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NUMERICAL STUDY OF A NONLINEAR DIFFUSION SYSTEM WITH BOUNDARY FLUXES

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Abstract. This paper considers a system of nonlinear diffusion-reaction equations with nonlinear boundary flows in a half-space. The focus is on the problem formulation, determination of a weak solution, and derivation of an energy estimate and a blow-up criterion. Self-similar solutions are constructed for the system, and numerical simulations are performed in 1D using an implicit scheme. The results demonstrate the development of solution peaks and the possible blow-up moment, as confirmed by 3D field evolution plots.

Keywords: numerical scheme, stability of the scheme, nonlinear diffusion, boundary problem, Picard method.

Chegaraviy oqim bilan berilgan chiziqsiz diffuziya sistemasining sonli tadqiqoti

Annotatsiya. Ushbu maqola yarim fazoda chiziqli bo'lmagan chegara oqimlari bilan chiziqli bo'lmagan diffuziya-reaksiya tenglamalari tizimini ko'rib chiqadi. Asosiy e'tibor muammoni shakllantirishga, kuchsiz yechimni aniqlashga va energiya bahosi va portlash mezonini olishga qaratilgan. Tizim uchun o'ziga o'xshash yechimlar qurilgan va raqamli simulyatsiyalar yashirin sxema yordamida 1D da amalga oshirilgan. Natijalar 3D maydon evolyutsiyasi grafiklari bilan tasdiqlanganidek, yechim cho'qqilarining rivojlanishini va mumkin bo'lgan portlash momentini ko'rsatadi.

Kalit so‘zlar: sonli-sxema, turg’unlik sharti, chiziqsiz diffuziya, chegaraviy masala, Pikard metodi.

Численное исследование системы нелинейной диффузии с граничными потоками

Аннотация. В данной работе рассматривается система нелинейных уравнений диффузии-реакции с нелинейными граничными потоками в полупространстве. Основное внимание уделено постановке задачи, определению слабого решения, получению энергетической оценки и критерия взрыва (blow-up). Для системы построены автомодельные решения и проведено численное моделирование в 1D с использованием неявной схемы. Результаты демонстрируют развитие пиков решения и возможный момент blow-up, что подтверждается 3D-графиками эволюции полей

Ключевые слова: численная схема, устойчивость схемы, нелинейная диффузия, краевая задача, метод Пикара.

Introduction. Nonlinear diffusion-reaction systems with boundary fluxes arise in models of chemical reactions, biological processes, and plasma physics. Such systems are characterized by complex dynamics, including the possibility of infinite growth of the solution over a finite time (blow-up). ([1-4]) .The aim of this work is to investigate the behavior of solutions to a system with nonlinear

fluxes using analytical and numerical methods, and to demonstrate the effectiveness of self-similar initial data for numerical modeling.

The system under consideration is

$$\begin{cases} u_t = \nabla\left(\left|\nabla u^{m_1}\right|^{p_1-2}\nabla u^{m_1}\right)+u^{\beta_1}, & x\in R_+^N,\ t>0,\\ u_t = \nabla\left(\left|\nabla \upsilon^{m_2}\right|^{p_2-2}\nabla \upsilon^{m_2}\right)+\upsilon^{\beta_2}, & x\in R_+^N,\ t>0, \end{cases} \tag{1}$$

with nonlinear flow boundary conditions

$$\begin{cases} -\left|\nabla u^{m_1}\right|^{p_1-2}\dfrac{\partial u^{m_1}}{\partial x_1}=\upsilon^{q_1}, & x_1=0,\ t>0,\\ -\left|\nabla \upsilon^{m_2}\right|^{p_2-2}\dfrac{\partial \upsilon^{m_2}}{\partial x_1}=u^{q_2}, & x_1=0,\ t>0, \end{cases} \tag{2}$$

and initial conditions

$$u(x,0)=u_0(x),\ \upsilon(x,0)=\upsilon_0(x),\ x>0, \tag{3}$$

The parameters satisfy the conditions $m_i>1,\ p_i>1+1/m_i,\ q_i>0(i=1,2),\ \beta>0$

where $R_+^N=\left\{(x_1,x')\,|\,x'\in R^{N-1},\ x_1>0\right\}$

Many works, such as [5-10], were also devoted to problems similar to problem (1)-(3)

