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Non-local model of aggregation in uniform polydispersed systems

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Aggregation and fragmentation of particles forming a disperse phase in multiphase flows play a great role in different chemical technological processes. Mass transfer processes in multiphase flows can be also accompanied by uninterrupted producing the new disperse phase induced by insoluble products of chemical reactions.
However, the well-known models don't allow describing the time non-locality of aggregation processes. The aim of our paper is to submit the relevant non-local modification of the Smoluchowski equation of binary aggregation. The model is constructed by the approach based on the relaxation transfer kernels theory.

1. Theoretical details

Aggregation of particles forming a dispersed phase in multiphase flows plays a great role in different chemical technological processes, metallurgy and nature phenomena. However, despite the fact that these processes are widely distributed in chemical technology and there are many approaches to their modeling, the authenticity methodology for modeling reactors in which these phenomena can be observed is weakly developed up to day.
For describing the evolution of the *i*-mers concentration in the apparatus we can use various modifications of Smoluchowski or Becker-Döring equations expanded by terms which correspond to the source of mass.
If there is not the fragmentation in the system then the well-known Becker-Döring equation transforms to the Smoluchowski equation adapted for binary coagulation (J.A.D. Wattis, 2006 and A.A. Lushnikov, 2006):

$$\frac{\partial C_i}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} \Phi_{i-j,j} C_{i-j} C_j - C_i \sum_{j=1}^{\infty} \Phi_{i,j} C_j \,, \tag{1}$$

where C_i is the concentration of the i-mers and $\Phi_{i,j}$ is the element of an aggregation matrix.
However, the important aspect of modeling aggregation processes leaves to be none elaborated at present. The question is how to allow for a non-location of an aggregation

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process. Indeed, without allowing for this aspect it is impossible to describe the influence of characteristic times of aggregates formation on the process kinetics (V.M. Voloschuk, Y.S. Sedunov, 1975).

This paper deals with the non-local model based on the Smoluchowski equation. The model is constructed by the approach developed in our previous works (Brener A.M., 2006). According to this approach the time non-locality can be described by the model of relaxation transfer kernels. In our case the characteristic times $\tau_{i,j}$ of the aggregation of i and $j-$mers play a role of relaxation times.

Thus we submit the following non-local modification of the Smoluchowski equations for aggregation in the polydispersed system:

$$\frac{\partial C_i}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} \int dt_1 \Phi_{i-j,j}(t,t_1) C_{i-j}(t_1) C_j(t_1) - \\ - \sum_{j=1}^{\infty} \int dt_1 \Phi_{i,j}(t,t_1) C_i(t_1) C_j(t_1) \quad . \tag{2}$$

Equations for elements of the aggregation matrix read (Brener A.M., 2006)

$$\frac{\partial}{\partial t}\Phi_{i,j} + \frac{\Phi_{i,j}}{\tau_{i,j}} f^0_{i,j} = 0 \, . \tag{3}$$

Time-derivatives of the integral terms are

$$\frac{\partial}{\partial t}\int dt_1 \Phi_{i,j} C_i(t_1) C_j(t_1) = \Phi^0_{i,j} C_i(t) C_j(t) - \\ - \frac{f^0_{i,j}}{\tau_{i,j}} \Phi^0_{i,j} \int_0^t dt_1 C_i(t_1) C_j(t_1) \exp\left(- \frac{f^0_{i,j}}{\tau_{i,j}} (t - t_1) \right) . \tag{4}$$

Thus, the system of kinetic equations looks as follows

$$\frac{\partial C_i}{\partial t} = \frac{1}{2}\sum_{j=1}^{i-1} \int dt_1 \Phi^0_{i-j,j} \exp\left(- \frac{f^0_{i-j,j}}{\tau_{i-j,j}} (t - t_1) \right) C_{i-j}(t_1) C_j(t_1) - \\ \sum_{j=1}^{\infty} \int dt_1 \Phi^0_{i,j} \exp\left(- \frac{f^0_{i,j}}{\tau_{i,j}} (t - t_1) \right) C_i(t_1) C_j(t_1) \tag{5}$$

By time-differentiating we obtain

$$\frac{d^2C_i}{dt^2} = \frac{1}{2}\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) - \sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t) -$$
$$-\frac{1}{2}\sum_{j=1}^{i-1}\frac{f^0_{i-j,j}}{\tau_{i-j,j}}\int dt_1\Phi^0_{i-j,j}\exp\left(-\frac{f^0_{i-j,j}}{\tau_{i-j,j}}(t-t_1)\right)C_{i-j}(t_1)C_j(t_1) + \quad (6)$$
$$+\sum_{j=1}^{\infty}\frac{f^0_{i,j}}{\tau_{i,j}}\int dt_1\Phi^0_{i,j}\exp\left(-\frac{f^0_{i,j}}{\tau_{i,j}}(t-t_1)\right)C_i(t_1)C_j(t_1)$$

