Numerical and Analytical Solutions of the Aerosol Dynamic Equation in Reactor Containment

M.O. Shaker¹, M. Aziz², R. Ali², M. Sirwah¹, and M. Slama².

¹ Mathematics Department, Faculty of Science, Tanta University, Tanta, Egypt.
² National Center for Nuclear Safety and Radiation Control, Atomic Energy authority, Ahmed EL-Zomor st. P.O. Box: 7551 Nasr City, Cairo, Egypt.

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ABSTRACT

During a severe reactor accident, nuclear aerosol composed of fission products, actinides and structural material are released into the reactor containment at different locations and times. Methods and approximations inherent in modeling of aerosol dynamics and evolution for nuclear reactor source term estimation have been investigated. Several aerosol evolution problems are considered to assess numerical methods of solving the aerosol dynamic equation. The space-dependent aerosol dynamic equation is solved to assess implications of spatial homogenization of aerosol distributions. The sectional method of solving the aerosol dynamic equation is quite efficient in modeling of coagulation problems, but should be improved for simulation of deposition problems.

KeyWords: Nuclear Aerosol / General Dynamic Equations / Coagulation Kernel / Deposition rate / Sectional Technique.

INTRODUCTION

We present the numerical techniques for solving the aerosol dynamic equation, with description of the sectional method. The accuracy of the computed results is always of primary concern for practical applications of the methods. The accuracy may be assessed by applying these methods to various benchmark problems for which the analytical solutions are available, and then by comparing the numerical results against the corresponding analytical results. The results of the test will then give us benchmarks for the applicability of numerical techniques to solving arbitrary realistic problems.

We have considered two classes of benchmark problems to test the sectional method. The first class includes two coagulation problems which allow only the coagulation process for the particle evolution mechanism. The second class deals with a coagulation and deposition problem where the aerosol is allowed to evolve through simultaneous coagulation and deposition processes; this second class includes two problems.

GENERAL DYNAMIC EQUATIONS

The aerosol behavior involves several factors such as particle size, composition, shape, charge, spatial inhomogeneities, environmental conditions, and thermal hydraulics that influence the aerosol evolution process. This complex behavior of aerosols is expressed mathematically using general dynamic equations (GDEs) (1, 2, 3).

In this study, we will consider the conventional spatially homogeneous version of the aerosol dynamic equation as well as the space- and time-dependent aerosol dynamic equation. A detailed description of GDE can be found in references (4, 5, 6).
Where \( n(v, t) \) is number of aerosol particles which have volumes between \( v \) and \( v + \, dv \) at time \( t \) per unit volume of the fluid, \( K(u, v) \) is coagulation kernel between two particles of volume \( u \) and \( v \) per unit fluid volume, \( R(v, t) \) is deposition rate of particles of size \( v \) at time \( t \) per unit fluid volume, \( S(v, t) \) is number of particles of volume \( v \) at time \( t \) injected to the system per unit fluid volume and \( \alpha(v, t) \) is rate of particle release per unit volume into environment if the containment fails.

**NUMERICAL SOLUTION**

Aerosol dynamic equation (1) cannot be solved analytically in most realistic cases. Hence, one must resort to numerical methods to solve the equation except when some special rate models and initial conditions are employed. Several numerical techniques have been proposed to solve the equation. Of these, the power moments method, J-space transform method, and sectional method have received the most attention. By dividing the entire particle size domain into \( m \) arbitrary sections, one can define \( Q_i \) to be an integral quantity of aerosol in section \( i \),

\[
Q_i(t) = \int_{v_{i-1}}^{v_i} q(v, t) \, dv = \int_{v_{i-1}}^{v_i} a v^\gamma n(v, t) \, dv, \text{ for } i = 1, 2, 3, 4, \ldots, m
\]  

(2)

