# REPORTS OF THE NATIONAL ACADEMY OF SCIENCES OF THE REPUBLIC OF KAZAKHSTAN 

ISSN 2224-5227
Volume 3, Number 307 (2016), 78 - 86

# МЕТОД РЕЛАКСАЦИОННЫХ ЯДЕР В МАТЕМАТИЧЕСКОЙ МОДЕЛИ ПРОЦЕССОВ ПЕРЕНОСА И АГРЕГАЦИИ 

А.С. Муратов, А.М. Бренер, Л. Ташимов<br>Южно-Казахстанский государственный университет, Шымкент, Казахстан<br>Amb 52@mail.ru. brener@fromru.com asm 59@mail.ru


#### Abstract

Аннотация. В статье дан оббзорный анализ математических моделей для описания тепло- и массопереноса и агрегационных процессов с помощью метода релаксационных ядер переноса, который открывает новые возможности для детального изучения влияния иерархии времен релаксации на интенсивность высокоскоростных и нано-масштабных технологических процессов.

Ключевые слова: массо- и теплоперенос, времена релаксации, релаксационные ядра, перекрестные эффекты, агрегация.


# THE RELAXATION KERNELS APPROACH TO MATHEMATICAL MODELS OF TRANSFER AND AGGREGATION PROCESSES 

A.S. Muratov, A. M. Brener, L. Tashimov<br>South Kazakhstan State University, 5, Tauke Khan, Shymkent, 160012, Kazakhstan

Key words: Mass and Heat Transfer; Relaxation times; Relaxation kernels; Cross effects; Aggregation.
Abstract. The paper deals with mathematical models describing heat and mass transfer and aggregation processes with the help of relaxation transfer kernels approach, which opens up fresh opportunities for detailed study of influence of relaxation times hierarchy on the intensity of high rate and nano-scale technological processes.

## 1. Introduction

Consideration of relaxation times and long-range interaction of structural components of a medium is a great practical and theoretical problem [1-3] that is relevant in cases of high rate or nano-scale technological processes. The operation cycle of these processes is short, and the entire process may go on under the transient regime. In this connection, resources of effective controlling such processes are limited, and it is important to calculate correctly and select the best values of governing parameters.

Problems of modeling both high rate and nano-scale processes are in touch with construction of equations with retarded or divergent arguments that reflects the actual mechanism of transfer phenomena in the medium modeled as a system of interacting oscillators with a set of partial frequencies and interaction potentials [2,3].

At the same time, though realization of that investigation program is very tempting, it's unlikely to promise near creation of the reliable engineering methodology for calculating heat and mass transfer processes. The alternative approach to the problem is the methodology of relaxation transfer kernels, which can be calculated from model evolution equations [3]. In a few articles before we elaborated upon this approach to modeling heat and mass transfer in high rate processes [3-8].

In this article we summarize briefly our results in the area of description of time nonlocality applied to heat and mass transfer and try to develop this approach for describing time nonlocality in aggregation processes. We concentrate our attention upon a problem of equations structure, touching on the problem
of analytical solutions of government equations in the lesser degree.

## 2. Mass and heat transfer equations

### 2.1. Main concept

Relaxation transfer kernels are the kernels of integral transformations that, in the statistical theory of dissipation processes, relate fluxes with thermodynamic forces [1]. The general structure of these relations for components fluxes in a multicomponent system according this methodology is like that [6]

$$
\begin{equation*}
J_{i}(R, t)=J_{i}\left(R, t_{0}\right)+\sum_{k=1}^{n} \iint d t_{1} d R^{\prime} N_{i k}\left(R, R^{\prime}, t, t_{1}\right) F_{k}\left(R^{\prime}, t\right) \tag{1}
\end{equation*}
$$

Limiting one self to the time nonlocality in the multicomponent system, one can write expressions for the $n$ linearly independent mass fluxes $J_{i}$ of components and the heat flux $J_{h}$ as

$$
\begin{gather*}
J_{i}=-\sum_{k=1}^{n} \int_{0}^{t} d t_{1} N_{i k}\left(R, t-t_{1}\right) \nabla\left(\frac{v_{k}\left(R, t_{1}\right)}{T}\right)-\int_{0}^{t} d t_{1} N_{i T}\left(R, t-t_{1}\right) \frac{\nabla T}{T^{2}},  \tag{2}\\
J_{T}=-\sum_{k=1}^{n} \int_{0}^{t} d t_{2} N_{T k}\left(R, t-t_{2}\right) \nabla\left(\frac{v_{k}\left(R, t_{2}\right)}{T}\right)-\int_{0}^{t} d t_{2} N_{T T}\left(R, t-t_{2}\right) \frac{\nabla T}{T^{2}}, \tag{3}
\end{gather*}
$$

where $v_{i}$ is a chemical potential; $R$-space coordinates; $T$ - temperature; $t$ - time.
For a more compact description, let's assume $v_{n+1} \equiv-1$. Then, in expressions (2), (3), one can replace the subscript $h$ by $n+1$ and write a unified form for the mass fluxes and heat flux in the multicomponent system.