A rearrangement of the equation (6) by way of separate averaging over two groups of indices corresponding to appearance and disappearance of i -mers gives

$$\frac{d^2C_i}{dt^2} = \frac{1}{2}\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) - \sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t) -$$
$$-\frac{1}{2}B_1\sum_{j=1}^{i-1}\int dt_1\Phi^0_{i-j,j}\exp\left(-\frac{f^0_{i-j,j}}{\tau_{i-j,j}}(t-t_1)\right)C_{i-j}(t_1)C_j(t_1) + \quad (7)$$
$$+B_2\sum_{j=1}^{\infty}\int dt_1\Phi^0_{i,j}\exp\left(-\frac{f^0_{i,j}}{\tau_{i,j}}(t-t_1)\right)C_i(t_1)C_j(t_1)$$

The next time-derivatives give

$$\frac{d^3C_i}{dt^3} = \frac{d}{dt}\left(\frac{1}{2}\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) - \sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t)\right) -$$
$$-\frac{1}{2}\sum_{j=1}^{i-1}\frac{f^0_{i-j,j}}{\tau_{i-j,j}}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) +$$
$$+\frac{1}{2}\sum_{j=1}^{i-1}\left(\frac{f^0_{i-j,j}}{\tau_{i-j,j}}\right)^2\int dt_1\Phi^0_{i-j,j}\exp\left(-\frac{f^0_{i-j,j}}{\tau_{i-j,j}}(t-t_1)\right)C_{i-j}(t_1)C_j(t_1) + \quad (8)$$
$$+\sum_{j=1}^{\infty}\frac{f^0_{i,j}}{\tau_{i,j}}\Phi^0_{i,j}C_i(t)C_j(t) -$$
$$-\sum_{j=1}^{\infty}\left(\frac{f^0_{i,j}}{\tau_{i,j}}\right)^2\int dt_1\Phi^0_{i,j}\exp\left(-\frac{f^0_{i,j}}{\tau_{i,j}}(t-t_1)\right)C_i(t_1)C_j(t_1)$$

And the new rearrangement which is analogous to that we use for deriving (7) leads to the following equations

$$\frac{d^3C_i}{dt^3} = \frac{d}{dt}\left(\frac{1}{2}\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) - \sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t)\right) -$$
$$-\frac{1}{2}A_1\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) +$$
$$+\frac{1}{2}B_1^2\sum_{j=1}^{i-1}\int dt_1\Phi^0_{i-j,j}\exp\left(-\frac{f^0_{i-j,j}}{\tau_{i-j,j}}(t-t_1)\right)C_{i-j}(t_1)C_j(t_1) + \quad (9)$$
$$+A_2\sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t) -$$
$$-B_2^2\sum_{j=1}^{\infty}\int dt_1\Phi^0_{i,j}\exp\left(-\frac{f^0_{i,j}}{\tau_{i,j}}(t-t_1)\right)C_i(t_1)C_j(t_1)$$

Using expressions (7) and (9) we can obtain the following system of kinetic equations

$$\frac{d^3C_i}{dt^3} + (B_1+B_2)\frac{d^2C_i}{dt^2} + B_1B_2\frac{dC_i}{dt} =$$
$$= (B_1+B_2+\frac{d}{dt})(\frac{1}{2}\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) - \sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t)) - \quad (10)$$
$$-\frac{1}{2}A_1\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) + A_2\sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t)$$

At the zero approximation when we assume that relaxation times are independent on $i-$mers orders we can obtain the equation

$$\frac{d^2C_i}{dt^2} + \frac{f^0}{\tau}\frac{dC_i}{dt} = \frac{1}{2}\sum_{j=1}^{i-1}\Phi^0_{i-j,j}C_{i-j}(t)C_j(t) - \sum_{j=1}^{\infty}\Phi^0_{i,j}C_i(t)C_j(t). \quad (11)$$

The main peculiarity of the submitted equations is presence of solutions describing perturbations propagating with finite velocities.

Further we consider only high rate aggregation process supposing the relaxation times are sufficiently small as compared with the characteristic process time. We suppose also that coefficient at the first time-derivative and elements of the aggregation matrix have the same order. It seems that such an assumption is acceptable for practical use.