Where \( v_{i-1} \) is the volume of the smallest particle in section \( i \) (m\(^3\)), \( v_i \) is the volume of the largest particle in section \( i \) (m\(^3\)), \( v_0 \) is the volume of the smallest particle in section 1 (m\(^3\)), \( v_m \) is the volume of the largest particle in section \( m \) (m\(^3\)), \( a \) and \( \gamma \) are constants, \( v \) is volume of any aerosol particle (m\(^3\)), \( q(v, t) \) takes the following:

1. Aerosol number distribution if \( \alpha = 1 \) and \( \gamma = 0 \) \( [q(v, t) = n(v, t)] \).
2. Aerosol volume distribution if \( \alpha = 1 \) and \( \gamma = 1 \) \( [q(v, t) = vn(v, t)] \).
3. Aerosol surface area distribution if \( \alpha = \pi^{1/3} b^{2/3} \) and \( \gamma = 2/3 \) \( [q(v, t) = \pi^{1/3} b^{2/3} v^{2/3} n(v, t)] \).

Note that the upper bound of section \( i - 1 \) is equal to the lower bound of section \( i \) for \( i = 2, 3, 4, \ldots, m \).

We will present the sectional method that is the numerical technique we use in this study; in this manner one can obtain the following set of general sectional equations:

\[
\frac{dQ_i}{dt} = \frac{1}{2} \left( \sum_{j=1}^{i-1} \sum_{k=j}^{i-1} Q_j Q_k \beta_{j,k} - Q_i \sum_{k=1}^{i-1} Q_k \beta_{i,k} - \frac{1}{2} \beta_{i,i} Q_i^2 - Q_i \sum_{k=i+1}^{m} Q_k \beta_{i,k} \right)
\]  

(3)
\[-Q_2 \int_{v_{l-2}}^{v_l} \frac{R(v,t)}{(v_l-v_{l-2})} dv + \alpha \int_{v_{l-2}}^{v_l} S(v,t) dv, \quad \text{for } l = 1, 2, 3, \ldots, m\]

Where \( \beta_{l,i-1}^{1}, \beta_{l,i-1}^{2}, \beta_{l,i-1}^{3} \) and \( \beta_{l,i}^{4} \) are sectional coagulation coefficients, much more information is available on references (7, 8, 9).

**MODEL DESCRIPTION**

The model is based on dividing the particle size range into \( m \) sections. The particle volumes of section \( l \) range from \( v_{l-1} \) to \( v_l \) where \( l = 1, 2, 3, \ldots, m \). Imposing conservation of aerosol volumes and numbers for each component for all the processes given and approximating a form of particle size distribution function as a constant within each section results in a set of differential equations for the aerosol volume and number concentration \( Q_2 \). This set of equations is integrated in time using a Runge-Kutta-Fehlberg (10, 11).

Aerosol model is designed by wolfram mathematica 7 program and executed on PC-IBM computer, 3 GHz. These equations can be solved in two major steps. The first step is to calculate and store the sectional coagulation coefficients for all sections (400 sections). The second step is to solve the system of ordinary differential equations. The execution time for the first step consumes 12 hours when the gravitational, Brownian and turbulent collision efficiency are calculated. However without gravitational, Brownian and turbulent efficiency being calculated, it consumes only 15 minutes. Solving the system of ordinary differential equations based on 400 sections consumes 18 hours when all terms of equation (3) are considered.

**BENCHMARK C1: CONSTANT COAGULATION KERNEL**

GDE in equation (1) was solved in a particular case: constant coagulation kernel and without deposition rate of particles (neglect deposition rate) by Schumann as referred to in reference 12, the solution has been improved by Mulholland and Baum as referred to in reference 13. Scott as referred to in reference 14 has solved equation (1) analytically, using the Laplace transform technique and the initial exponential distribution. The analytical solution is given by

\[ n(v,t) = \frac{4 N_0}{v_{min} (2 + N_0 K t)} \exp \left(-\frac{2}{v_{min} (2 + N_0 K t)} \right), \]  

(4)

Where \( K \) is constant coagulation kernel (m³/sec).