$$
\begin{equation*}
J_{i}=-\sum_{k=1}^{n+1} \int_{0}^{t} d t_{1} N_{i k}\left(R, t-t_{1}\right) \nabla\left(\frac{v_{k}\left(R, t_{1}\right)}{T}\right) \tag{4}
\end{equation*}
$$

Let's also introduce notation for the integral terms

$$
\begin{equation*}
I_{i k}=\int_{0}^{t} d t_{1} N_{i k}\left(R, t-t_{1}\right) \nabla\left(\frac{v_{k}\left(R, t_{1}\right)}{T}\right) \tag{5}
\end{equation*}
$$

Now, instead of equations (2), (3) we get

$$
\begin{equation*}
J_{i}=-\sum_{k=1}^{n+1} I_{i k} \tag{6}
\end{equation*}
$$

For calculating the relaxation transfer kernels we can use various approximations which are based on information about the physical mechanism of the processes [1,2]. However, the analyses of various data $[1,2]$ as well as our own experience [4-8] allow us to submit the heuristic unified model equation for relaxation kernels

$$
\begin{equation*}
\frac{\partial N_{i}}{\partial}=-N_{i} \tau_{i i}^{-1}+\sum_{\substack{k=1 \\ k \neq i}}^{n} N_{k} \tau_{i k}^{-1} \tag{7}
\end{equation*}
$$

where, in order to be in agreement with the Onsager principle, it is assumed that $\tau_{i k}=\tau_{k i}$.
Of course, it's impossible to warrant that form (7) is actually universal. But we shall consider equation (7) as the base model for our further constructions.

The matrix of system (7) is symmetrical; therefore, all its eigenvalues are real. In this connection, solution (7) can be represented as the sum of the forward and cross terms of the transfer kernels [6]:

$$
\begin{equation*}
N_{i}=\sum_{k=1}^{n} N_{i k} \tag{8}
\end{equation*}
$$

where all items are real exponents and $N_{i k}=N_{k i}$.

As it is shown in [6] with the help of the above model we can infer the following relations for integrals (5):

$$
\begin{equation*}
\frac{\partial I_{i k}}{\partial t}=\eta_{i k} \nabla\left(\frac{v_{k}}{T}\right)-\frac{I_{i k}}{\tau_{i k}} \tag{9}
\end{equation*}
$$

where for isotropic medium we suppose [3]

$$
\begin{equation*}
\frac{\partial \eta_{i k}}{\partial R}=0 \tag{10}
\end{equation*}
$$

So then, as a result of the repeated differentiation of (4) up to derivatives of the $(n+1)$-th order, the following relationships are obtained (where for any function $\frac{\partial^{0} Z}{\partial t^{0}} \equiv Z$ ):

$$
\begin{equation*}
\frac{\partial^{m} J_{i}}{\partial t^{m}}=\sum_{s=0}^{m-1}(-1)^{s+1} \frac{\partial^{m-1-s}}{\partial t^{n-1-s}}\left(\sum_{k=1}^{n+1} \frac{\eta_{i k} \nabla\left(v_{k} / T\right)}{\tau_{i k}^{s}}\right)+(-1)^{m+1} \sum_{k=1}^{n+1} \frac{I_{i k}}{\tau_{i k}^{m}} \tag{11}
\end{equation*}
$$

Thus, for each of the components we obtain a system which consists of $(n+1)$ equations connecting the component flux with its derivatives up to $(n+1)$ order inclusive.

The matrices $M_{i}$ of the obtained systems are not degenerate

$$
\begin{equation*}
\operatorname{det} M_{i}=\operatorname{det}\left(\frac{(-1)^{m-1}}{\tau_{i k}^{m}}\right) \neq 0 \tag{12}
\end{equation*}
$$

In this connection, from the $(n+1)$ equations that are linear relative to integrals $I_{i k}$, one can express all these integrals through the derivatives of fluxes $J_{i}$ and then substitute the obtained expressions into equation (6).