Using this approach we introduce the small parameter ε as follows

$$\varepsilon = \tau / f_0 . \quad (12)$$

Adhering to the known scheme, we can look for i -mers concentrations in form of

$$C_i = C_i^{(0)} + \varepsilon C_i^{(1)} + \varepsilon^2 C_i^{(2)} + \ldots \tag{13}$$

Using the multi-scale coordinates

$$\xi = \frac{t}{\varepsilon}, T = t, \tag{14}$$

and substituting expression (13) into equation (11) we get the following equations for the approximations of zero and first orders

$$\frac{\partial^2 C_i^{(0)}}{\partial \xi^2} + \frac{\partial C_i^{(0)}}{\partial \xi} = 0, \tag{15}$$

$$\frac{\partial^2 C_i^{(1)}}{\partial \xi^2} + \frac{\partial C_i^{(1)}}{\partial \xi} = -2\frac{\partial^2 C_i^{(0)}}{\partial \xi \partial T} - \frac{\partial C_i^{(0)}}{\partial T} + \frac{1}{2}\sum_{j=1}^{i-1} \Phi_{i-j,j}^0 C_{i-j}^{(0)} C_j^{(0)} - \\ - \sum_{j=1}^{\infty} \Phi_{i,j}^0 C_i^{(0)} C_j^{(0)} \tag{16}$$

The system of (15), (16) as well as equations for next orders can be investigated by methods of the secular perturbation theory (Dodd, R.K., Eilbeck, J.C., Gibbon, J.D., Morris, H.C., 1984) or by numerical experiment.
Under the numerical experiment we use the following form of the aggregation matrix:

$$a_{i,j} \approx \frac{k}{(i+j)^{\beta}} + c_2 \left(\frac{i-j}{i+j}\right)^2, \tag{17}$$

where parameters k, c_2 and β will be dependent on system physical properties (Brener A.M., Balabekov B.Ch., Golubev V.G., Bekaulova A.A., 2008).

2. Results and Discussion

Figure 1 depicts some results of the numerical experiment. The continuous curves show the time history of the concentrations of i-mers according to the local Smoluchowski equations, and the dotted curves show the time history of i-mers concentrations according to the submitted non-local model. Number of the curve corresponds to the i-mer order, i.e. it denotes “i”. At the moment $t = 0$ we suppose $C_i = 0$ for $i > 1$. Although we didn’t observe a qualitative distinction for the behavior of curves but rates of aggregation processes at the initial period were essentially different. The concentration of i-mers of orders close to 2 passes through the maximum, and the points of maximum in calculations with allowing for the relaxation times are displaced to latest moments. Investigations should be continued for various aggregation matrices.

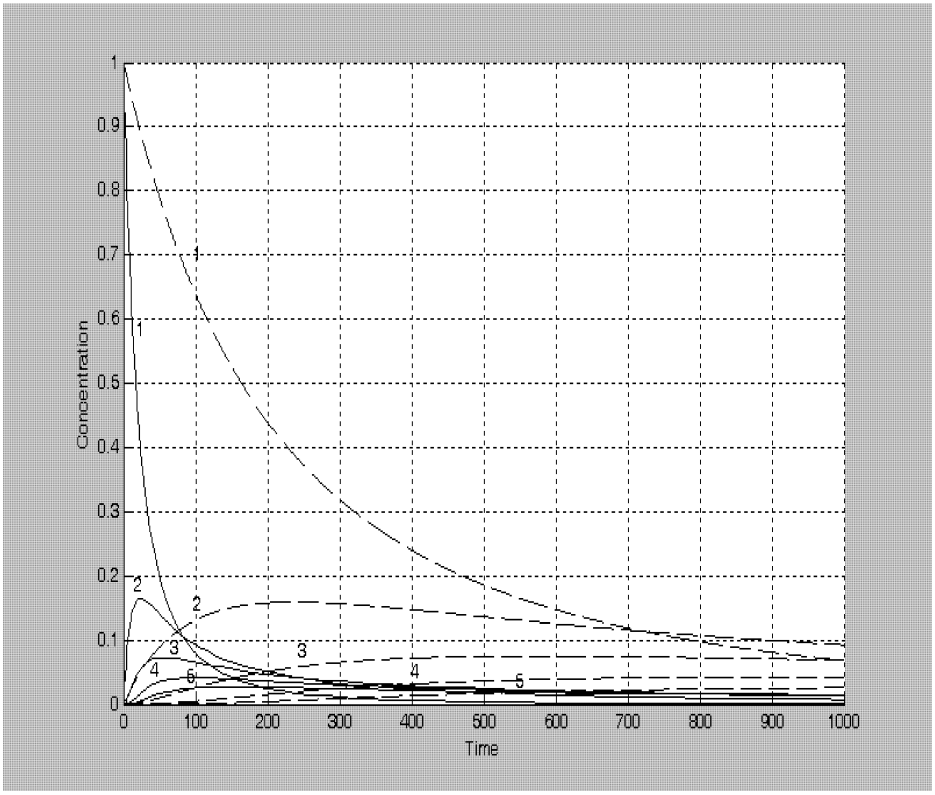

Figure1- Time history of i-mers concentrations according to the local (continuous curves) and non-local (dotted curves) models.

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