Numerical modeling of cross-diffusion processes

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Abstract. The paper studied the processes represented by a system of equations of a particular product of the parabolic type. For the solution of mutual diffusion problems, evaluations were obtained according to the environmental parameters and the dimensions of the space. Computational schemes, algorithms, and software packages in programming environments were developed, and the obtained solutions were visualized to solve the studied problems.

1 Introduction

The spread of industrial emissions in the atmosphere occurs due to their adjective transfer by air masses and diffusion due to turbulent air pulsations. If the impurities emitted into the air consist of large particles, then propagating in the atmosphere, they begin to fall under the influence of gravity at a certain constant speed according to the Stokes law. Naturally, almost all impurities eventually settle on the earth's surface, and heavy ones are mainly under the action of the gravitational field and light ones - because of the diffusion process. For the environment, gaseous impurities such as oxides are the most dangerous; we will restrict ourselves to considering only light compounds [1-3].

Of great importance in the theory of the spread of pollution are fluctuations in the speed and direction of the wind over a long period (about a year), when the air masses, entraining impurities from the source, repeatedly change direction and speed. Such long-term changes are usually described by a special diagram called the wind rose, in which the vector value is proportional to the number of recurring events associated with the movement of air masses in a given direction, i.e., the maxima of the wind rose diagram correspond to the prevailing winds in the area [4-7].

In [4], the results of an experiment on the study of temperature fields in the boundary layer of air above a capillary-porous plate are presented when the evaporation of liquid into the flow occurs directly from the body's pores. In this case, the smallest particles of moist air enter the boundary layer of air due to the pressure difference in the dry layer of the

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material, which then evaporates in the air above the surface of the plate. The presence of a negative heat source in the air's boundary layer intensifies the heat and mass transfer process between the body and the environment.

In [8], modeling of aerosol propagation in a cloudy jet is given, taking into account such phenomena as turbulence generation due to flow instability at high Reynolds numbers, its viscous dissipation, and convective-diffusion transport. The paper prefers a complex turbulence model based on a system of two partial differential equations. The advantage of this approach is that it allows one to calculate an important parameter, the turbulence scale, with acceptable accuracy.

2 Qualitative analysis of cross-diffusion processes

Let us consider the following problem, which represents the process of mutual diffusion:

$$\begin{cases} \dfrac{\partial u}{\partial t} = \dfrac{\partial}{\partial x}\left(u^{\sigma_1}\dfrac{\partial u}{\partial x}\right) - v^{\beta_1}\left|\dfrac{\partial u}{\partial x}\right|^{p_1}, \\ \dfrac{\partial v}{\partial t} = \dfrac{\partial}{\partial x}\left(v^{\sigma_2}\dfrac{\partial v}{\partial x}\right) - u^{\beta_2}\left|\dfrac{\partial v}{\partial x}\right|^{p_2}, \end{cases} \tag{1}$$

$$\begin{cases} u(x,0) = u_0(x), \\ v(x,0) = v_0(x), \end{cases} \quad x \in R, \tag{2}$$

$$\begin{matrix} u(0,t) = u_1(t), & u(1,t) = u_2(t), \\ v(0,t) = v_1(t), & v(1,t) = v_2(t), \end{matrix} \quad 0 \le t \le T, \tag{3}$$

here $\sigma_1,\ \sigma_2,\ \beta_1,\ \beta_2,\ p_1,\ p_2$ are given real numbers.

We look for the solution to the problem (1)-(3) in the following form:

$$\begin{cases} u = A\left(a - \dfrac{x}{\ell(t)}\right)_+^{\gamma_1}, \\ v = B\left(a - \dfrac{x}{\ell(t)}\right)_+^{\gamma_2}, \end{cases} \tag{4}$$

here $a > 0$, $D_+ = \max(0, D)$,

$$\gamma_1 = \frac{(2-p_1)(\sigma_1+2-p_1)(\sigma_2+2-p_2) + \beta_1\left((2-p_2)(\sigma_1+2-p_1) + \beta_2(2-p_1)\right)}{(\sigma_1+2-p_1)\left((\sigma_1+2-p_1)(\sigma_2+2-p_2) - \beta_1\beta_2\right)} > 0,$$

$$\gamma_2 = \frac{(2-p_2)(\sigma_1+2-p_1) + \beta_2(2-p_1)}{(\sigma_1+2-p_1)(\sigma_2+2-p_2) - \beta_1\beta_2} > 0,$$

$$A=\left(\frac{\gamma_1^{p_1}}{\gamma_1\left(\sigma_1\left(\gamma_1+1\right)-1\right)}B^{\beta_1}\right)^{\frac{1}{\gamma_1+1-p_1}},\quad B=\left(\frac{\gamma_2^{p_2}}{\gamma_2\left(\sigma_2\left(\gamma_2+1\right)-1\right)}\right)^{\frac{1+\sigma_1-p_1}{(\sigma_1+1-p_1)(\sigma_2+1-p_2)-\beta_1}}.$$

