RESEARCH ARTICLE

Computer Simulation of Diffusion in a Mixture of Ideal Gases Considering the Dependence of the Diffusion Coefficient on the Entropy of Mixing Using Finite Element Method

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Abstract

The objective of the research was to perform computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing according to the proposed mathematical model. Computer simulation was carried out in one-dimensional and two-dimensional settings using finite element method and Python programming language with the use of NumPy and SciPy libraries. The obtained results show that the proposed mathematical model of diffusion in a mixture of ideal gases could be used to solve computer simulation tasks of gas diffusion satisfying the principle of mass conservation, because the entropy is considered via the chemical potential.

Keywords: computer modeling, mathematical modeling, gas diffusion, entropy of gas mixing, chemical potential, finite element method, numerical methods.

Submitted: 29 September 2025
Accepted: 12 October 2025
Published: 29 October 2024

Vol. 1, **No.** 2, 2025.
10.62762/JNSPM.2025.504999

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1 Introduction

The process of gas diffusion is fundamental for solving certain problems in various areas of human activity, such as agricultural industry and ecology [1], engineering [2], biology [3], medicine [4], veterinary science [5] et al. But despite the fact that lots of studies were devoted to the description of diffusion in gases [1–5], there still are some gaps in this description which were described by the great scientists a century ago [6, 7] which remain unfilled to this day. Thus, J. Gibbs, in analyzing the change in entropy during gas diffusion [6], established that the increase in entropy caused by mixing different types of gases at constant temperature and pressure does not depend on the nature of these gases, while the displacement of two masses of the same ideal gas does not cause an increase in entropy. Thus, the mixing of two identical gases cannot be considered as a limiting case of mixing two different gases, and when moving from mixing

Citation
Shalkevich, P., & Tsvikevich, N. (2025). Computer Simulation of Diffusion in a Mixture of Ideal Gases Considering the Dependence of the Diffusion Coefficient on the Entropy of Mixing Using Finite Element Method. *Journal of Numerical Simulations in Physics and Mathematics*, 1(2), 60–66.

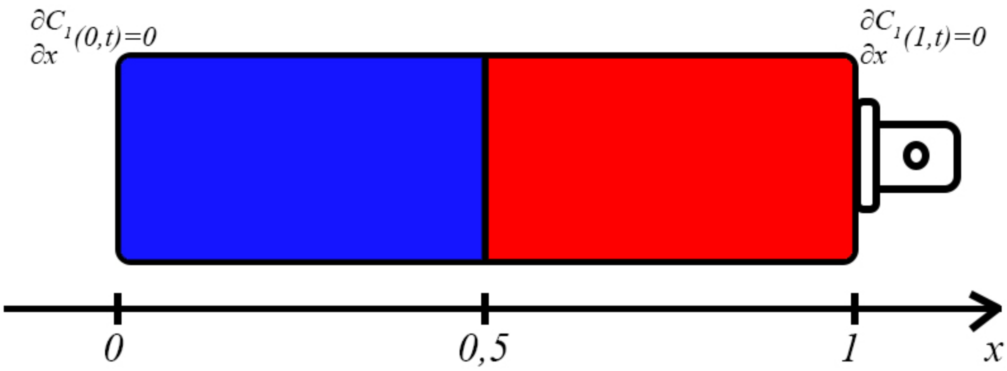


Figure 1. The initial conditions for computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting, $D_{eff} = 0.002$.

arbitrarily close gases to mixing identical gases, the change in entropy experiences a jump (Gibbs paradox) [6]. And A. Einstein in his work on the quantum theory of an ideal gas, drew attention to the paradox [7] to which this theory leads, which consists in the fact that a mixture of degenerate gases of N_1 atoms with mass m_1 and N_2 atoms with mass m_2 (arbitrarily slightly different from m_1) at a given temperature has a different pressure than a simple gas with the number of atoms $N_1 + N_2$, which has practically the same mass of atoms and is in the same volume.