Definition. Functions $u,v\in L^{\infty}\left(0,T;L^2\left(R_+^N\right)\right)$ are called weak solutions of problem (1)-(3) if for all test functions $\phi,\psi\in C_0^{\infty}\left(R_+^N\times[0,T)\right)$ integral identities hold:

$$\int_0^T\int_{R_+^N}\left[-u\phi_t+\left|\nabla u^{m_1}\right|^{p_1-2}\nabla u^{m_1}\cdot\nabla\phi-u^{\beta_1}\phi\right]dxdt=\int_{R_+^N}u_0(x)\phi(x,0)dx,$$

$$\int_0^T\int_{R_+^N}\left[-v\psi_t+\left|\nabla v^{m_2}\right|^{p_2-2}\nabla v^{m_2}\cdot\nabla\psi-v^{\beta_2}\psi\right]dxdt=\int_{R_+^N}v_0(x)\psi(x,0)dx.$$

For a weak solution, energy function is introduced

$$E(t)=\int_{R_+^N}\frac{1}{m_1}\left|\nabla u^{m_1}\right|^{p_1}+\frac{1}{m_2}\left|\nabla v^{m_2}\right|^{p_2}dx-\int_{R_+^N}\frac{1}{\beta_1+1}u^{\beta_1+1}+\frac{1}{\beta_2+1}v^{\beta_2+1}dx.$$

Using integration by parts and boundary conditions, we obtain the inequality

$$\frac{d}{dt}\int_{R_+^N}\left(u^2+v^2\right)dx\le C\int_{R_+^N}\left(u^{\beta_1+1}+v^{\beta_2+1}\right)dx,$$

which allows you to monitor energy growth and identify a possible blow-up. The system can experience a blow-up if the following condition is met for certain parameters:

$$\beta_i>p_im_i,\ i=1,2,$$

and the initial data are sufficiently large. In this case, the maximum of the solution becomes infinite in a finite time. Numerical experiments confirm this criterion.

To obtain the initial data, it is convenient to use self-similar solutions of the form

$$u_0(x)=A\left(1-x^2\right)^{1/(m_1-1)},\ v_0(x)=B\left(1-x^2\right)^{1/(m_2-1)}$$

where A, B — scaling constants. Such functions provide a smooth "hump" for the initial conditions and allow for the correct initiation of numerical simulations.

Numerical solutions. Consider a one-dimensional spatial domain $[0,L]$. Introduce a uniform spatial grid $x_i=i\Delta x$, where $\Delta x=L/N$, and a uniform time grid $t^n=n\Delta t$, $n=0,1,2,\text{K}$ The unknown functions $u(x,t)$ and $v(x,t)$ approximated by the grid values $u_i^n\approx u\left(x_i,t^n\right)$ and $v_i^n\approx v\left(x_i,t^n\right)$

To approximate the equation for the component u, we use a fully implicit scheme of the form:

$$\frac{u_i^{n+1}-u_i^n}{\Delta t}=\frac{F_{i+1/2}^{n+1}-F_{i-1/2}^{n+1}}{\Delta x}+\left(u_i^n\right)^{\beta_1},\ i=1,\text{K},N-1 \tag{4}$$

where $F_{i+1/2}^{n+1}$ denotes the numerical flux on the half-cell $[x_i,x_{i+1}]$.

The nonlinear diffusion flux is defined by:

$$F_{i+1/2}^{n+1}=\left|\frac{\left(u_{i+1}^{n+1}\right)^{m_1}-\left(u_i^{n+1}\right)^{m_1}}{\Delta x}\right|^{p_1-2}\frac{\left(u_{i+1}^{n+1}\right)^{m_1}-\left(u_i^{n+1}\right)^{m_1}}{\Delta x}. \tag{5}$$

Similarly, a fully implicit scheme is constructed for the component v:

$$\frac{v_i^{n+1}-v_i^n}{\Delta t}=\frac{G_{i+1/2}^{n+1}-G_{i-1/2}^{n+1}}{\Delta x}+\left(v_i^n\right)^{\beta_2}, \tag{6}$$

where $G_{i+1/2}^{n+1}$ is defined analogously to (5) with the substitutions u a v,m_1 a m_2,p_1 a p_2.