As a result, one can come to the linear differential equation of the $(n+1)$ th order for the fluxes of each of the components [6]

$$
\begin{equation*}
L\left(\frac{\partial^{n+1} J_{i}}{\partial t^{n+1}}, \frac{\partial^{n} J_{i}}{\partial t^{n}}, \ldots J_{i} ; v_{1}, \ldots, v_{n}\right)=0 \tag{13}
\end{equation*}
$$

where $L$ is the linear operator.
The succeeding deduction is based on the conservation laws:

$$
\begin{equation*}
\frac{\partial v_{i}}{\partial t}+\nabla \cdot J_{i}=0 \tag{14}
\end{equation*}
$$

Acting on expression (13) by the nabla operator and using equation (14), we can obtain the differential equation of the $(n+2)$ th time-order for the potential of each of the components

$$
\begin{equation*}
L\left(\frac{\partial^{n+2}\left(v_{i}\right)}{\partial t^{n+2}}, \frac{\partial^{n+1}\left(v_{i}\right)}{\partial t^{n+1}}, \ldots, \frac{\partial v_{i}}{\partial t} ; v_{1}, \ldots, v_{n} ; \nabla^{2} v_{1}, \ldots, \nabla^{2} v_{n}\right)=0 \tag{15}
\end{equation*}
$$

The nonlinear generalization of equation (4) can be represented in a nonlocal quadratic form with tensor kernels $[6,8]$

$$
\begin{align*}
& J_{i}=-\sum_{k=1}^{n+1} \int_{0}^{t} d t_{1} N_{i k}^{(1)}\left(R, t-t_{1}\right) \cdot \nabla\left(\frac{v_{k}\left(R, t_{1}\right)}{T}\right)- \\
& -\sum_{k=1}^{n+1} \sum_{p=1}^{n+1} \int_{0}^{t} \int_{0}^{t} d t_{1} d t_{2} N_{i k p}^{(2)}\left(R, t-t_{1}, t-t_{2}\right): \nabla\left(\frac{v_{k}\left(R, t_{1}\right)}{T}\right) \nabla\left(\frac{v_{p}\left(R, t_{2}\right)}{T}\right), \tag{16}
\end{align*}
$$

In the weakly nonlinear approximation, we can assume [8]

$$
\begin{equation*}
\left\|N_{i k p}^{(2)}\right\|=\varepsilon\left\|N_{i k}^{(1)}\right\|\left\|N_{i p}^{(1)}\right\|, \tag{17}
\end{equation*}
$$

where $\varepsilon$ is the series expansion parameter.
One can evaluate the small parameter $\varepsilon$ as the ratio of the two Knudsen numbers that are calculated by two characteristic spatial scales for the elastic and inelastic molecular collisions, respectively [8]

### 2.2. Examples

As the first example let's consider mass and heat transfer in two-component systems like high dilute solutions. In this case the cross fluxes may be disregarded [3, 4].

Thus we use simplest form of relaxation kernels

$$
\begin{equation*}
N_{i}\left(R, t-t_{1}\right)=\eta_{i}(R, t) \exp \left(-\left(t-t_{1}\right) / \tau_{i}\right) \tag{18}
\end{equation*}
$$

Relations for mass and heat fluxes read

$$
\begin{align*}
J_{1} & =\int_{0}^{t} d t_{1} N_{1}\left(R, t-t_{1}\right) \nabla v\left(R, t_{1}\right),  \tag{19}\\
J_{2} & =\int_{0}^{t} d t_{2} N_{2}\left(R, t-t_{2}\right) \nabla \beta\left(R, t_{2}\right) . \tag{20}
\end{align*}
$$

Thus, operating under the above methods applied to an isotropic media we are led to the following transfer equations of a hyperbolic type [3]:

$$
\begin{align*}
& \tau_{1} \frac{\partial^{2} v}{\partial t^{2}}=\left(1-\tau_{1} \frac{\partial}{\partial t} \ln \eta_{1}\right) \frac{\partial v}{\partial t}+\eta_{1} \nabla^{2} v  \tag{21}\\
& \tau_{2} \frac{\partial^{2} \beta}{\partial \partial^{2}}=\left(1-\tau_{2} \frac{\partial}{\partial t} \ln \eta_{2}\right) \frac{\partial \beta}{\partial t}+\eta_{2} \nabla^{2} \beta \tag{22}
\end{align*}
$$

The case of a non-isotropic media is also considered in [3].
Equations (21), (22) closely resemble transfer equations for media with memory that are presented in [2]. It's easy to check also that under the exponential relaxation kernel the heat transfer equation (22) corresponds with the Maxwell - Kattaneo law:

$$
\begin{equation*}
q+\tau \frac{\partial q}{\partial}=-\lambda \nabla T \tag{23}
\end{equation*}
$$

where

$$
\begin{equation*}
\tau=\frac{\tau_{2}}{1-\tau_{2} \frac{\partial}{\partial} \eta_{2}}, \lambda=\frac{\eta_{2}}{1-\tau_{2} \frac{\partial}{\partial} \eta_{2}}\left(1 / T^{2}\right) . \tag{24}
\end{equation*}
$$

Under the relaxation times that are far less than the observation time the above equations can be considered by the methods of singular perturbations.

