

Modeling source strength modification due to coagulation in a diffusing aerosol puff

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The particles released into the atmosphere from combustion and explosive sources are concentrated at the release point ($>10^6$ - 10^7 particles/cc) with sizes predominantly less than 50 nm. The concentration decreases rapidly due to the combined effect of coagulation and dispersion as the plume spreads and becomes a part of the background aerosol. It is important to estimate the fraction of the emitted particles surviving coagulation along with the modification in the size spectra, by the time they are completely dispersed in the atmosphere. Although realistic situation can only be addressed after due considerations are given to the details of meteorology and source characteristics, model studies will be useful in understanding the relative importance of coagulation vis-à-vis dispersion in governing survival fraction (Turco & Yu, 1997). To this end, we have examined coagulation-diffusion problems from an analytical and numerical framework.

In a recent study (Anand & Mayya, 2009), we employed Jaffe approximation technique, borrowed from ion-recombination theory, to obtain approximate analytical solutions to coagulation-diffusion equation. If N_a particles are emitted from a Gaussian puff of radius of gyration R_g , and if K is the mean coagulation coefficient of particles and D is diffusion coefficient in the atmosphere, then the fraction of particles surviving coagulation as the puff completely disperses may be shown to be

$$F_\infty = (1+A)^{-1} \quad (1)$$

$$A = 3^{1/2} KN_a / (16 (\pi)^{3/2} R_g D).$$

While this formula captures the qualitative features of the processes, it under-predicts the survival fraction as compared to that obtained by accurate numerical computations. This calls for seeking more accurate approximations. For this we have now developed what may be called as beyond-Jaffe approximation. The Jaffe technique assumes the validity of diffusion laws for the spatial dispersion of the puff. In the beyond Jaffe approximation, allowance is made for a non-diffusive evolution of spatial variance due to coagulation. We illustrate the technique for the decay of the total number concentration $N(r,t)$ in a spherically symmetric puff for constant diffusion coefficient and coagulation kernel. The equation is

$$\frac{\partial N(r,t)}{\partial t} = D \nabla^2 N(r,t) - \frac{1}{2} K [N(r,t)]^2 \quad (2)$$

Given an initial Gaussian puff, we assume the following functional form for its evolution:

$$N(r,t) = \frac{N_a}{\pi^{3/2} \xi(t)^{3/2}} \exp(-r^2 / \xi(t)) F(t) \quad (3)$$

where, $\xi(t)$ (measure of variance) and $F(t)$ (survival fraction) are yet to be determined. Upon taking spatial moments of Eq.(2), we obtain coupled equations for $\xi(t)$ and $F(t)$, which may be exactly solved in the limit, $t \rightarrow \infty$, to yield

$$F_\infty = \left(1 + \frac{5A}{4}\right)^{-4/5} \quad (4)$$

For small A , Eq.(4) approaches Eq.(1). As the parameter A increases, the two equations differ noticeably. In figure 1, we have compared the two solutions with numerical solutions of Eq.(2) obtained using Mathematica (Wolfram, 2005). As may be seen the “beyond Jaffe approximation” is quite close to the accurate solutions even for very large values of A .

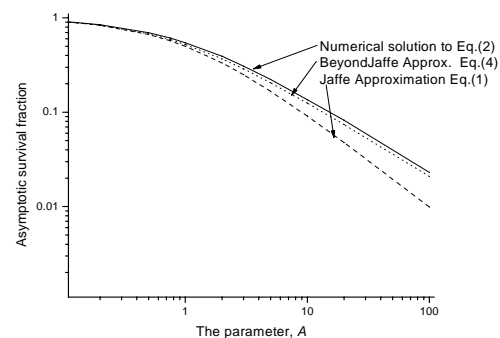


Figure 1: Variation of survival fraction with A .

The approach proposed may be extended for estimating modification of the size spectra during dispersion. It is also possible to include homogeneous non-constant kernels and space and time dependent diffusion coefficients. From a practical point of view, the A value will be low (~ 0.1) for dilute puffs in highly dispersive atmospheres and can be large (1-10) for dense puffs in calm atmospheres such as those arising from intense fireworks in festive seasons. In general, the formulae can be viewed as environmental source modifiers for particle releases from localized sources.

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