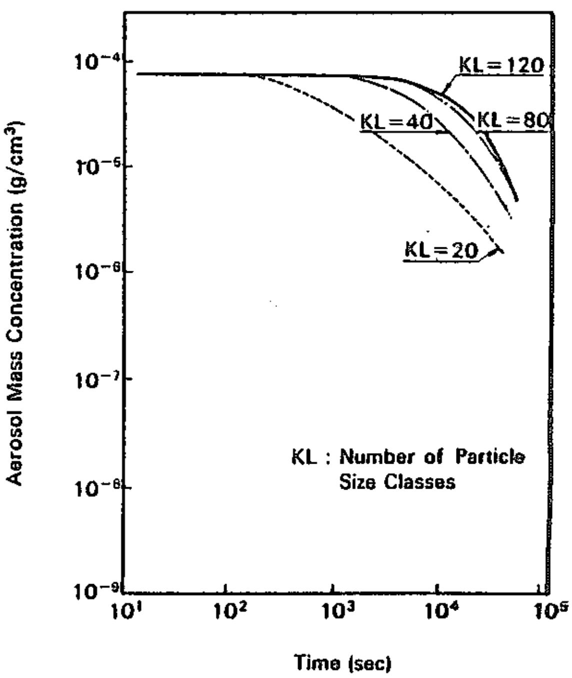

Fig.2 Changes in Mass Concentration by ABC-3C at Different Particle Size Classes

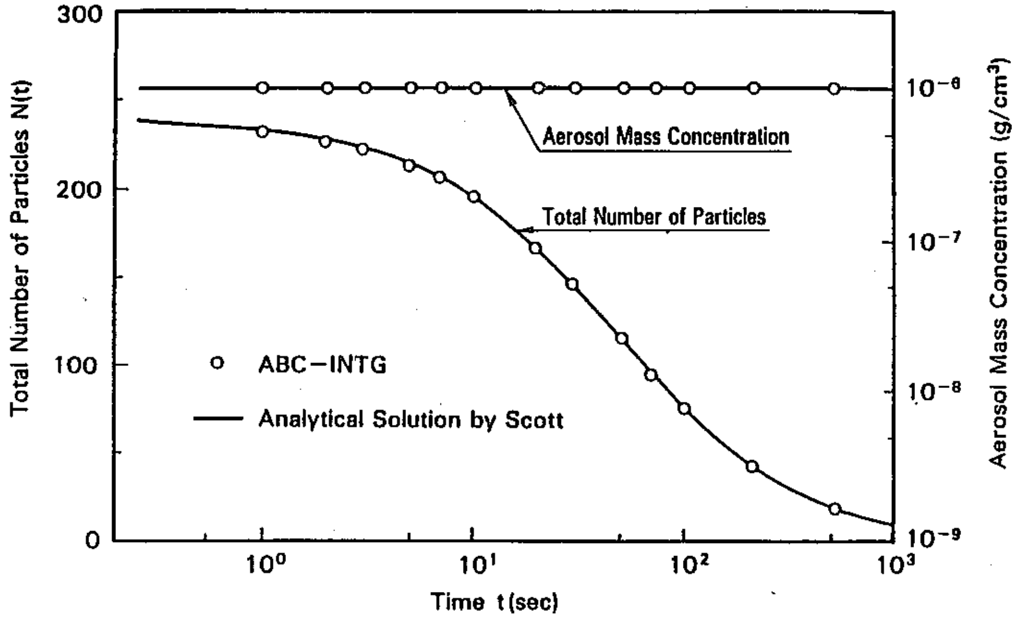

Fig.3 Comparisons of the ABC-INTG Predictions with the Analytical Solutions by Scott

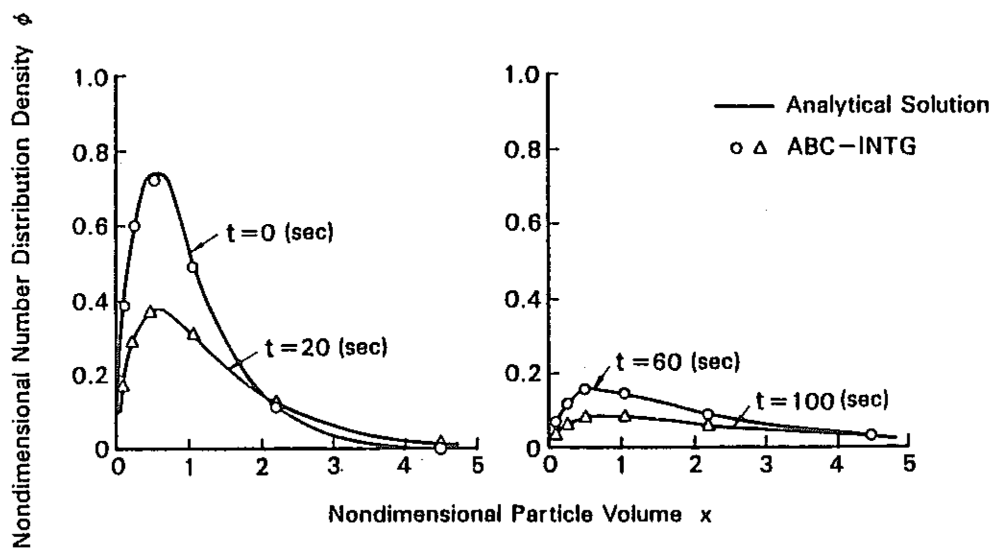

Fig.4 Comparisons of the ABC-INTG Predictions with The Analytical Solutions by Scott (Particle Size Distribution Density)