The next example we consider is mass and heat transfer in diluted two-component systems with allowing for cross effects like the thermal diffusion and the Soret effect [4]. Model system for the
relaxation kernels reads

$$
\begin{align*}
& \frac{\partial N_{m}}{\partial t}=-N_{m} \tau_{m}^{-1}+N_{h} \tau_{\times}^{-1},  \tag{25}\\
& \frac{\partial N_{h}}{\partial t}=N_{m} \tau_{\times}^{-1}-N_{h} \tau_{h}^{-1}, \tag{26}
\end{align*}
$$

The choice of signs in equations (25) and (26) is determined by the conditions of coupling distortions of the temperature and concentration fields [4].

The solution of equations (25) and (26) can be written in the form

$$
\begin{align*}
& N_{m}=N_{m m}+N_{m h},  \tag{27}\\
& \quad N_{h}=N_{h h}+N_{h m}, \tag{28}
\end{align*}
$$

Here:

$$
\begin{gather*}
N_{m m}=\frac{\eta_{m}}{\lambda_{2}-\lambda_{1}}\left[\left(\lambda_{2}+\frac{1}{\tau_{m}}\right) \exp \left(\lambda_{1} s\right)-\left(\lambda_{1}+\frac{1}{\tau_{m}}\right) \exp \left(\lambda_{2} s\right)\right],  \tag{29}\\
N_{h h}=\frac{\eta_{h}}{\lambda_{2}-\lambda_{1}}\left[\left(\lambda_{2}+\frac{1}{\tau_{h}}\right) \exp \left(\lambda_{1} s\right)-\left(\lambda_{1}+\frac{1}{\tau_{h}}\right) \exp \left(\lambda_{2} s\right)\right],  \tag{30}\\
N_{m h}=N_{h m}=\frac{\eta_{\times}}{\tau_{\times}\left(\lambda_{2}-\lambda_{1}\right)}\left[\exp \left(\lambda_{1} s\right)-\exp \left(\lambda_{2} s\right)\right], \tag{31}
\end{gather*}
$$

were $\lambda_{1}, \lambda_{2}$ are eigenvalues of the system (25), (26).
From the condition of damping the perturbations in quasi-equilibrium systems it is readily available that both eigenvalues should be negative. From this, one can obtain the inequality:

$$
\begin{equation*}
\tau_{\times}>\sqrt{\tau_{m} \tau_{h}} \tag{32}
\end{equation*}
$$

The time dependence of cross transfer kernels has a maximum. This phenomenon is caused by the influence of thermal diffusion or the Soret effect [4, 8]. The peak of the time dependence of cross transfer kernels determines the period of increasing initial perturbations of the temperature and concentration fields. This period is easily evaluated [8]:

$$
\begin{equation*}
\tau_{\uparrow}=s_{c r}=\frac{\ln \left(\lambda_{2} / \lambda_{1}\right)}{\lambda_{1}-\lambda_{2}} \tag{33}
\end{equation*}
$$

As it follows from (15) we can obtain equations of the 3rd time-order for heat and mass transfer in the considered case.

## 3. Aggregation kinetic equations

Particles aggregation is widespread in different chemical technological processes, metallurgy and nature, and there are many approaches to modeling this phenomenon [9]. At the same time, certain important aspects in description of aggregation processes leave to be none elaborated at present. One of these important but weakly developed questions is time non-locality of aggregation processes. Indeed, without allowing for this aspect it is impossible to describe the influence of characteristic times of aggregates formation on the process kinetics [10]. It is justified especially in reference to nanotechnological processes.

For describing the evolution of $i$-mers concentration in the apparatus we can use various modifications of Smoluchowski or Becker-Dцring equations expanded as required by terms which correspond to a source of mass [11, 12].

This section deals with the non-local modification of Smoluchowski equation based on the approach presented in the previous section. We don't discuss here such especially physical problems as particles nucleation, etc. But we try to understand and to emphasize some difficulties emerging in the act of deriving non-local aggregation equations.