**BEHAVIOR OF THE NUMBER OF AEROSOL PARTICLES**

The value of the error for the aerosol number between numerical and analytical solutions to the equation GDE is less than \( 10^{-11} \) as evident in Figure (1). This indicates that our calculations are fully equivalent to analytical solution. Properties of the sectional method in this benchmark are 1- with increasing in the time at nuclear aerosol number decreasing. 2-nuclear aerosols, which have a smaller size, coagulate to become a nuclear aerosol with a largest size then nuclear aerosol move from a less section to a large section in size; Figures (3A), (3B) and (3C) show these properties. Figures (3A), (3B) and (3C) illustrate that the last 55, 25 and 20 sections do not contain aerosol by respectively.

The value of the error can be calculated in a manner which is more in-depth by counting the error on each section, as in Figure (2). The field of nuclear aerosols has been divided into sections using
more than one division such as 50, 100, 200 and 400 sections; and by calculating the error value for these different divisions, it appears that all the values of the error in divisions 200 and 400 are less than $10^{-11}$, as in Figure (2). By demonstrating the error value output from each section in the different divisions, we find that the value of the error resulting from the divisions 200 and 400 sections is much lower than the error resulting from the divisions 50 and 100 sections, as in Figure (2).

**Fig. (1):** the value of the error for the aerosol number between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles $N_0$ ($10^{14}$, $10^{13}$ and $10^{12}$ particle/m$^3$) at the constant coagulation alone and divided aerosol particle range into 400 sections.

**Fig. (2):** the error value for the number of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C1.

. (3A): the number of nuclear aerosols after 2 hours by using benchmark C1.

**Fig. (3A):** the number of nuclear aerosols after 2 hours by using benchmark C1.

**Fig. (3B):** the number of nuclear aerosols after 12 hours by using benchmark C1.

**Fig. (3C):** the number of nuclear aerosols after 24 hours by using benchmark C1.

**BEHAVIOR OF THE VOLUME OF AEROSOL PARTICLES**

The volume of aerosol particles fixed value in this benchmark C1 because there is no deposition rate of nuclear aerosol, whether on the land or walls of the reactor. The value of the error for the aerosol number between numerical and analytical solutions to the equation GDE is less than $10^{-10}$ as evident in Figure (4). This indicates that our calculations are fully equivalent to analytical solution.
Figures (6A), (6B) and (6C) show that the volume of nuclear aerosol constant before and after the coagulation kernel after 2, 12 and 24 hours respectively.

Figure (5) shows the value of the error for the aerosol volume between numerical and analytical solutions by using different divisions of the aerosol range within 24 hours. The value of the error can be calculated in a manner which is more in-depth by using counting the error on each section, as in Figures (5).

Fig. (4): the value of the error for the aerosol volume between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 \) (\( 10^{14}, 10^{13} \) and \( 10^{12} \) particles \( \text{m}^{-3} \)) at the constant coagulation alone and divided aerosol particle range into 400 sections.

Fig. (5): the error value for the volume of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C1.

Fig. (6A): the volume of nuclear aerosols after 2 hours by using benchmark C1.

Fig. (6B): the volume of nuclear aerosols after 12 hours by using benchmark C1.

g. (6C): the volume of nuclear aerosols after 24 hours by using benchmark C1.

**BENCHMARK C2: LINEAR COAGULATION KERNEL**

GDE in equation (1) was solved in a particular case: linear coagulation kernel \( K(u,v) = b(u+v) \) and without deposition rate of particles by Williams and Loyalka as referred in
reference 1. Golvin as referred in reference 15 has solved equation (1) analytically, using the Laplace transform technique and initial exponential distribution. The analytical solution is given by

\[
n(t, \tau) = \frac{N_0 \exp[-b N_0 v_{m0} \tau]}{(1 - \exp[-b N_0 v_{m0} \tau])^2} \left[ 2 - \frac{\exp[-b N_0 v_{m0} \tau]}{v_{m0}} \right] I_n \left[ \frac{2(1 - \exp[-b N_0 v_{m0} \tau])^{1/2}}{v_{m0}} \right]
\]

Where \( I_n \) is a modified Bessel function and \( b \) is coefficient in a linear coagulation kernel.