The above largely explains the existing practice and approaches in the field of computer simulation of gas mixing [8–11], which, with a certain reliability, does not explain the entire nature of diffusion processes of gas mixing. These historical paradoxes and limitations of current practices highlight the need for diffusion models that incorporate fundamental thermodynamic principles.

This paper presents results of computer simulation of diffusion in a mixture of ideal gases using mathematical model which considers the dependence of the diffusion coefficient on the entropy of mixing. Computer simulation was carried out in one-dimensional and two-dimensional settings using finite element method and Python programming language (using NumPy and SciPy libraries).

2 Computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting

Considering that the entropy of a mixture of ideal gases is equal to the sum of entropies of all of its components, taken at the temperature of the mixture and partial pressures P_i of each i component. In such a case, the entropy of mixing can be represented in the following form

$$\Delta S_{mix} = -R\left(\sum_{i=1}^{n}\frac{M_i}{\nu_i}\right)\left(\sum_{i=1}^{n} x_i \ln(x_i)\right), \quad (1)$$

where x_i is the molar concentration of each component i of the mixture, M_i is the mass of the i gas, and v_i is the molar mass of the i gas. Considering the entropy of mixing for a mixture of ideal gases, the mass flow of component x_i will be determined not only by its gradient, but also by the degree of disorder of the mixture, i.e., the entropy of mixing:

$$q_i = -D_i \Delta S_{mix} x_i \nabla \mu_i, \quad (2)$$

where D_i is the diffusion coefficient of the x_i component, S_{mix} is the entropy of mixing, and μ_i is the chemical potential of the gas i.

It should be noted that the diffusion coefficient of component 1 is not equal to the diffusion coefficient of component 2.

The chemical potential for an ideal gas at low pressures is known [12]:

$$\mu_i = RT\ln(x_i) + \mu_0(T) \quad (3)$$

Hence,

$$\nabla\mu_i = \nabla RT\ln(x_i) = R\ln(x_i)\nabla T + \frac{RT}{x_i}\nabla x_i. \quad (4)$$

Considering that $\ln(f) = f'/f$, for a binary mixture in a unit volume we obtain the equality

$$\vec{q}_i = -D_i \Delta S_{cx_i} R x_i \nabla \mu_i = -D_{ieff}\left(T\nabla x_i + ln x_i \nabla T\right). \quad (5)$$