So we submit the following non-local modification of the Smoluchowski equation for aggregation in the uniform system:

$$
\begin{equation*}
\frac{d C_{i}}{d t}=\frac{1}{2} \sum_{j=1}^{i-1} \int_{0}^{t} \int_{0}^{t} N_{j, i-j} C_{j}\left(t_{1}\right) C_{i-j}\left(t_{2}\right) d t_{1} d t_{2}-\sum_{j=1}^{\infty} \int_{0}^{t} \int_{0}^{t} N_{i, j} C_{i}\left(t_{1}\right) C_{j}\left(t_{2}\right) d t_{1} d t_{2} \tag{34}
\end{equation*}
$$

$C_{i}$ denotes the concentration of $i$-mer.
In our case the characteristic times $\tau_{i, j}$ of the aggregation of $i$ and $j$-mers play a role of relaxation times. The simplest model equation for elements of the aggregation matrix can be constructed by analogy with model equation (6) for transfer kernels. We submit this equation as follows:

$$
\begin{equation*}
r_{i} \frac{\partial N_{i, j}}{\partial s_{i}}+r_{j} \frac{\partial N_{i, j}}{\partial s_{j}}+\frac{f_{i, j}^{0}}{\tau_{i, j}} N_{i, j}=0, \tag{35}
\end{equation*}
$$

where $s_{i}=t-t_{1} \quad s_{j}=t-t_{2}$
In equation (35) the coefficients $r_{i}$ on a level with relaxation time $\tau_{i j}$ play a part of control parameters of globules "inertness", the parameter $f$ answers for media and particles characteristics.

Independent integrals of equation (35) read

$$
\Psi_{1}=\frac{s_{i}}{r_{i}}-\frac{s_{j}}{r_{j}} ; \quad \Psi_{2}^{l}=N_{i, j} \exp \left(\frac{f_{i, j}^{0}}{r_{i} \tau_{i, j}} s_{i}\right) \quad \text { or } \quad \Psi_{2}^{I I}=N_{i, j} \exp \left(\frac{f_{i, j}^{0}}{r_{j} \tau_{i, j}} s_{j}\right)
$$

Thus the aggregation matrix, satisfying equation (35) and coming up to the condition of fast relaxation in time $t \gg \tau_{i, j}$, can be written as

$$
\begin{equation*}
N_{i, j}=\eta_{i, j}^{0} \exp \left(-\frac{f_{i, j}^{0}}{2 \tau_{i, j}}\left(\frac{s_{i}}{r_{i}}+\frac{s_{j}}{r_{j}}\right)\right) \tag{36}
\end{equation*}
$$

Let's assume at the beginning $r_{i}=r_{j}=1$ and $\frac{f_{i, j}^{0}}{\tau_{i, j}} \equiv a_{i, j}=a=$ const .
Thus we have

$$
\begin{equation*}
\frac{d C_{i}}{d t}=\frac{1}{2} \exp (-a t) \sum_{1} \eta_{j, i-j} I_{1} I_{2}-\exp (-a t) I_{3} \sum_{2} \eta_{i, j} I_{2} \tag{37}
\end{equation*}
$$

Here $\sum_{1}$ means $\sum_{j=1}^{i-1} ; \sum_{2}$ means $\sum_{j=1}^{\infty} ; I_{1}=\int_{0}^{t} \exp (a s / 2) C_{i-j}(s) d s ;$

$$
I_{2}=\int_{0}^{t} \exp (a s / 2) C_{j}(s) d s ; I_{3}=\int_{0}^{t} \exp (a s / 2) C_{i}(s) d s
$$

We didn't find way to rigorous reducing equation (37) to an ODE form even in that case. However, we try to simplify the problem by using asymptotic behaviour of integrals in (37). Namely, it is supposed that for small relaxation times we can use Laplace method in the neighbourhood of the time point $t$. But immediate substitution of the integrals expansions into equation (37) requires multiplying asymptotic sequences. Such procedure is dangerous, as it may lead to utter loss of checking orders of approximation.

Therefore we rearrange the equations to the form which is free from a product of integrals:

$$
\begin{equation*}
\frac{d^{2} C_{i}}{d t^{2}}+a \frac{d C_{i}}{d t}=\frac{1}{2} \exp \left(-\frac{a t}{2}\right) \sum_{1} \eta_{j, i-j}\left(C_{j} I_{1}+C_{i-j} I_{2}\right)-\exp \left(-\frac{a t}{2}\right)\left[C_{i} \sum_{2} \eta_{i, j} I_{2}+I_{3} \sum_{2} \eta_{i, j} C_{j}\right] . \tag{38}
\end{equation*}
$$