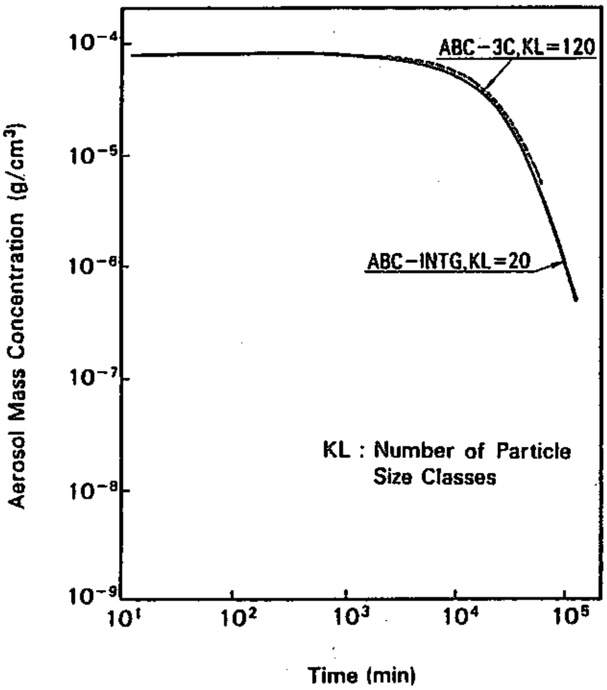

Fig.5 Comparison of the ABC-INTG Prediction with that by ABC-3C

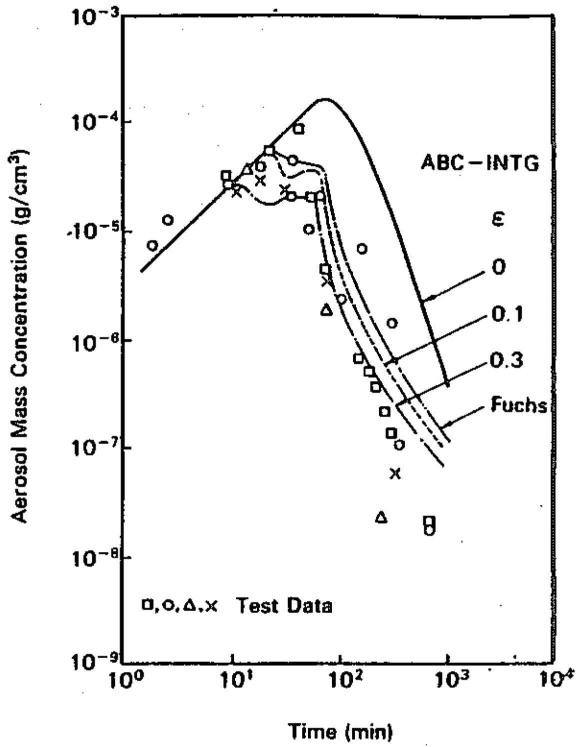

Fig.6 Comparisons of the ABC-INTG Predictions with LTV No.3 Test, Atomics International

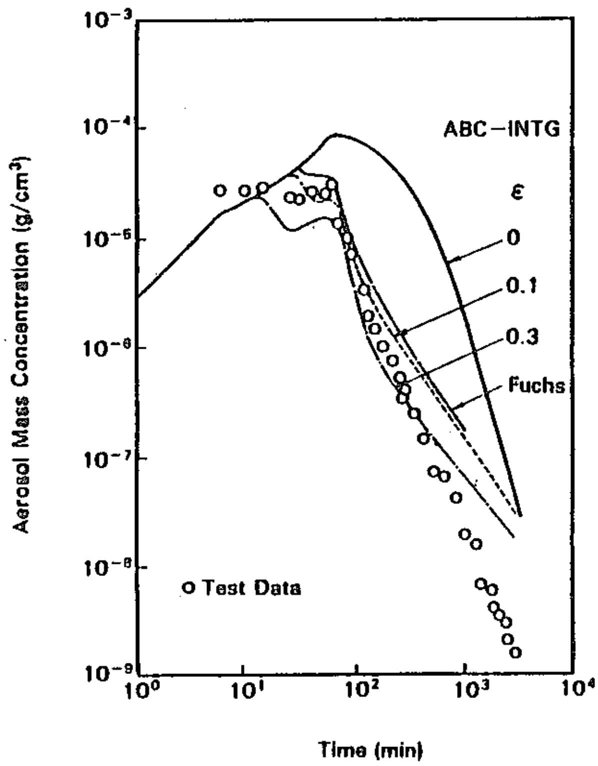

Fig.7 Comparisons of the ABC-INTG Predictions with CSTF AB1 Test by Hanford Engineering Development Laboratory