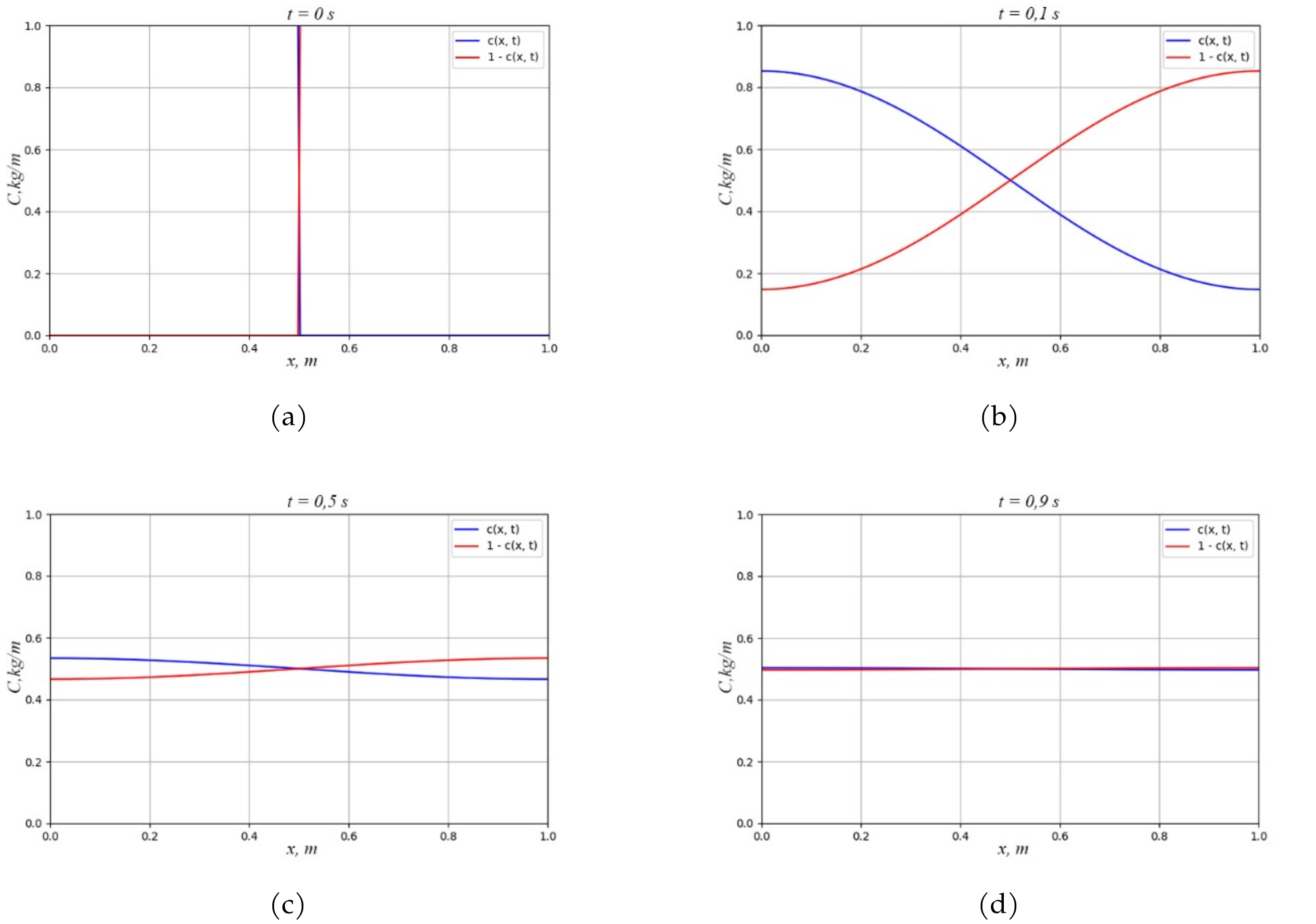


Figure 2. Results of the computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting: (a) at the initial time; (b) at time t = 0.1 s; (c) at time t = 0.5 s; (d) at time t = 0.9 s.

Therefore, the effective diffusion coefficient for a mixture of ideal gases, considering the entropy of mixing, is determined by the following expression:

$$D_{ieff} = D_i \Delta S_{mixx_i} R. \tag{6}$$

So, for computer simulation of diffusion in a mixture of ideal gases, considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting, the diffusion equation will have the following form

$$\frac{\partial C_1}{\partial \tau} = \frac{\partial}{\partial x}\left(D_{eff} C_1 \frac{\partial}{\partial x}\left(T ln C_1\right)\right), \tag{7}$$

where C_1 is the concentration of gas 1 at the X point at time t (%), D_{eff} is the effective diffusion coefficient ($K^o \cdot s/m^2$), and T is the temperature of the gas mixture (K^o).

As the initial conditions for computer simulation of diffusion in a mixture of ideal gases, considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting, we use the following: gases 1 and 2 are separated by an impermeable membrane and are located in a 1 m long cylinder (Figure 1). The membrane is located at a distance of 0.5 m from the ends of the cylinder. At a certain point in time, the membrane is removed and diffusion mixing of gases 1 and 2 occurs. It is required to find the evolution in time and the dependence on the coordinate x of the concentration of gases 1 and 2. In this case, C_2 is the concentration of gas 2 at the X point at time t.

Initial and boundary conditions have the following form:

$$\begin{aligned} &C_1 + C_2 = 1, \quad C_1(x,0) = 1, \forall x \in [0;0.5], \\ &C_1(x,0) = 0, \forall x \in [0.5;1] \end{aligned} \tag{8}$$

$$\frac{\partial C_1}{\partial x}(0,t) = 0, \forall t > 0, \quad \frac{\partial C_2}{\partial x}(1,t) = 0, \forall t > 0 \tag{9}$$

Equations (9) show that the gas mass flows on the left and the right walls of the vessel are zero.