Using then Laplace method we obtain the understandable asymptotic relations in which the orders of equations and approximations are concerted

$$
\begin{gather*}
I_{1}^{(1)}=\frac{2}{a}\left[\exp \left(\frac{a t}{2}\right) C_{i-j}(t)-C_{i-j}(0)\right]-\frac{4}{a^{2}}\left[\exp \left(\frac{a t}{2}\right) \frac{d C_{i-j}}{d t}-\frac{d C_{i-j}(0)}{d t}\right],  \tag{39}\\
I_{2}^{(1)}=\frac{2}{a}\left[\exp \left(\frac{a t}{2}\right) C_{j}(t)-C_{j}(0)\right]-\frac{4}{a^{2}}\left[\exp \left(\frac{a t}{2}\right) \frac{d C_{j}}{d t}-\frac{d C_{j}(0)}{d t}\right],  \tag{40}\\
I_{3}^{(1)}=\frac{2}{a}\left[\exp \left(\frac{a t}{2}\right) C_{i}(t)-C_{i}(0)\right]-\frac{4}{a^{2}}\left[\exp \left(\frac{a t}{2}\right) \frac{d C_{i}}{d t}-\frac{d C_{i}(0)}{d t}\right] . \tag{41}
\end{gather*}
$$

As a result we get

$$
\begin{align*}
& \frac{d^{2} C_{i}}{d t^{2}}+a \frac{d C_{i}}{d t}=\frac{2}{a} \sum_{1} \eta_{j, i-j}\left[C_{j} C_{i-j}-\frac{1}{a} \frac{d}{d t}\left(C_{j} C_{i-j}\right)\right]-\frac{4}{a} \sum_{2} \eta_{i, j}\left[C_{i} C_{j}-\frac{1}{a} \frac{d}{d t}\left(C_{i} C_{j}\right)\right]- \\
& -\frac{1}{a} \exp \left(-\frac{a t}{2}\right) \sum_{i} \eta_{i, i-j}\left[C_{j}\left(C_{i-j}(0)-\frac{2}{a} \frac{d C_{i-j}(0)}{d t}\right)+C_{i-j}\left(C_{j}(0)-\frac{2}{a} \frac{d C_{j}(0)}{d t}\right)\right]+  \tag{42}\\
& +\frac{2}{a} \exp \left(-\frac{a t}{2}\right) \sum_{2} \eta_{i, j}\left[C_{i}\left(C_{j}(0)-\frac{2}{a} \frac{d C_{j}(0)}{d t}\right)-C_{j}\left(C_{i}(0)-\frac{2}{a} \frac{d C_{i}(0)}{d t}\right)\right]
\end{align*}
$$

Let's consider now the general case.
The evolution equation reads

$$
\begin{equation*}
\frac{d C_{i}}{d t}=\frac{1}{2} \sum_{1} \eta_{j, i-j} \exp \left(-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) t\right) I_{1} I_{2}-\sum_{2} \eta_{i, j} \exp \left(-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) t\right) I_{3} I_{4} \tag{43}
\end{equation*}
$$

Here $g_{m, n}^{(i)}=\frac{a_{m, n}}{2 r_{i}} ; g_{m, n}^{(j)}=\frac{a_{m, n}}{2 r_{j}}$;

$$
\begin{gathered}
I_{1}=\int_{0}^{t} \exp \left(g_{j, i-j}^{(i-j)} s\right) C_{i-j}(s) d s ; I_{2}=\int_{0}^{t} \exp \left(g_{j, i-j}^{(j)} s\right) C_{j}(s) d s \\
I_{3}=\int_{0}^{t} \exp \left(g_{i, j}^{(j)} s\right) C_{j}(s) d s ; I_{4}=\int_{0}^{t} \exp \left(g_{i, j}^{(i)} s\right) C_{i}(s) d s
\end{gathered}
$$

By time-differentiating the evolution equation we obtain

$$
\begin{align*}
& \frac{d^{2} C_{i}}{d t^{2}}=\frac{1}{2} \sum_{1} \eta_{j, i-j}\left\{-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) \exp \left(-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) t\right) I_{1} I_{2}+\right. \\
& \left.+\exp \left(-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) t\right)\left[\exp \left(g_{j, i-j}^{(i-j)} t\right) C_{i-j} I_{2}+\exp \left(g_{j, i-j}^{(j)} t\right) C_{j} I_{1}\right]\right\}-  \tag{44}\\
& -\sum_{2} \eta_{i, j}\left\{-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) \exp \left(-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) t\right) I_{3} I_{4}+\right. \\
& \left.+\exp \left(-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) t\right)\left[\exp \left(g_{i, j}^{(j)} t\right) C_{j} I_{4}+\exp \left(g_{i, j}^{(i)} t\right) C_{i} I_{3}\right]\right\}
\end{align*}
$$

Unlike the first case we can't now get rid of the products of integrals with the help of equation (34). That is why we are forced to resort to separate averaging of sums containing $I_{1} I_{2}$ and $I_{3} I_{4}$ [10].

