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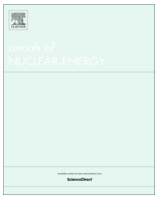

Benchmark problems in aerosol evolution: Comparison of some exact and DSMC results

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ABSTRACT

Aerosols are generated in many normal or accident situations associated with the nuclear enterprise. For a good understanding and modeling of the nuclear source term, for example, good experimental data and computational programs relating to aerosol evolution are needed. In the past several years there has been an effort to explore use of the Direct Simulation Monte Carlo (DSMC) approach for such estimations to improve fidelity of computations to the actual physics and chemistry of the accidents. An integral part of these efforts has been verification and validation of the DSMC technique against other available results wherever possible. This paper explores verification of DSMC against one existing and two new benchmark problems covering condensation, coagulation, deposition and two-component aerosols. The simulations compare well with the exact results, providing further confidence in the use of DSMC.

1. Introduction

Aerosols are generated in many normal or accident situations associated with the nuclear enterprise. In particular, for a good understanding and modeling of the nuclear source term, good experimental data and computational programs relating to aerosol evolution are needed. The fundamental aerosol science and computational models and practices have been discussed in the nuclear literature in the past (Sher and Hobbins, 2011; Williams and Loyalka, 1991), and continual progress is being made in both acquisition of new data and computational tools. While the source term computer programs rely on deterministic methods for estimation of aerosol evolution, in the past several years there has been an effort to explore use of the Direct Simulation Monte Carlo (DSMC) approach for such estimations to improve fidelity of computations to the actual physics and chemistry of the accidents (Campbell and Loyalka, 2015; Campbell et al., 2016; Loyalka, 2003; Palaniswaamy and Loyalka, 2007a, b, 2008; Palsmeier and Loyalka, 2013; Rangaraj and Loyalka, 2004). An integral part of these efforts has been verification and validation of DSMC against other available results wherever possible. We should note that in addition to the above work on nuclear aerosols, some other authors have also explored applications of DSMC or related Monte Carlo methods to model aerosol evolution in other areas (Efendiev and Zachariah, 2002; Liu et al., 2017; Smith et al., 1999; Sun et al., 2004; Wei, 2013).

The aerosol evolution equation itself is a nonlinear, integro-differential equation of considerable complexity (Williams and Loyalka, 1991). Assuming aerosols of multiple species (N) are well-mixed, a general form of this equation is:

$$\begin{aligned}&\frac{\partial}{\partial t}n(\boldsymbol{v},\boldsymbol{m},t)+R(\boldsymbol{v},\boldsymbol{m},t)n(\boldsymbol{v},\boldsymbol{m},t)+\sum_{p=1}^{N}\frac{\partial}{\partial v_p}[I_p(\boldsymbol{v},\boldsymbol{m},t)n(\boldsymbol{v},\boldsymbol{m},t)]\\&=\frac{1}{2}\int_0^\infty d\boldsymbol{u}\int_0^\infty d\boldsymbol{w}\int_0^\infty d\boldsymbol{q}\int_0^\infty d\boldsymbol{s}\;n(\boldsymbol{u},\boldsymbol{q},t)n(\boldsymbol{w},\boldsymbol{s},t)K(u,q|w,s)\\&\quad\prod_{p=1}^{N}\delta(v_p-u_p-w_p)\delta(m_p-q_p-s_p)\\&-n(\boldsymbol{v},\boldsymbol{m},t)\int_0^\infty d\boldsymbol{u}\int_0^\infty d\boldsymbol{q}\,K(u,q|v,m)n(\boldsymbol{u},\boldsymbol{q},t)+S(\boldsymbol{v},\boldsymbol{m},t)\end{aligned}\tag{1}$$

where $n(\boldsymbol{v},\boldsymbol{m},t)=n(v_1,v_2,\ldots,v_N;m_1,m_2,\ldots,m_N,t)$ is the aerosol distribution function as dependent on time, species volume and mass. One desires a solution of this equation subject to a prescribed initial condition $n(\boldsymbol{v},\boldsymbol{m},0)$ and the models for the rates $R(\boldsymbol{v},\boldsymbol{m},t)$,

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$I(\boldsymbol{v}, \boldsymbol{m}, t)$ and $K(u, q|w, s)$ for deposition, condensation and coagulation, respectively, and the source term $S(\boldsymbol{v}, \boldsymbol{m}, t)$.

It is our purpose here to report on some additional benchmarks of DSMC against some exact analytical solutions. We have used one problem and its analytical result that is already available, and have also obtained new analytical results for two additional problems that enlarge the number of exact problems available covering mixed aerosols, condensation, and deposition. We have of course used simplified rate processes and initial conditions as the analytical results can be obtained only for specialized cases. Nevertheless, these cases present significant tests for DSMC, or any other computational process. We believe the availability of these new analytical solutions will also aid in further benchmarking of all aerosol computational techniques, and that the work reported here will be of wider significance than the benchmarking of DSMC alone.