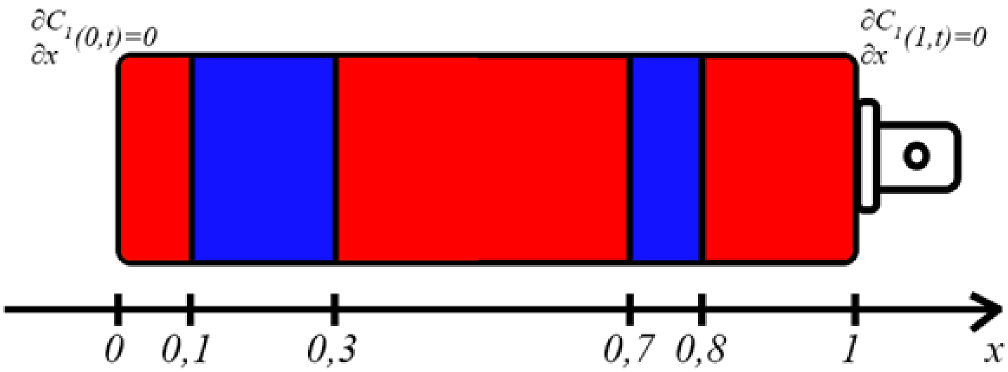


Figure 3. The initial conditions for computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting of the more complicated task, $D_{eff} = 0.002$.

Computer simulation was carried using finite element method and NumPy and SciPy libraries of Python programming language. The results are shown in Figure 2, where the change in concentration of gas 1 is shown in red and gas 2 – in blue.

The task described above is the simplest case two gases mixing, but in real conditions, it is necessary to solve more complex tasks. Therefore, it makes sense to consider the solution of the task with the following conditions:

$$C_1(x,0) = 1, \forall x \in [0.1; 0.3] \cup [0.7; 0.8]. \tag{10}$$

Moreover, on intervals not shown in (7), the next condition is met:

$$C_1(x,0) = 0. \tag{11}$$

A schematic interpretation of the problem with the initial conditions described in (10), (11) is shown in Figure 3.

Computer simulation of the task described in the Figure 3 was carried out using the finite element method and NumPy and SciPy libraries of Python programming language. The results are shown in Figure 4, where the change in concentration of gas 1 is shown in red and gas 2 – in blue.

3 Computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a two-dimensional setting

Let us consider a closed square with a side length of 1 (Figure 5). A small closed square is placed in it and filled with gas A (red). Outside the small square, the large square is filled with gas B (blue). When the walls of the small square are removed diffuse mixing of gases A and B begins. The concentration of gases A and B at any point at any time should be calculated.

Equation (1) for a two-dimensional setting will take the following form:

$$\frac{\partial C_1}{\partial \tau} = \frac{\partial}{\partial x}\left(D_t C_1 \frac{\partial}{\partial x}(TlnC_1)\right) + \frac{\partial}{\partial y}\left(D_t C_1 \frac{\partial}{\partial y}(TlnC_1)\right). \tag{12}$$

To solve the task at hand, it is necessary to fulfill the following conditions

$$C_1(x,y,t) = 1, \forall x \in \left[0,4;0,6\right], \forall y \in \left[0,4;0,6\right], \tag{13}$$

$$C_1\left(x,y,t\right) = 0, \forall x, \quad C_1\left(x,0\right) = 0, \tag{14}$$