There are not indisputable grounds for such procedure but we assume that (44) can be rewritten in the following form using coefficients $A_{i}$ and $B_{i}$ as functions of time $t$ :

$$
\begin{align*}
& \frac{d^{2} C_{i}}{d t^{2}}=-\frac{1}{2} A_{i} \sum_{1} \eta_{j, i-j} \exp \left(-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) t\right) I_{1} I_{2}+  \tag{45}\\
& +B_{i} \sum_{2} \eta_{i, j} \exp \left(-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) t\right) I_{3} I_{4}+\Phi
\end{align*}
$$

Here

$$
\begin{align*}
& \Phi=\frac{1}{2} \sum_{1} \eta_{j, i-j} \exp \left(-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) t\right)\left[\exp \left(g_{j, i-j}^{(i-j)} t\right) C_{i-j} I_{2}+\exp \left(g_{j, i-j}^{(j)} t\right) C_{j} I_{1}\right]+  \tag{46}\\
& +\sum_{2} \exp \left(-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) t\right)\left[\exp \left(g_{i, j}^{(i)} t\right) C_{j} I_{4}+\exp \left(g_{i, j}^{(j)} t\right) C_{i} I_{3}\right] .
\end{align*}
$$

By repeated time-differentiating we get

$$
\begin{align*}
& \frac{d^{3} C_{i}}{d t^{3}}=\frac{1}{2}\left(A_{i}^{2}-\frac{d A_{i}}{d t}\right) \sum_{1} \eta_{j, i-j} \exp \left(-\left(g_{j, i-j}^{(j)}+g_{j, i-j}^{(i-j)}\right) t\right) I_{1} I_{2}- \\
& -\left(B_{i}^{2}-\frac{d B_{i}}{d t}\right)_{2} \eta_{i, j} \exp \left(-\left(g_{i, j}^{(i)}+g_{i, j}^{(j)}\right) t\right) I_{3} I_{4}+\frac{d \Phi}{d t} . \tag{47}
\end{align*}
$$

The scheme of subsequent transformations is like that.

1. From (43) and (45) we infer the expressions for sums containing $I_{1} I_{2}$ and $I_{3} I_{4}$.
2. Then we substitute these expressions to equation (47) and use asymptotic relations for integrals once again.

By realizing this clear scheme we obtain the three-order ODE of rather unwieldy form, and it is no need to presenting this equation here.

In any case, it is possible to conclude at once that account of an interference of non-simultaneous perturbations of $i$-mers concentration field may be important on close examination of aggregation processes. This shade was missed in our work [10].

## 4. Conclusion

In this paper we submit a brief introduction to the problem of time nonlocality both of mass and heat transfer and aggregation processes. In essence, here we give only formulation of the problem and then try to show that the relaxation kernels approach may be advantageous for deriving governing evolution equations with accounting of hierarchy of relaxation times.

Now it has become evident that transfer equations based on the Fourier and Fick laws don't give an adequate description of high rate or nano-scale technological processes. As for aggregation processes, an importance of accounting relaxation phenomena is obvious. In this paper we didn't submit results of our numerical experiments because these results were dependent on the form of a static part of coagulation kernels $\eta_{i, j}$, but discussion in this problem was not our goal here. Some results of these experiments can be found in our works [10-12, 13].

The approach of relaxation transfer kernels can be tested for modification of the Becker-During aggregation-fragmentation equation too [14, 15]. It may be interesting also to consider the problems of the gelation behaviour and other dynamical phenomena in the systems described by new evolution equations [16-18].

In our opinion, the relaxation kernels approach may be considered as the unified method for creating engineering models of transfer and aggregation processes [19, 20]. We think, this problem merits closer inspection of investigators.