**BEHAVIOR OF THE NUMBER OF AEROSOL PARTICLES**

Numbers of aerosol particles in reactor containment were studied in this case as in Figures (9A), (9B) and (9C). Figure (7) shows the value of the error for the aerosol number between numerical and the analytical solutions in this benchmark C2 using all sections within 24 hours. Figures (9A), (9B) and (9C) show that the rate of coagulation kernel in this benchmark C2 is less than it in the previous benchmark C1.

Figure (8) shows the error value for the numbers of nuclear aerosols in the reactor containment, using different divisions of the aerosol field during 24 hours. The same figure shows that the best way to divide the field of aerosol is 400 sections, and that the error value is less than \( 10^{-3} \) when dividing the aerosol field into the 400 sections.

![Fig. (7): the value of the error for the aerosol number between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 \) (10\(^{14}\), 10\(^{13}\) and 10\(^{12}\) particle /m\(^3\)) at the linear coagulation alone and divided aerosol particle range into 400 sections.](image)

![Fig. (8): the error value for the number of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C2.](image)
The volume of aerosol particles fixed value in this benchmark C2 because there is no deposition rate of nuclear aerosol, whether on the land or walls of the reactor. The value of the error for the aerosol volume between numerical and analytical solutions to the equation GDE is less than $10^{-10}$ as evident in Figure (10). This indicates that our calculations are fully equivalent to analytical solution. Figures (12A), (12B) and (12C) show that the volume of nuclear aerosol constant before and after the coagulation kernel after 2, 12 and 24 hours.

Figure (11) shows the value of the error for the aerosol volume between numerical and analytical solutions to the behavior of the volume of aerosol particles by using different divisions of the aerosol range within 24 hours, the value of the error for the aerosol volume, using the divisions of the field of nuclear aerosol to 100, 200 and 400 sections less than the value of the error by using the division of the field of nuclear aerosol to 50 sections.

(10): the value of the error for the aerosol volume between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles $N_0$ ($10^{14}$, $10^{13}$ and $10^{12}$ particle /m$^3$) at the linear coagulation alone and divided aerosol particle range into 400 sections.

Fig. (11): the error value for the volume of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C2.
BENCHMARK C3: CONSTANT COAGULATION KERNEL AND CONSTANT DEPOSITION RATE OF PARTICLES

Loss of particles to the internal surfaces of the containment can also be an important factor in altering shapes of particle size distributions. Major mechanisms for particle removal due to deposition are gravitational settling and diffusion. Simulation of these mechanisms, in the presence of others, is thus an interesting subject for testing the current numerical technique.

GDE in equation (4.8) was solved in a particular case: constant coagulation kernel $K(u,v) = K$ and constant deposition rate of particles $R(v,t) = R$ by Williams and Loyalka as referred to in reference 1. The particle size distribution at any time is given by

$$n(v,t) = \frac{G N}{v \tau} \exp \left[ -G \frac{v}{v \tau} \right]$$  \hspace{1cm} (6)

Where $G = \frac{N + \frac{5}{2}R}{N + \frac{5}{2}R}$ and $N = \frac{2R}{K} \frac{\exp[-R \tau]}{\left[1 + \frac{2R}{K v \tau} \exp[-R \tau]\right]}$

BEHAVIOR OF THE NUMBER OF AEROSOL PARTICLES

The value of the error for the aerosol number between numerical and analytical solutions to the equation GDE is less than $10^{-11}$ as evident in Figure (13). This indicates that our calculations are fully equivalent to analytical solution. Figures (15A), (15B) and (15C) show the behavior of aerosol in nuclear reactor in this benchmark C3 after 2, 12 and 24 hours respectively.