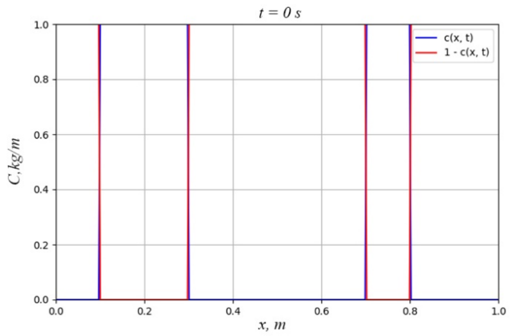
$$\frac{\partial C_1}{\partial x}(0,y,t) = 0, \quad \frac{\partial C_1}{\partial x}(1,y,t) = 0, \quad \frac{\partial C_1}{\partial y}(x,0,t) = 0, \tag{15}$$

$$\frac{\partial C_1}{\partial y}(x,1,t) = 0, \quad D_t = 0,002, \quad T = 283K^o. \tag{16}$$

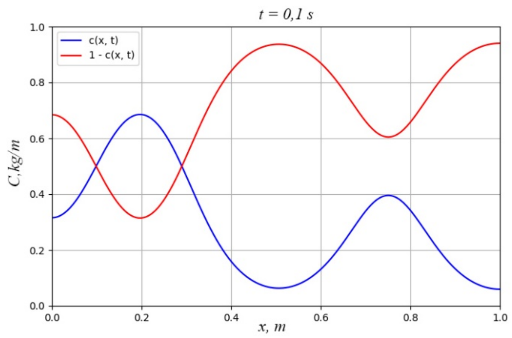
The results of computer simulation of the task which was carried out using finite element method and Python programming language (using NumPy and SciPy libraries) are shown in Figure 6.

4 Conclusion

The conducted research and the obtained solutions show that proposed mathematical model of diffusion in a mixture of ideal gases which considers the dependence of the diffusion coefficient on the entropy of mixing could be used to solve computer simulation tasks of diffusion in a mixture of gases. In addition, this research demonstrates an approach that allows to model diffusion processes of gas mixtures considering the basic thermodynamics provisions by taking into



(a)



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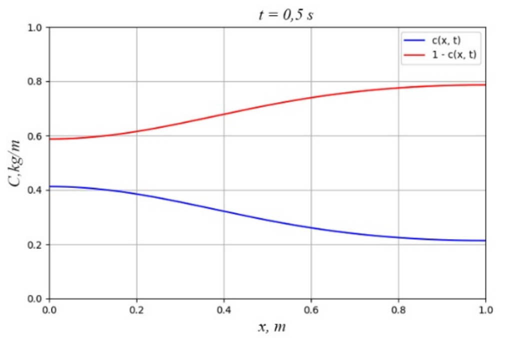

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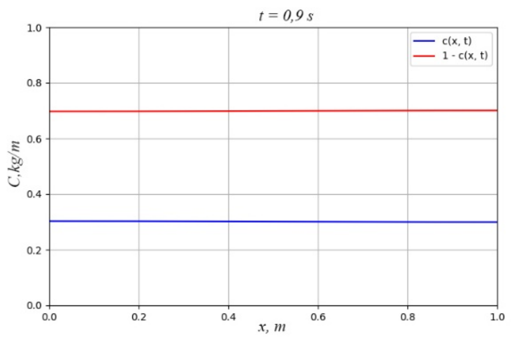


(d)

Figure 4. Results of the computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a one-dimensional setting of the more complicated task: a) at the initial time; b) at time t = 0.1 s; c) at time t = 0.5 s; d) at time t = 0.9 s.