The use of a fully implicit approximation significantly increases the stability of the numerical method in the presence of stiff nonlinear reaction terms.

The boundary conditions are incorporated into the numerical scheme through the values of the fluxes at the domain boundaries. At the left boundary $x=0$, nonlinear boundary fluxes are imposed:

$$F_{-1/2}^{n+1}=-\left(v_0^{n+1}\right)^{q_1},\ G_{-1/2}^{n+1}=-\left(u_0^{n+1}\right)^{q_2}$$

At the right boundary $x=L$, homogeneous Neumann conditions are used, which correspond to zero fluxes:

$$F_{N+1/2}^{n+1}=0,\ G_{N+1/2}^{n+1}=0$$

This approach ensures the conservativeness of the scheme and the correct transmission of the influence of nonlinear boundary conditions on the solution dynamics.

Since the schemes (4)-(6) are nonlinear, the Picard iterative method is applied at each time step. At the k - iteration, approximations $u^{(k+1)},v^{(k+1)}$ are computed using the values from the previous iteration $u^{(k)},v^{(k)}$ in the diffusion fluxes.

The iterative process continues until the convergence criterion

$$\max_i\left|u_i^{(k+1)}-u_i^{(k)}\right|<\varepsilon,\ \max_i\left|v_i^{(k+1)}-v_i^{(k)}\right|<\varepsilon$$

where $\varepsilon>0$ — is a prescribed tolerance.

The performed numerical experiments demonstrate the formation of localized peaks of the solutions near the boundary $x=0$, which is caused by the nonlinear boundary fluxes and superlinear reaction terms. In several regimes, a sharp growth of the maximum values of the solution is observed, indicating the possibility of blow-up in finite time.

For the analysis of the dynamics, three-dimensional plots of the evolution of the solutions $u(x,t)$ and $v(x,t)$ are used, which make it possible to clearly trace the influence of nonlinear diffusion and boundary interactions on the solution development. The obtained results are in good agreement with theoretical predictions for nonlinear porous-medium-type equations with reaction.