2. Problems

2.1. Benchmark 1: Single species with constant coagulation, condensation, and deposition rates

This problem is an extension of Ramabhadran et al. (1976) for a single component aerosol with constant coagulation and condensation rates. We have included a constant deposition rate.

2.2. Benchmark 2: Two species with constant coagulation and condensation rates

This problem is for a two-component aerosol with constant coagulation and condensation rates. Its formulation and solution were given by Gelbard and Seinfeld (1978), and these are described also in Williams and Loyalka (1991).

2.3. Benchmark 3: Two species with constant coagulation and deposition rates

This problem is a variation on 2.2 above for a two-component aerosol with constant coagulation and deposition rates, but condensation is not included.

All of the above cases use Laplace transforms (on size or mass) and methods of characteristics to solve the resulting partial differential equations for the transforms. Analytic inversion of the Laplace transforms is possible for some specific initial conditions only. We describe the problems and their solution briefly.

3. Analytical solutions

3.1. Benchmark 1: Single species with constant coagulation, condensation, and deposition rates

For a single species, with no source, and taking, $K(u, v) = K_0$ (coagulation) and $R(v, t) = R_0$ (deposition) as constants, and $I(v, t) = \sigma_1 v$ (condensation) with σ_1 a constant, Eq. (1) becomes:

$$\frac{\partial}{\partial t} n(v,t) = -\sigma_1 \frac{\partial}{\partial v}(v\, n(v,t)) + \frac{1}{2} K_0 \int_0^v n(v-u,t) n(u,t) du - K_0 n(v,t) \int_0^\infty n(u,t) du - R_0\, n(v,t) \tag{2}$$

We also assume an initial condition:

$$n(v,0) = \frac{N_0}{v_0} exp\left[-\frac{v}{v_0}\right] \tag{3}$$

where N_0 is the total number of particles at time $t = 0$ s.

To construct the analytical solution, we define:

$$N(t) = \int_0^\infty n(v,t) dv \tag{4}$$

Integrating Eq. (2) on v from 0 to ∞, using the convolution theorem, and using definition (4) we obtain:

$$\frac{d}{dt} N(t) = -\frac{1}{2} K_0 N^2(t) - R_0 N(t) \tag{5}$$

which has the solution:

$$N(t) = \frac{2N_0 R_0}{-N_0 K_0 + \exp(R_0 t)(2R_0 + N_0 K_0)} \tag{6}$$

Taking the Laplace transform of equation (2) and the initial condition (3) on v, and using the above result, we obtain the partial differential equation and the initial condition:

$$\frac{\partial}{\partial t} \bar{n}(s,t) = \sigma_1 s \frac{\partial}{\partial s}(\bar{n}(s,t)) + \frac{K_0}{2} \bar{n}^2(s,t) - K_0 \bar{n}(s,t) \frac{2N_0 R_0 K_0 \bar{n}(s,t)}{-N_0 K_0 + \exp(R_0 t)(2R_0 + N_0 K_0)} - R_0 \bar{n}(s,t) \tag{7}$$

$$\bar{n}(s,0) = N_0 / \left(\left(s + \frac{1}{v_0} \right) v_0 \right) \tag{8}$$

The method of characteristics (we used Mathematica's DSolve program, and some algebraic manipulations) now gives,

$$\bar{n}(s,t) = \frac{4N_0 R_0^2 (s e^{\sigma_1 t})^{R_0/\sigma_1}}{(e^{R_0 t}(2R_0 + N_0 K_0) - N_0 K_0)\left(v_0 e^{\sigma_1 t} s^{\frac{R_0+\sigma_1}{\sigma_1}} (e^{R_0 t}(2R_0 + N_0 K_0) - N_0 K_0) + 2R_0 (s e^{\sigma_1 t})^{R_0/\sigma_1} \right)} \tag{9}$$

Taking the inverse Laplace transform (we again used Mathematica and some algebraic manipulations), we get:

Table 1

Summary of aerosol evolution equations with their respective initial conditions and exact solutions for single-component aerosols (Benchmark 1).

Equation to Solve	$\frac{\partial}{\partial t} n(v,t) = -\sigma_1 \frac{\partial}{\partial v}\ (v1n(v,t)) + \frac{1}{2} K_0 \int_0^v n(v-u,t)\, n(u,t) du - K_0 n(v,t) \int_0^\infty n(u,t) du - R_0\, n(v,t)$
Initial Condition	$n(v,0) = \frac{N_0}{v_0} exp[-\frac{v}{v_0}]$
Exact Solution	$n(v,t) = 4N_0 R_0^2 \frac{\exp(-\sigma_1 t - \xi) \exp(\sigma_1 t)^{R_0/\sigma_1}}{v_0 (N_0 K_0 - \exp(R_0 t)(2R_0 + N_0 K_0))^2}$ where : $\xi = \frac{2R_0\, v \exp(\sigma_1 t)^{-1+\frac{R_0}{\sigma_1}}}{v_0(-N_0 K_0 + \exp(R_0 t)(2R_0 + N_0 K_0))}$