Verification of the building materials production process mathematical model

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Abstract. We consider a new mathematical model of the process of production of building materials based on the reaction of autocatalysis in the case of two reagents. The considered mathematical model takes into account the terms of a higher order of smallness for a small parameter. The results obtained when considering a reaction in an infinite cylinder with a random distribution of chemical reagents at the initial moment of time using two different mathematical models are compare.

1. Introduction
We consider the process of production of building materials based on the autocatalytic reaction of two reagents. The kinetic system of Carleman equations can be used for the mathematical description of this process [1-13]. Recently, a new model has been proposed to describe the process under study, taking into account members of a higher order of accuracy [14]. To verify the model, we compare the results obtained using both models. The comparison is carried out for the case of a reaction in an infinite cylinder, provided that the distribution of reagents is random, which corresponds to the actual technological process.

2. Problem formulation
We consider the process of autocatalytic reaction of two reagents in an infinite cylinder. The density of the first reagent is denoted by $u(t,x)$ the density of the second reagent is denoted by $w(t,x)$. We assume that at the initial moment of time, the densities of both reagents are stationary random processes that have a Gaussian distribution with the same mathematical expectations and the same correlation functions. To describe this process, a system of Carleman equations can be used

\[
\begin{align*}
\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} &= -\frac{1}{\varepsilon} (u^2 - w^2) \\
\frac{\partial w}{\partial t} - c \frac{\partial w}{\partial x} &= \frac{1}{\varepsilon} (u^2 - w^2)
\end{align*}
\]

where $\varepsilon$ is a small parameter [1-13]. In [14], a new mathematical model is proposed that takes into account higher-order terms and makes it possible to describe the process under study more correctly from a mathematical point of view.
Thus, we compare solutions of two Cauchy problems with the same initial conditions, which are stationary random processes that have a Gaussian distribution

\[ u(0,x) = u^0(x) \]
\[ w(0,x) = w^0(x) \]

with mathematical expectations equal to 1 and correlation functions equal to 0.0025exp(-|\alpha\tau|). For a fixed \( t \), the solution to each of the two Cauchy problems will be a pair of stationary random processes, but due to the non-linearity of the problems, they will not have a Gaussian distribution for positive \( t \).

In practice, when modeling a technological process, the main interest is the time it takes to implement it, that is, the equilibrium position will be reached. As a measure of deviation from the equilibrium position, we take the values of the correlation functions of the solution components at \( \tau = 0 \).

For the numerical solution of the Cauchy problem, we use a finite-difference scheme of the second order of accuracy. To study the probabilistic characteristics, we use the method considered in [15].

3. Results

We consider the mathematical models for values of the parameter \( \epsilon = 0.02 \). In Fig. 1 fragments of implementations of the initial conditions of the studied problems are presented.

![Figure 1. Initial condition \( u^0(x), w^0(x) \).](image)

In Fig. 2, 3 we can see the correlation functions of initial random processes obtained by the method detailed in [15]. This figures demonstrate the accuracy of correlation function calculations.
Figure 2. The correlation function of initial condition $u_0(x)$.

Figure 3. The correlation function of initial condition $w_0(x)$.

The evolution of the densities of both reagents described by the new mathematical model can be seen in figures 4-8 for the time values: 0.005, 0.05, 0.5, 5, and 10. The interaction of the reactants leads to a rapid "pumping" of the reagents. In Fig. 5 at $t = 0.05$, we can see almost complete coincidence of the densities of both reagents. Next, we can observe the tendency of the solution to the equilibrium position.
Figure 4. The solution components of second model at $t = 0.005$.

Figure 5. The solution components of second model at $t = 0.05$.

Figure 6. The solution components of second model at $t = 0.5$. 
In Figures 9-11, we can see a comparison of the solution components of the first problem $w_2$ and the solution components of the second problem $w_1$ for the time values: 0.005, 0.05, and 0.5.
Figure 10. The solution components of the first model $w_{22}$ and of the second model $w_{12}$ at $t = 0.05$

Figure 11. The solution components of the first model $w_{32}$ and of the second model $w_{31}$ at $t = 0.5$

Figure 12. The correlation function of the components solution of the first problem $c_{fw42}$ and of the second one $c_{fw41}$ at $t = 0.5$
In Figures 12-13, we can see the correlation functions of the components of solutions to both problems. It can be noted that if the behavior of the process characteristics is the same, there are quantitative differences in the reaction time.

4. Conclusions
We consider the process of autocatalytic reaction of two reagents in an infinite cylinder. This example compares two mathematical models: a kinetic model and a model that takes into account members of a higher order of smallness. It is possible to note the same nature of changing characteristics of the process. However, taking into account members of a higher order of smallness, leads to a quantitative change in characteristics, even for small values of the parameter.

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