The analytical description of the dynamics of the impurity redistribution in the composite particles by coagulation

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The description of the composite particles formation consisting of mixture of different materials is important for many practical problems, such as the analysis of accidental releases in atmosphere, the description of multiphase processes in chemical reactors and others. The programs developed for the numerical simulation of these processes require optimization of computational methods and verification. For these purposes it is convenient to use the solutions of the kinetics equations for composite particles in concise form (impurity integrated) (Piskunov, 2013). This report focuses on the new results on the development of this approach.

Statement of the problem. The complete kinetic equation for two-component system has the form (Lushnikov, 1976; Piskunov, 2013):

$$\frac{\partial C}{\partial t}=\frac{1}{2}\int_0^g\int_0^\alpha K(g-s,\alpha-\beta;s,\beta)C(g-s,\alpha-\beta)C(s,\beta)ds\,d\beta$$

$$-C(g,\alpha)\int_0^\infty\int_0^\infty K(g,\alpha;s,\beta)C(s,\beta)ds\,d\beta \equiv S\left(C,g,\alpha,t\right) \qquad (1)$$

where $C(g,\alpha,t)$ is the concentration of particles containing at time t the total mass g and the impurity mass α, $K(g,\alpha;s,\beta)$ are coagulation coefficients.

In the concise description the one component (impurity) is taken integrally by using the zero $n(g,t)$ and the first $m(g,t)$ moments of entire spectrum (Simons, 1981; Piskunov et al., 1997):

$$n(g,t)=\int_0^\infty C(g,\alpha,t)d\alpha\,; \quad m(g,t)=\int_0^\infty \alpha C(g,\alpha,t)d\alpha \qquad (2)$$

The ratio $m(g,t)/gn(g,t)$ determines the average impurity mass in a particle. In the concise description the equation (1) is replaced by the following chain of equations:

$$\partial_t n=\frac{1}{2}\int_0^g K(g-s,s)n(g-s)n(s)ds-n(g)\int_0^\infty K(g,s)n(s)ds\,, \qquad (3)$$

$$\partial_t m=\int_0^g K(g-s,s)n(g-s)m(s)ds-m(g)\int_0^\infty K(g,s)n(s)ds\,. \qquad (4)$$

Analytical solutions. The general analytical solution of the kinetic equation (1) for the additive kernel $K(g_1,g_2) = K_0(g_1+g_2) = K_0(x_1+y_1+x_2+y_2)$ (where x and y are the mass of the individual components, and $g=x+y$) was obtained by Fernandez-Diaz and Gomez-Garcia (2007). In the case of the exponential initial distribution

$$C(x,y,t=0)=ab\mathrm{e}^{-ax-by}=ab\theta(g-\alpha)\mathrm{e}^{-ag-(b-a)\alpha}=C_0(g,\alpha) \qquad (5)$$

(a, b are parameters; $\theta(g)$=0, if g<0 and $\theta(g)$=1, if g>0, and $\alpha = y$) this solution is:

$$C(g,\alpha,\tau)=\theta(g-\alpha)ab(1-\tau)\mathrm{e}^{-\left(a+\frac{ab\tau}{a+b}\right)g-(b-a)\alpha}\sum_{k=0}^{\infty}\frac{\left(\dfrac{a^2b^2\tau g\alpha(g-\alpha)}{a+b}\right)^k}{(k+1)!(k!)^2} \qquad (6)$$

where $\tau=1-\exp\left(-(a+b)K_0t/ab\right)$ is the dimensionless time. Integrating the solution (5) we find the expressions for the values $n(g,t)$ and $m(g,t)$ that can also be obtained by solving the system of equations (3-4):

$$n=\frac{1-\tau}{g\sqrt{\tau}}\mathrm{e}^{-ag(1+\tau)}I_1(2ga\sqrt{\tau})\,;\; m=\frac{a(1-\tau)}{b-a}\mathrm{e}^{-ag(1+\tau)}I_0(2ga\sqrt{\tau})\,, \qquad (7)$$

where I_0 and I_1 are the modified Bessel functions of the first kind.

Relaxation to the uniform distribution. The dynamics of the impurity redistribution in the composite particles with time is important for practical problems. In (Piskunov, 2013) a large number of analytical solutions were obtained for the initial particle spectra in which the relative mass of the impurity is uniformly distributed by size. The general results of the stability of the uniform distribution of the impurity were formulated and were proved. In the case of the non-uniform initial distribution of impurity we express its mass concentration $m_1(g,t)$ through the mass concentration for uniform distribution $m_0(g,t)= gn_0(g,t)$ and we introduce the quantity $\eta(g,t)$ that takes into account the difference between the two cases:

$$m_1(g,t)=m_0(g,t)\left[1+\eta(g,t)\right] \qquad (8)$$

Substituting this expression into equation (4) and using (3) in the case of the constant kernel $K(x,y) = K_0$ and the exponential distribution $n_0(g,t)=(N^2/M)\mathrm{e}^{-gN/M}$ (where $N = N_0/(1+K_0N_0t/2)$ and M are total number and mass concentrations) we obtain the solution for $\eta(g,t)$:

$$\eta(g,\tau)=\eta_0(g)\exp(-N_0\tau g/M)+$$
$$+\frac{N_0\tau g}{M}\int_0^1 y\eta_0(gy)\mathrm{e}^{-\frac{N_0\tau g}{M}y}\left(2+\frac{N_0\tau g}{M}(1-y)\right)dy, \qquad (9)$$

where $\tau=1-N/N_0$ is the dimensionless time. This solution allows to define the asymptotic behavior for $\eta(g,t)$. For example, for $\eta_0(g) = A\mathrm{e}^{ag}$ with parameters A, a (a<N_0/M) we obtain that at $g\to\infty$ and $t\to\infty$:

$$\eta(g,\tau)\approx A/\left(1-aM/N_0\right)^2=\text{const}\,, \qquad (10)$$

i.e. the non-uniform initial distribution of impurity at large times becomes the uniform one for a large part of the spectrum of composite particles (except for the small g). Moreover, the relaxation time coincides with the coagulation time.

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