Aerosol deposition rate has a significant impact on the behavior of aerosol in nuclear reactor, and it shows in the result of calculating the value of the error between numerical and the analytical solutions using different divisions of the aerosol field, as evident in Figure (14).
Fig. (13): the value of the error for the aerosol number between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \(N_0 (10^{14}, 10^{13} \text{ and } 10^{12} \text{ particle/m}^3)\) at constant coagulation kernel and constant deposition rate and divided aerosol particle range into 400 sections.

Fig. (14): the error value for the number of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C3.

Fig. (15A): the number of nuclear aerosols after 2 hours by using benchmark C3.

Fig. (15B): the number of nuclear aerosols after 12 hours by using benchmark C3.

Fig. (15C): the number of nuclear aerosols after 24 hours by using benchmark C3.

BEHAVIOR OF THE VOLUME OF AEROSOL PARTICLES

Different volumes of aerosols in nuclear reactor in this case take the same behavior, because of the aerosol deposition rate fixed, as evident in Figure(16). Figure (16) shows the value of the error for the aerosol volume between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \(N_0 (10^{14}, 10^{13} \text{ and } 10^{12} \text{ particle/m}^3)\) at constant coagulation kernel and constant deposition rate and divided aerosol particle range into 400 sections. The error value for the aerosol volume between numerical and analytical solutions to equal, although there is disagreement values the initial total number distribution, because different volumes of aerosols take the same behavior. Figures (18A), (18B) and (18C) show the volume of nuclear aerosol in a decrease with constant coagulation kernel and constant deposition rate after 2, 12 and 24 hours respectively. Figure (17) shows the value of the error for the aerosol volume between numerical and analytical solutions by using different divisions of the aerosol range within 24 hours.
Fig. (16): the value of the error for the aerosol volume between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 (10^{14}, 10^{13} \text{ and } 10^{12}\text{ particle } /\text{m}^3) \) at constant coagulation kernel and constant deposition rate and divided aerosol particle range into 400 sections.

Fig. (17): the error value for the volume of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C3.

Fig. (18A): the volume of nuclear aerosols after 2 hours by using benchmark C3.

Fig. (18B): the volume of nuclear aerosols after 12 hours by using benchmark C3.

Fig. (18C): the volume of nuclear aerosols after 24 hours by using benchmark C3.

**BENCHMARK C4: LINEAR COAGULATION KERNEL AND CONSTANT DEPOSITION RATE OF PARTICLES**

GDE was solved in a particular case: linear coagulation kernel \( K(u, v) = K(u + v) \) and constant deposition rate of particles \( \mathcal{R}(v, t) = \mathcal{R} \) by Williams and Loyalka as referred to in reference 1. Ramabhadran and Perterson have found the analytical solution of equation (4.8) for the case of a linear
coagulation kernel and constant deposition rate based on the exponential initial distribution. Their analytical solution can be written as

\[
\eta(v, t) = \frac{N_0 T \exp \left[ \frac{1-1}{\theta} \right]}{\theta \tilde{v}} \exp \left[ \frac{(1 + \theta) \nu}{v_m0} \right] \left[ \frac{2 \tilde{g}^2 \nu}{v_m0} \right]^t,
\]

Where \( \theta = \frac{R}{v_m0} \), \( \tau = N_0 v_m0 K t \), \( T = \exp[1 - \tau \theta] \) and \( g = 1 - \exp \left[ \frac{1-1}{\theta} \right] \).}

**BEHAVIOR OF THE NUMBER OF AEROSOL PARTICLES**

Figure (19) shows the value of the error for the aerosol number between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 (10^{14}, 10^{13} \text{ and } 10^{12} \text{ particle / m}^3) \) at linear coagulation kernel and constant deposition rate coagulation alone and divided aerosol particle range into 400 sections.

Figure (20) shows the error value for the number of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C4.

Figure (19) shows the value of the error for the aerosol number between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 (10^{14}, 10^{13} \text{ and } 10^{12} \text{ particle / m}^3) \) at linear coagulation kernel and constant deposition rate coagulation alone and divided aerosol particle range into 400 sections.