To find the rule of motion of the front, we use the method of integral relations for a single equation of the problem (1) - (3)

$$\frac{d}{dt}\int_0^{\ell(t)}u(t,x)\,dx=u^{\sigma_1}\left.\frac{\partial u}{\partial x}\right|_{x=0}-\int_0^{\ell(t)}\left|\frac{\partial u}{\partial x}\right|^{p_1}v^{\beta_1}\,dx$$

and as a result we have the following differential equation for the front:

$$\frac{d\ell}{dt}=\ell^{-1}\left(\frac{C}{M}\ell^{p_1+1}-\frac{Y}{M}\right),$$

Here

$$M=\frac{a^{\gamma_1+1}-(a-1)^{\gamma_1+1}}{\gamma_1+1}A,\qquad Y=\frac{a^{\sigma_1+\gamma_1-1}}{\gamma_1-1}A^{\sigma_1+1},$$

$$C=\frac{a^{p_1(\gamma_1-1)+\beta_1\gamma_2+1}-(a-1)^{p_1(\gamma_1-1)+\beta_1\gamma_2+1}}{p_1(\gamma_1-1)+\beta_2\gamma_2+1}(\gamma_1-1)A^{p_1}B^{\beta_1}.$$

According to the resulting differential equation, the results are as follows.

1) $\gamma_1>1$.

In this case $\ell'(t)<0,\ t<T_0$, dust and moisture migration in limited $0<T_0<+\infty$ occurs in a limited area of time and is for the front

$$x_{\max}=\left(\frac{Y}{C}\right)^{\frac{1}{p_1+1}}$$

expression is appropriate.

2) $0<\gamma_1<1$, $\quad\ell'(t)<0,\ \forall t>0$.

In this case $\ell(t)$, function $t\to+\infty$ dust and moisture migration occurs in the limited field.

$$x_{\max}=\left(\frac{Y}{C}\right)^{\frac{1}{p_1+1}}$$

In particular, let's see what happens when $p_1=1$. Solve () differential equation

$$\int \frac{\ell}{\ell^2 - Y/C} d\ell = \frac{C}{M} t + const$$

$$\ell(t) = \left(e^{\frac{2C}{M}t+\eta} + \frac{Y}{C} \right)^{\frac{1}{2}}, \eta - const \tag{5}$$

Similarly, for the front of the second equation of problem (1) - (3), we can get the same result as (4).

Now, look at the algorithm for solving problems (1) - (3).

Numerical problem-solving algorithm

This is a differential scheme for the system

$$\begin{cases} \dfrac{u_i^{j+1} - u_i^j}{\tau} = \dfrac{1}{h^2}\left(a(y_{i+1}^j)\left(u_{i+1}^{j+1} - u_i^{j+1}\right) - a\left(u_i^j\right)\left(u_i^{j+1} - u_{i-1}^{j+1}\right)\right) - Q(v)\left(v_i^j\right)^{\beta_1} \\ \dfrac{v_i^{j+1} - v_i^j}{\tau} = \dfrac{1}{h^2}\left(a(y_{i+1}^j)\left(v_{i+1}^{j+1} - v_i^{j+1}\right) - a\left(v_i^j\right)\left(v_i^{j+1} - v_{i-1}^{j+1}\right)\right) - Q(u)\left(u_i^j\right)^{\beta_2} \end{cases}$$

in the form, here $a(y)$ s calculated using the following formulas:

a) $a(y) = \left(\dfrac{y_{i-1}^j + y_i^j}{2} \right)^{\sigma}$,

b) $a(y) = \dfrac{\left(y_{i-1}^j\right)^{\sigma} + \left(y_i^j\right)^{\sigma}}{2}$.

$Q(y)$ is linearized by the following methods:

1) $Q(y) = \left[\dfrac{\overset{s}{y}{}_{i+1}^j - \overset{s}{y}{}_i^j}{h} \right]^p$ - Picar method [1, 2],

2) $Q(y) = \dfrac{\overset{s+1}{y}{}_{i+1}^j - \overset{s+1}{y}{}_i^j}{h} \left[\dfrac{\overset{s}{y}{}_{i+1}^j - \overset{s}{y}{}_i^j}{h} \right]^{p-1}$ - special method [1,2],

