

UDC 516.9

NUMERICAL SOLUTIONS OF MULTIDIMENSIONAL CROSS-DIFFUSION PROBLEMS WITH NONLINEAR BOUNDARY CONDITIONS AND VARIABLE DENSITY

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Abstract. This article studies the asymptotic behavior of self-similar solutions within a nonlinear cross-diffusion system characterized by nonlocal boundary conditions. The principal term of the asymptotic behavior of self-similar solutions has been established. A method for selecting the initial approximation for the iterative process in the numerical study of the problem is proposed. Numerical computations and result analysis were conducted utilizing asymptotic formulas as a preliminary approximation for the iterative procedure.

Keywords: cross-diffusion, nonlocal boundary condition, self-similar.

1 INTRODUCTION

Cross-diffusion is when the parts of a mixture interact with each other by having their own spatial distribution that affects the other parts. In cross-diffusion, one part affects how another part moves. In normal diffusion, each part moves on its own from high to low concentration. This interaction is very important in systems with more than one phase, like chemical solutions, groups of living cells, or processes in ecosystems.

Cross-diffusion is one of the most fundamental phenomena in the modeling of multicomponent transport processes. The initial development of this concept is associated with the work of Shigesada, Kawasaki, and Teramoto [1], who first substantiated the possibility of spatial segregation of species due to cross-flows. Similar ideas were developed in the studies of Gurtin [2], Bazykin [3], as well as in classical models of taxis and chemotaxis reviewed by Horstmann [4].

Cross-diffusion arises as a result of the interaction of several physical mechanisms, including thermomigration and thermal diffusion (the Soret and Dufour effects) [5, 6], autocatalytic chemical reactions [7], predation and avoidance in biological systems [8, 9], chemotaxis and taxis of bacteria [10], and combined heat and mass transfer in porous media [11].

Cross-diffusion mechanisms are widely manifested in physics, chemistry, and engineering. Multicomponent gas mixtures Maxwell–Stefan models describe the interaction of gas flows during co-diffusion [12, 13]. Thermal diffusion and thermomigration Soret and Dufour effects lead to the movement of matter under the action of temperature gradients [5, 6]. Chemical reaction-diffusion systems nonlinear diffusion causes various blow-up regimes in reaction-diffusion processes [7]. Engineering problems and nanofluids cross-diffusion plays an important role in heat and mass transfer processes in porous media [14], nanofluids [15], MHD systems [16], rotating disk flows [17].

2 PROBLEM STATEMENT

The paper examines the asymptotic behavior of solutions within a multidimensional cross-diffusion system characterized by nonlinear boundary conditions.

$$\rho(x) \frac{\partial u}{\partial t} = \nabla \cdot (v^{m_1-1} \nabla(u)), \quad \rho(x) \frac{\partial v}{\partial t} = \nabla \cdot (u^{m_2-1} \nabla(v)), \quad x \in R_+, \quad t > 0, \quad (1)$$

$$-v^{m_1-1} \frac{\partial u}{\partial x_1}(0, t) = u^{q_1}(0, t), \quad -u^{m_2-1} \frac{\partial v}{\partial x_1}(0, t) = v^{q_2}(0, t), \quad t > 0, \quad (2)$$

$$u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), \quad x \in R_+, \quad (3)$$

where $R_+^N = \{(x_1, x') \mid x' \in R^{N-1}, x_1 > 0\}$, $\rho(x) = (1 + |x|)^n$, $m_i > 1$, $q_i > 0 (i=1,2)$, u_0 and $v_0(x)$ are non-negative continuous functions with compact support in R_+^N .

Cross-diffusion refers to the phenomenon whereby the spatial displacement of one entity, defined by a certain variable, transpires as a result of the diffusion of another entity, defined by a different variable [18].

The principles of cross-diffusion are evident across multiple domains of natural sciences, including physical systems, chemical systems dynamics of electrolytic solutions, biological systems cross-diffusion transfer, population dynamics, ecology (forest age structure dynamics), and seismology, exemplified by the Burridge-Knopoff model of tectonic plate interactions. Cross-diffusion mathematical models are extensively employed in the analysis of biological population dynamics and tectonic plate movement [22, 23]. In [26, 27], the authors investigated the criteria for global solvability and non-solvability of the solution over time and established an estimate of the solution in proximity to the blow-up time of the nonlocal diffusion problem.