The number of nuclear aerosols to be finished and the results show that the total number of nuclear aerosols after 24 hours is equal to 150 particle /m³ in the case \( N_0 = 10^{12} \text{ particle / m}^3 \), as evident in Figure (21C).

Figure (20) shows the error value for the number of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using linear coagulation kernel and constant deposition rate.
BEHAVIOR OF THE VOLUME OF AEROSOL PARTICLES

Different volumes of aerosols in nuclear reactor in this case take the same behavior, because of the aerosol deposition rate fixed, as evident in Figure (22). Figure (22) shows the value of the error for the aerosol volume between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 \) (\( 10^{14}, 10^{13} \) and \( 10^{12} \) particle/m³) at linear coagulation kernel and constant deposition rate and divided aerosol particle range into 400 sections. The error value for the aerosol volume between numerical and analytical solutions to equal, although there is disagreement values the initial total number distribution, because different volumes of aerosols take the same behavior. Figures (24A), (24B) and (24C) show that the volume of nuclear aerosol in a decrease with linear coagulation kernel and constant deposition rate after 2, 12 and 24 hours respectively. Figure (23) shows the value of the error for the aerosol volume between numerical and analytical solutions by using different divisions of the aerosol range within 24 hours.

Fig. (21A): the number of nuclear aerosols after 2 hours by using benchmark C4.

Fig. (21B): the number of nuclear aerosols after 12 hours by using benchmark C4.

Fig. (21C): the number of nuclear aerosols after 24 hours by using benchmark C4.

Fig. (22): the value of the error for the aerosol volume between numerical and analytical solutions within 24 hours and the effect of different values of initial total number distribution of real particles \( N_0 \) (\( 10^{14}, 10^{13} \) and \( 10^{12} \) particle/m³) at linear coagulation kernel and constant deposition rate and divided aerosol particle range into 400 sections.

Fig. (23): the error value for the volume of nuclear aerosol for the different divisions using the whole field of aerosol through 24 hours, by using benchmark C4.
The purpose of this research had been to overcome the limitations of and eliminate use of assumptions made in the present-day computer programs and eventually develop a production computer program to predict and evaluate the dynamics and behavior of aerosols without compromising the physics of collisions. We have investigated overall aspects relating to methods and approximations inherent in modeling of aerosol dynamics and evolution. We have considered benchmark problems, use and construction of better rate process models, and implications of spatial homogenization of aerosol distributions.

The sectional method of solving the aerosol dynamic equation was tested for various benchmark problems for which it is possible to compare the numerical results against the corresponding analytical results. Various benchmark problems are considered and the simulation results are compared to the corresponding analytical results to assess the accuracy of the sectional technique through the study of the effect of different values for initial total number distribution $N_0$ and the effect of the different divisions of the aerosol range for the number and volume of nuclear aerosol in reactor containment in each benchmark. Results of chapter IV have led to the following observations:

1. A comparison on numerical results against the analytical results showed that numerical results were in excellent agreement with the analytical results, for all the benchmark problems involving aerosol coagulation and deposition processes.
2. The numerical results compared well (maximum error $10^{-3}$ %) with the analytical results for pure coagulation problems employing either a constant kernel or a linear kernel. For simultaneous coagulation and deposition problems, the numerical results were also quite acceptable (maximum error $10^{-6}$ %).
3. The numerical errors are negligible for deposition cases (benchmarks C3 and C4).
4. We find that the value of the error resulting from the divisions 200 and 400 sections is much lower than the error resulting from the divisions 50 and 100 sections.

Overall, the accuracy of the sectional technique is within an acceptable range for coagulation and deposition problems. Sectional method is complex and efficient. The effect of the spatial inhomogeneity can be substantial on source term estimation depending on conditions in the aerosol system, and hence the "well-mixed" assumption needs further research and clarification.
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