3) $Q(y) = \left[\dfrac{\overset{s}{y}{}_{i+1}^j - \overset{s}{y}{}_i^j}{h} \right]^p + \beta \left(\dfrac{\overset{s}{y}{}_{i+1}^j - \overset{s}{y}{}_i^j}{h} \right)^{p-1} \left(\dfrac{\overset{s+1}{y}{}_{i+1}^j - \overset{s+1}{y}{}_i^j}{h} - \dfrac{\overset{s}{y}{}_{i+1}^j - \overset{s}{y}{}_i^j}{h} \right)$ - Newton's method [1,2]

where s is the step in the iterative process.
We can solve it numerically using one of the iterative methods and the sweep method [3]

$$\begin{cases} \dfrac{\overset{s+1}{u}{}_i^{j+1}-\overset{s}{u}{}_i^{j}}{\tau}=\dfrac{1}{h^2}\left(a(\overset{s}{y}{}_{i+1}^{j})\left(\overset{s+1}{u}{}_{i+1}^{j+1}-\overset{s+1}{u}{}_i^{j+1}\right)-a\left(\overset{s}{y}{}_i^{j}\right)\left(\overset{s+1}{u}{}_i^{j+1}-\overset{s+1}{u}{}_{i-1}^{j+1}\right)\right)-Q(y)\left(v_i^j\right)^{\beta_1}, \\ \dfrac{\overset{s+1}{v}{}_i^{j+1}-\overset{s}{v}{}_i^{j}}{\tau}=\dfrac{1}{h^2}\left(a(\overset{s}{y}{}_{i+1}^{j})\left(\overset{s+1}{v}{}_{i+1}^{j+1}-\overset{s+1}{v}{}_i^{j+1}\right)-a\left(\overset{s}{y}{}_i^{j}\right)\left(\overset{s+1}{v}{}_i^{j+1}-\overset{s+1}{v}{}_{i-1}^{j+1}\right)\right)-Q(y)\left(u_i^j\right)^{\beta_2}. \end{cases}$$

An algorithm for numerical problem-solving and visualization was developed, according to which the software was created.
•Developed software was tested using various examples, and positive results were obtained.
•Mutual diffusion processes are visualized.

3 Computational

Experiment. Solution of the problem of cross-diffusion

$$\begin{cases} \dfrac{\partial u}{\partial t}=\dfrac{\partial}{\partial x}(v^{\sigma_1}\dfrac{\partial u}{\partial x})\pm\gamma(t,x)\dfrac{\partial u}{\partial x}, \\ \dfrac{\partial v}{\partial t}=\dfrac{\partial}{\partial x}(v^{\sigma_2}\dfrac{\partial v}{\partial x})\pm\gamma(t,x)\dfrac{\partial v}{\partial x}, \end{cases}$$

$$u|_{t=0}=u_0(x)\ge 0, \qquad v|_{t=0}=v_0(x)\ge 0,$$
$$u|_{x=x_1}=\psi_1(t)\ge 0, \qquad v|_{x=x_1}=\varphi_1(t)\ge 0,$$
$$u|_{x=x_2}=\psi_2(t)\ge 0, \qquad v|_{x=x_2}=\varphi_2(t)\ge 0.$$

Below are some results of the dust and moisture migration process in a two-component environment.

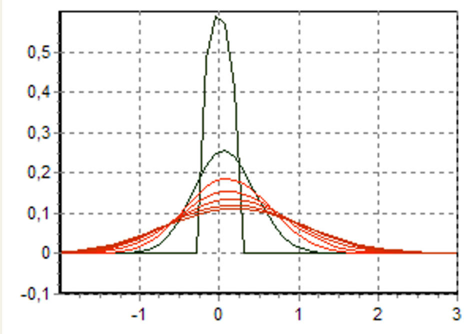

Fig. 1. $\sigma_1 = 2;\ \sigma_2 = 3;\ \nu_1 = 1;\ \nu_2 = 2;\ x_0 = -4;\ x_n = 8.$

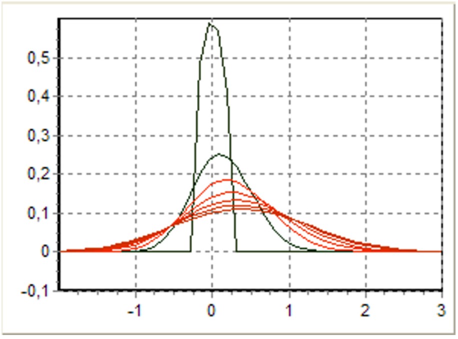

Fig. 2. $\sigma_1 = 2;\ \sigma_2 = 4;\ \nu_1 = 2;\ \nu_2 = 4;\ x_0 = -4;\ x_n = 8.$

4 Conclusions

The problem of mutual diffusion, represented by a system of nonlinear differential equations of the given parabolic type, was modeled following the numerical solution methods. An algorithm for numerical problem-solving and visualization was developed, according to which software was created using programming environments. Developed software was tested using various samples, and positive results were obtained. Mutual diffusion processes were visualized.

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