$$u_t = u_{xx}, \quad v_t = v_{xx}, \quad x > 0, \quad 0 < T < \infty, \quad (4)$$

$$-u_x(0, t) = u^\alpha v^p, \quad -v_x(0, t) = u^q v^\beta, \quad 0 < t < T, \quad (5)$$

$$u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), \quad x > 0. \quad (6)$$

If $pq \leq (1-\alpha)(1-\beta)$, then it is proven that each solution of problem (4) - (6) is global. The following problems were studied in [10]:

$$u_t = (u^n)_{xx}, \quad v_t = (v^k)_{xx}, \quad x \in R_+, \quad t > 0, \quad (7)$$

$$-(u^n)_x(0, t) = v^p(0, t), \quad -(v^k)_x(0, t) = u^q(0, t), \quad t > 0, \quad (8)$$

$$u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), \quad x \in R_+, \quad (9)$$

It is shown that the solution to problem (7) - (8) is global in $pq \leq (n+1)(k+1)/4$. For the numerical parameters of systems (7) - (9), conditions are obtained under which the solution of the problem blows up in finite time.

It is also noteworthy that in [29], system (7) was studied with the following boundary conditions.

$$-(u^n)_x(0, t) = u^\alpha v^p(0, t), \quad -(v^k)_x(0, t) = u^q v^\beta(0, t), \quad t > 0.$$

The following equality is proven: $\min\{y_1 - r_1, y_2 - r_2\} = 0$, where

$$r_1 = \frac{2p+k+1-2\beta}{4pq-(k+1-2\alpha)(n+1-2\beta)}, \quad r_2 = \frac{2p+n+1-2\beta}{4pq-(k+1-2\alpha)(n+1-2\beta)},$$

$$y_1 = \frac{1-r_1(n-1)}{2}, \quad y_2 = \frac{1-r_2(k-1)}{2},$$

is a critical exponent of the Fujita type.

The examination of requirements for global solvability and non-solvability of problems (1) - (3) across diverse numerical parameter values has been the focus of numerous investigations [18-34].

3 METHOD OF SOLUTION

This research focuses on the asymptotic analysis of self-similar solutions to problems (1) - (3). In the scenario of slow diffusion ($m_i, m_2 > 1$), multiple self-similar solutions to problems (1) - (3) are formulated, illustrating the asymptotic behavior of the solutions to the given problem. Proposed are methods for selecting suitable initial approximations for the iterative process in numerical research that maintain the qualitative aspects of problems (1) - (3). A methodical methodology was established, and numerical computations were executed, illustrating swift convergence to the precise solution.

The system of equations (1) delineates processes characterized by a finite propagation speed of disturbances when $m_i > 1 (i=1,2)$. Equations (1) are degenerate at $u(x, t), v(x, t) = 0$, so problem (1) - (3) permits a generalized solution that is deficient in requisite smoothness at the sites of degeneracy.

The system (1) possesses compactly supported self-similar solutions characterized by the form

$$\begin{cases} \underline{u}(x,t) = (T+t)^{-\alpha_1} f(\xi), \\ \underline{v}(x,t) = (T+t)^{-\alpha_2} \varphi(\xi), \end{cases} \tag{10}$$

where $\xi = |\zeta|$, $\zeta_1 = (x_1 + h_1)(T+t)^{-\beta}$, $\zeta_i = x_i(T+t)^{-\beta}$, $(i = 2, \dots, N)$, $T > 0$, $\beta = \frac{q_1 - m_2}{2q_1 - m_2 - 1} = \frac{q_2 - m_1}{2q_2 - m_1 - 1}$, $\alpha_1 = \frac{1}{2q_1 - m_2 - 1}$, $\alpha_2 = \frac{1}{2q_2 - m_1 - 1}$ and $(f(\xi), \varphi(\xi))$ are solutions to the following problems

$$\begin{cases} \xi^{N-1} \frac{d}{d\xi} \left(\xi^{1-N} \varphi^{m_1-1} \frac{df}{d\xi} \right) + \beta \xi^{n+1} \frac{df}{d\xi} + \alpha_1 \xi^n f = 0, \\ \xi^{N-1} \frac{d}{d\xi} \left(\xi^{1-N} f^{m_2-1} \frac{d\varphi}{d\xi} \right) + \beta \xi^{n+1} \frac{d\varphi}{d\xi} + \alpha_2 \xi^n \varphi = 0, \end{cases} \tag{11}$$

$$\begin{cases} -\varphi^{m_1-1} \frac{df}{d\xi}(0) = f^{q_1}(0), \\ -f^{m_2-1} \frac{d\varphi}{d\xi}(0) = \varphi^{q_2}(0), \end{cases} \tag{12}$$

This is obtained by substituting (10) into (1) - (3) and performing some simplifications. Let us consider the following functions

$$\begin{cases} \tilde{f}(\xi) = (a - \xi^2)^{\frac{1}{m_2-1}}, \\ \tilde{\varphi}(\xi) = (a - \xi^2)^{\frac{1}{m_1-1}}, \end{cases} \tag{13}$$

where $a > 0$.