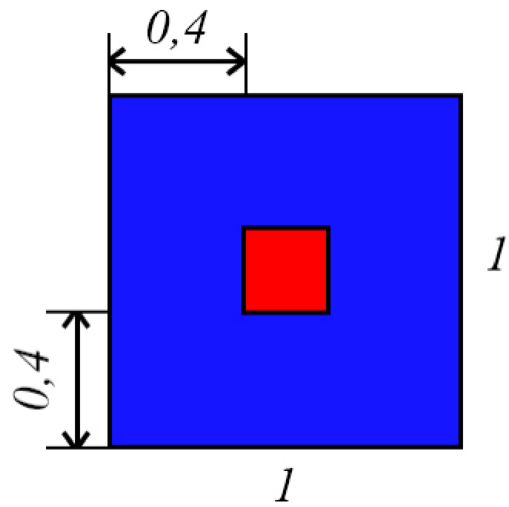
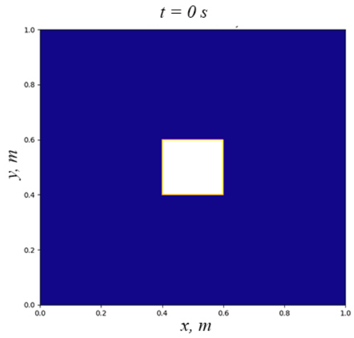
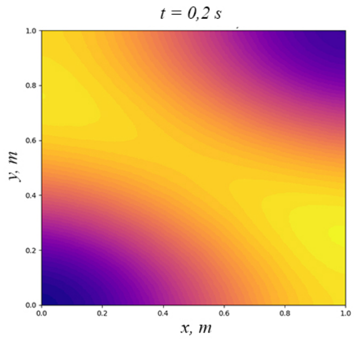


Figure 5. The initial conditions for computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a two-dimensional setting.

account the effect of the temperature gradient on diffusion. The presented approach of gas diffusion modeling allows to predict the mass transfer coefficient solving tasks of convective drying in conditions when the concentrations of steam and air are comparable, basing on the fact that the mass flow can be used to determine the chemical potential. It is also important to highlight the difference between the proposed gas diffusion model and other gas diffusion entropy models which were used to solve heat and mass transfer tasks. The application of that models requires considering the entropy function jump caused by the Gibbs paradox, which in practical use causes problems associated with the impossibility of fulfilling the principle of mass conservation due to the entropy function discontinuity. Whereas the proposed gas diffusion model demonstrates the classical approach to solving heat and mass transfer tasks using entropy indirectly, considering the dependence of the diffusion coefficient on the entropy of mixing. And, since the entropy is considered via the chemical potential, which can be determined using the mass flow, the proposed model satisfies the principle of mass conservation. On the same basis, there are prospects for applying the proposed gas diffusion model which considers the dependence of the diffusion coefficient on the entropy of mixing to solve isotope separation tasks and the tasks of cross effects in structurally inhomogeneous media. Also, considering that the entropy approach can be used to model gas flow and adsorption in porous media [13], the proposed model can also be used to improve the author's previously developed



(a)



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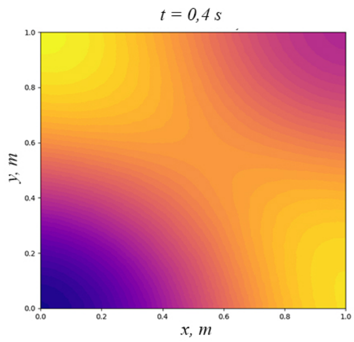

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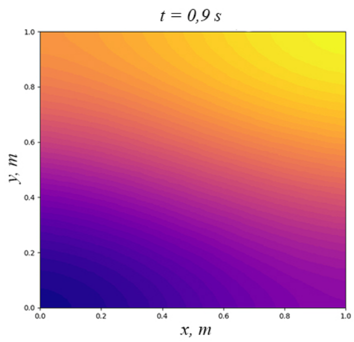

(d)

Figure 6. Results of the computer simulation of diffusion in a mixture of ideal gases considering the dependence of the diffusion coefficient on the entropy of mixing in a two-dimensional setting: a) at the initial time; b) at time t = 0.2 s; c) at time t= 0.4 s; d) at time t= 0.9 s.

model of pollutants migration in soils [14].

Despite the fact that calculation of the entropy of gas mixing was not the purpose of this study, the definition of the diffusion coefficient obtained in the presented work makes it possible to evaluate the change of the entropy in subsequent works. Also, it should be noted that the numerical evaluation of the change of the entropy of gas mixing according to the proposed model, as well as the verification of this model and the search for the most acceptable numerical methods for its solution will be the topics of further researches.

Data Availability Statement

Data will be made available on request.

Funding

This work was supported without any funding.

Conflicts of Interest

The authors declare no conflicts of interest.

Ethical Approval and Consent to Participate

Not applicable.

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