## REFERENCES

[1] Rudyak, V.Yu., Statisticheskaya teoriya dissipativnykh protsessov v gazakh i zhidkostyakh (Statistical Theory of Dissipative Processes in Gases and Liquids), Novosibirsk: Nauka, 1987, p. 272.
[2] Jou, D., Casas-Vazquez, J., and Criado-Sancho, M., Thermodynamics of Fluids under Flow, Berlin: Springer, 2001, p. 231.
[3] Kim, L.A. and Brener, A.M., On the Time Nonlocality in the Heat- and Mass-Transfer Equations for High-Rate Processes, Theor. Found. Chem. Eng., 1996, vol. 30, pp. 233-235
[4] Kim, L.A. and Brener, A.M., Nonlocal Equations of Heat and Mass Transfer with Allowance for Cross Effects, Theor. Found. Chem. Eng., 1998, vol. 32, no. 3, pp. 213-215
[5] Kim, L., Brener, A.M., and Berdalieva, G.A., The Consideration of Cross Effects in Non-Local Equations of Heat and Mass Transfer, Proc. 1st European Congress on Chemical Engineering, Florence, Italy, May 4-7, 1997, vol. 3, pp. 1809-1813.
[6] Brener, A.M., Muratov, A.S., and Tashimov, L., Non-Linear Model of Time Dependent Relaxation Cores for the Systems with Cross Transfer Effects, Proc. VIII Int. Conf. on Advanced Computational Methods in Heat Transfer, Lisbon, Portugal, March 24-26, 2004, pp. 321-332.
[7] Brener, A.M., Serimbetov, M.A., and Musabekova, L.M., Non-Local Equations for Concentration Waves in Reacting Diffusion Systems, Proc. XII Int. Conf. on Computational Methods and Experimental Measurements, Malta, June 20-22, 2005, pp. 93-103
[8] A.M. Brener. Nonlocal Equations of the Heat and Mass Transfer in Technological Processes Theoretical Foundations of Chemical Engineering, 2006, Vol.40, No. 6, pp. 564-572.
[9] J.A.D. Wattis. An introduction to mathematical models of coagulation-fragmentation processe: A discrete deterministic mean-field approach. Physica D 222 (2006), 1-20.
[10] Brener A., Balabekov B., Kaugaeva A. Non-local model of aggregation in uniform polydisparsed systems. Chem. Eng. Transactions, 2009, 17, 783-788.
[11] Brener A., Balabekov B.Ch., Golubev V.G., Bekaulova A.A. Modeling of aggregation processes in physico-chemical systems. Proc. of the $23^{\text {rd }}$ Europ. Symp. on Appl. Thermodyn., Cannes, May 29-June1, 2008, 123-126.
[12] Brener A., Makhatova A., Yakubova R. Modeling of aggregation processes in multiphase chemical reactors. Proc. of $11^{\text {th }}$ Int. Conf. on Multiphase Flow in Ind. Plants, Palermo, 2008, 611-618.
[13] Brener A.M. Nonlocal model of aggregation in polydispersed systems. Theor. Found. Chem. Eng. 2011. V. 45. № 3. P. 349.
[14] Boehm A.B., Poor C., Grant S.B. Particle coagulation and the memory of initial conditions. J. Phys. A 31. 1988. 9241.
[15] Meakin P. Fractal aggregates. Advances in Colloid and Interface science.1987.V.28.P. 249.
[16] Vepa R. Dynamics of smart structures. John Wiley \& Sons, 2010.
[17] Meakin P. Fractal aggregates. Advances in Colloid and Interface science.1987.V.28.P. 249.
[18] F. Family, Daoud M., Herrmann H.J., Stanley H.E. Scaling and Disordered Systems. World Scientific, 2002.
[19] Leyvraz F. The "active perimeter" in cluster growth models: a rigorous bound. J. Phys. A.: Math. Gen. 1985. V. 18, P. 941.
[20] Leyvraz F. Scaling theory and exactly solved models in the kinetics of irreversible aggregation. Phys. Reports. 2003. V. 383. P. 95.

# ТАСЫМАЛДАУ ЖӘНЕ АГРЕГАЦИЯЛАУ ПРОЦЕСТЕРІНІҢ МАТЕМАТИКАЛЫК МОДЕЛІНДЕ РЕЛАКСАЦИЯЛЫҚ ЯДРОЛАРЫНЫН ӘДІСІ 

А.С. Муратов, А.М. Бренер, Л. Ташимов<br>Оңтүстік Қазақстан мемлекеттік университеті, Шымкент, Қазақстан

Түйін сөздер: масса және жылу тасымалдау, релаксация уақыттары, релаксациялық ядролар, қиылысу тиімділіктері, агрегация.

Аннотация. Мақалада жогары жылдамдықты және нано-масштабты технологиялық процестердің интенсивтілігін релаксациялық уақыт иерархиясының эсерін бөлектеп біліп шығуга жаңа мүмкіндіктерді ашатын, релаксациялық ядролар тасыматдау әдісінің көмегімен жылу және масса тасымалдауды және агрегациялық процестерді сипаттау үшін математикалық моделдерін жалпылай талдау берілген.