Theorem. Suppose $m_1 > 1$ and $m_2 > 1$, then the compactly supported solution of the system of equations (11) has $\xi \rightarrow \sqrt{a}$ the asymptotics

$$\begin{cases} f(\xi) = c_1 \tilde{f}(\xi)(1 + o(1)), \\ \varphi(\xi) \simeq c_2 \tilde{\varphi}(\xi)(1 + o(1)), \end{cases} \tag{14}$$

where $c_1 = \left(\frac{\beta(m_2 - 1)}{n + 2} \right)^{1/(m_1 - 1)}$, $c_2 = \left(\frac{\beta(m_1 - 1)}{2} \right)^{1/(m_2 - 1)}$.

The theorem is proven as in [30].

4 RESULTS

The numerical system is formulated using the finite difference approach. Equations (1) are approximated with second-order precision in spatial coordinates and first-order precision in time for this purpose. An iterative procedure is established, whereby node values are computed utilizing the expansion approach during the inner iteration phases. In general, the primary challenge in numerically resolving the nonlinear problem (1) - (3) lies in choosing a suitable initial approximation for the iterative procedure.

Functions that include certain characteristics of the desired solutions are employed while addressing particular problems. These functions are derived from a qualitative investigation of the issue. This challenge is surmounted by effectively choosing initial approximations based on the values of the numerical parameters in the equations. An established asymptotic formula is employed in the computations for this purpose. Numerical computations were conducted based on the aforementioned results. Below are shown some outcomes of the numerical methodologies and computer experiments.

A computational experiment was conducted using the aforementioned numerical schemes. Some results of the numerical experiments are presented below. The grid step is very small, $h = 0.05$, the number

of nodes is $N = 2500$, and the $\varepsilon = 10^{-3}$ iteration accuracy is specified. The calculation was carried out up to $t = 22$ with $\tau = 0.02$ time steps. Formulas (10) and (14) were used as the initial approximation for the iterative process.

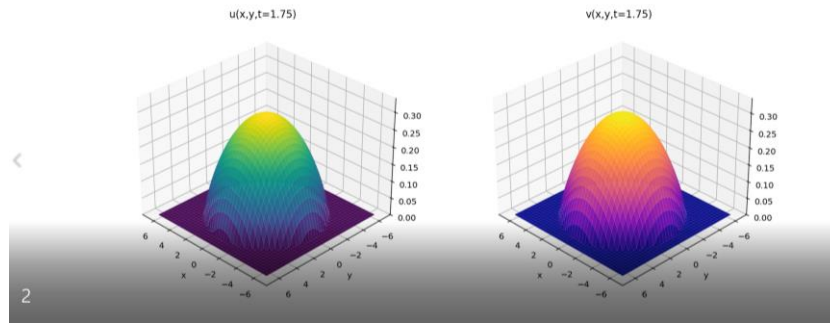


Fig. 1. The numerical solution of problem (1) - (3), $T=1.75$. $q_1 = 4.75, q_2 = 5.5, m_1 = 1.15, m_2 = 1.35$

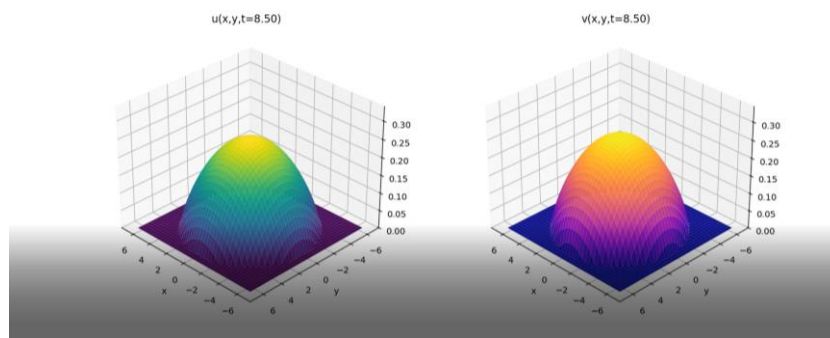


Fig. 2. The numerical solution of problem (1) - (3), $T=8.5$. $q_1 = 4.75, q_2 = 5.5, m_1 = 1.15, m_2 = 1.35$