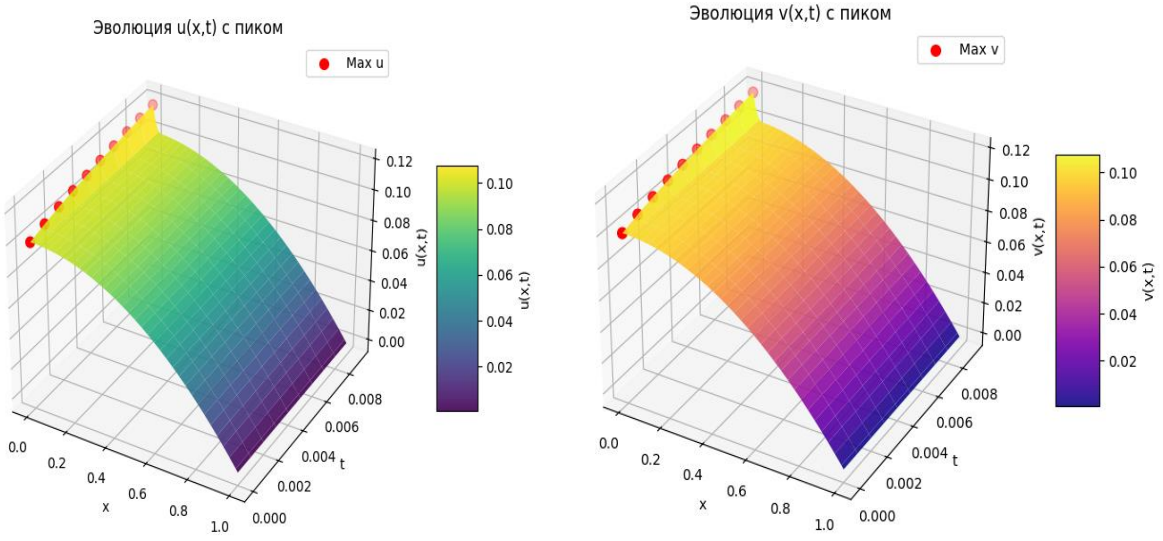

Figure 1: Evolution $u(x,t)$ and $v(x,t)$ with solution peaks with parameters: $m_1 = 2, m_2 = 2$, $p_1 = 3, p_2 = 3, \beta_1 = 2, \beta_2 = 2$, $q_1 = 1.5, q_2 = 1.5$

Stability of the scheme. Let us consider the stability of the proposed fully implicit finite-difference scheme. Note that the presence of nonlinear diffusion operators and superlinear reaction terms significantly complicates a rigorous analysis. However, for the scheme under consideration, it is possible to obtain a priori estimates that guarantee the numerical stability of the solution up to the moment of a possible blow-up.

Let's consider the component u . Multiply the difference equation (4) by u_i^{n+1} and sum over $i = 1, \text{K}, N-1$:

$$\sum_{i=1}^{N-1} \frac{u_i^{n+1} - u_i^n}{\Delta t} u_i^{n+1} = \sum_{i=1}^{N-1} \frac{F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}}{\Delta x} u_i^{n+1} + \sum_{i=1}^{N-1} \left(u_i^{n+1}\right)^{\beta_1+1}.$$

The left-hand side can be rewritten as

$$\sum_{i=1}^{N-1} \frac{1}{2\Delta t} \left(\left|u_i^{n+1}\right|^2 - \left|u_i^n\right|^2 + \left|u_i^{n+1} - u_i^n\right|^2 \right)$$

which reflects the dissipative nature of the time discretization. Using discrete integration by parts for the flux term, we obtain

$$\sum_{i=1}^{N-1} \frac{F_{i+1/2}^{n+1} - F_{i-1/2}^{n+1}}{\Delta x} u_i^{n+1} = -\sum_{i=1}^{N-1} F_{i+1/2}^{n+1} \frac{u_{i+1}^{n+1} - u_i^{n+1}}{\Delta x} + B_u^{n+1}$$

where B_u^{n+1} denotes the contribution of the boundary fluxes. Substituting the expression for the flux (5), we obtain

$$-\sum_{i=0}^{N-1} \left| \frac{\left(u_{i+1}^{n+1}\right)^{m_1} - \left(u_i^{n+1}\right)^{m_1}}{\Delta x} \right|^{p_1},$$

which is a nonpositive quantity and accounts for the energy dissipation caused by nonlinear diffusion. Analogous arguments apply to the component v . Thus, up to the blow-up time, the following a priori estimate holds:

$$\left\|u^{n+1}\right\|_{l^2}^2 + \left\|v^{n+1}\right\|_{l^2}^2 + \Delta t \sum_{k=0}^{n} \left(\left\|\nabla_h \left(u^{m_1}\right)^{k+1}\right\|_{l^{p_1}}^{p_1} + \left\|\nabla_h \left(v^{m_2}\right)^{k+1}\right\|_{l^{p_2}}^{p_2} \right) \le C\left(t^n\right),$$

where ∇_h denotes the discrete gradient, and the function $C(t)$ is finite for all $t < t^*$, where t^* - is the possible blow-up time. Consequently, the fully implicit scheme is conditionally stable up to the onset of solution singularity. The obtained estimate confirms the correctness of the numerical method and explains its ability to reliably reproduce the solution dynamics up to blow-up..

Conclusion. A nonlinear diffusion system with boundary flows is considered. The definition of a weak solution, energy estimation, and a blow-up criterion allow us to understand the system's dynamics. Self-similar initial data ensure a correct start to the numerical solution. Numerical experiments in 1D demonstrate peak growth and a possible blow-up, which is confirmed by 3D plots. This work can be extended to multidimensional problems and more complex nonlinearities.

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