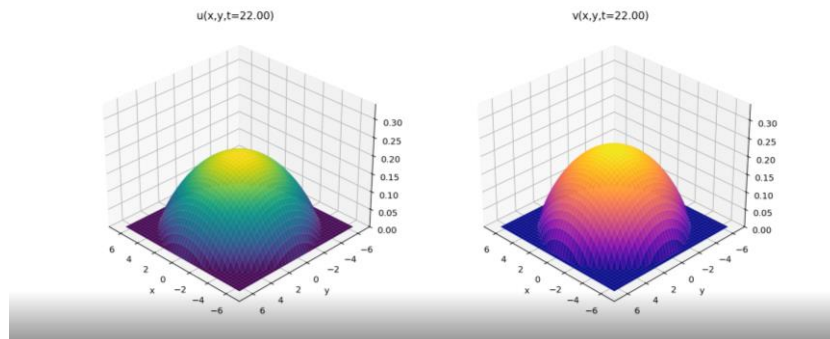


Fig. 3. The numerical solution of problem (1) - (3), $T=22$. $q_1 = 4.75, q_2 = 5.5, m_1 = 1.15, m_2 = 1.35$

Figures 1-3 show the results of the numerical solution of problem (1) - (3), corresponding to the case of slow diffusion. Asymptotic formulas $m_i > 1$ ($i = 1, 2$) (10), (14) and graphs demonstrate that the body moves at a finite velocity. The propagation depth of the diffusion wave depends on time and the wave front (the point where $\underline{u}(x,t), \underline{v}(x,t)$ vanishes), and for each medium, it is located at the endpoint. The asymptotic formulas $x_\phi = \sqrt{a}(T+t)^\beta < \infty$, (10), (14) and graphs indicate that the body moves at a finite velocity.

5 CONCLUSION

The mathematical model formulated in equations (1) - (3) was studied for the numerical solution of a multidimensional cross-diffusion process with nonlinear boundary conditions. In this case, density is of crucial importance in determining the dynamics of diffusion. The results show that the addition of density-dependent terms has a significant effect on the rate and direction of mass transfer in the system. Changes

in density gradients change the diffusion rate and the stability of the resulting structures. This clearly demonstrates the strong dependence between the concentration and density distribution in multicomponent media. The analysis shows that under conditions of slow diffusion, diffusion "particles" propagate in the medium at a finite speed and the depth of the diffusion wave develops over time. In this case, the wave front corresponds to the boundary of each medium. In multidimensional conditions, this process becomes even more complicated, since density inhomogeneities and nonlinear boundary effects together determine the spatial location and development of diffusion fronts. These results are especially important for studying real-world physical systems where diffusion processes depend on density changes. For example, they are used in the fields of oil transport, biophysical diffusion (such as drug delivery through tissues), and materials science. They also give useful information for controlling how substances spread in heterogeneous media and making more accurate models of transport phenomena that depend on density and selectivity.

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Received: July 25, 2025

Citation: Urunbaev J.E. 2025. Numerical solutions of multidimensional cross-diffusion problems with nonlinear boundary conditions and variable density. *International journal of theoretical and applied issues of digital technologies*. Volume 8, Issue 4, pp. 123-128. <https://doi.org/10.62132/ijdt.v8i4.312>.

ЧИСЛЕННОЕ РЕШЕНИЕ МНОГОМЕРНЫХ ЗАДАЧ КРОСС-ДИФФУЗИИ С НЕЛИНЕЙНЫМИ ГРАНИЧНЫМИ УСЛОВИЯМИ И ПЕРЕМЕННОЙ ПЛОТНОСТЬЮ

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Аннотация. В данной статье исследуется асимптотическое поведение автомодельных решений в нелинейной системе кросс-диффузии, характеризующейся нелокальными граничными условиями. Установлен главный член асимптотики автомодельных решений. Предложен метод выбора начального приближения для итерационного процесса при численном исследовании задачи. Численные расчеты и анализ результатов проводились с использованием асимптотических формул в качестве предварительного приближения для итерационной процедуры.

Ключевые слова: кросс-диффузия, нелокальное граничное условие, автомодельный.