

Modeling mass transfer processes in multicomponent capillary–porous bodies under mixed boundary conditions

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In this study, we present a physicomathematical model for convective drying of a multicomponent body of the capillary-porous structure, considering moisture transfer dynamics at both macro and micro levels. Recognizing the impact of the material's local structure on drying processes, particularly in phase transformations, the model integrates the continuum-thermodynamic approach pioneered by Ya. Burak, Ye. Chaplya, and B. Gayvas. This approach addresses the interrelated mechanical, thermal, and diffusion processes occurring in heterogeneous, nonequilibrium systems, where local thermodynamic equilibrium assumptions allow equilibrium state descriptions by conjugate physical parameters. The unique dual-level approach captures moisture exchange between an individual grain and the grain bed, enabling realistic simulations of the drying process by directly accounting for phase transformations and material structure influences. The presented methodology allows simultaneous solving of mass transfer equations for the grain bed and individual grains, supported by numerical experimentation. The results reveal distinct moisture distribution patterns across the grain bed and within individual grains, with variations influenced by drying agent velocity. The novelty of this approach lies in its simultaneous treatment of grain-scale and bed-scale moisture transfer, providing a detailed perspective on moisture dynamics. This model has potential applications in optimizing industrial drying processes for capillary-porous materials, enhancing efficiency and cost-effectiveness.

Keywords: *drying; capillary-porous; moisture concentration; moisture diffusion; mixed boundary condition; phase transition; continuum-thermodynamics; mass transfer.*

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1. Introduction

The dynamics of drying processes are directly or indirectly influenced by the local (microscopic) structure of the material. Such influences are particularly related to the presence of physically distinct states of moisture particles, which differ in mobility and undergo phase transformations. The rate of moisture movement within the material primarily depends on the types of moisture bonding with the body, which should be considered on a microscopic level.

The continuum-thermodynamic approach to constructing physicomathematical models of solid solution mechanics, describing interconnected mechanical, thermal, and diffusion processes that account for local changes in the states of constituent components, was developed in the works of Ya. Burak and Ye. Chaplya, and was further advanced in the heat-moisture transfer models in capillary-porous bodies by B. Gayvas. This approach is based on the following principles: for spatially heterogeneous and nonequilibrium systems, the hypothesis of local thermodynamic equilibrium is assumed, which implies that the state of physically small subregions of the system is determined by conjugate physical parameters describing the equilibrium state. For mechanical, physical, and chemical processes, the conjugate parameters include pressure and volume, stress and strain tensors, absolute temperature and entropy for thermal conduction, and chemical potential and particle concentration for diffusion. Balance and kinetic relations, as well as equations of state, are used to determine changes in mass, energy, and momentum.

This approach is applied to the problem of convective drying of a layer of multicomponent capillary-porous material under mixed boundary conditions, where the displacement vector and the deviation of moisture concentration are taken as the solving functions.

2. Literature overview

The field of thermodynamics and statistical mechanics owes much of its foundation to J. Willard Gibbs, who, in his 1902 work, “Elementary Principles in Statistical Mechanics”, laid out essential principles that continue to guide scientific approaches to understanding equilibrium and non-equilibrium states in complex systems. Following Gibbs, significant contributions to the thermodynamics of irreversible processes were made by S. R. de Groot in “Thermodynamics of Irreversible Processes” and I. Gyarmati in “Non-Equilibrium Thermodynamics: Field Theory and Variational Principles”, who developed frameworks for describing energy dissipation in non-equilibrium systems. Similarly, the work of A. V. Luikov on heat and mass transfer in capillary-porous bodies extended these ideas specifically into drying processes, providing a basis for understanding diffusion and phase transitions within porous materials.

In Ukrainian science, Ya. Burak and Ye. Chaplya have made significant contributions to the development of continuum-thermodynamic models that integrate mechanical, thermal, and diffusion processes in capillary-porous materials [1–3]. Their collaboration with O. Chernukha advanced the principles of local thermodynamic equilibrium, introducing mathematical models that account for local changes in the states of the constituent components in solid solutions [1]. By the 1990s, Ye. Chaplya extended these continuum-thermodynamic models further by incorporating diffusion and structural effects within porous media, as detailed in his foundational works on the theory of solid solutions [2, 4].

B. Gayvas extended this approach to specific cases of convective drying, analyzing wood and other porous materials under realistic environmental conditions in a series of studies that refined the theoretical framework and practical application of these models [5–7, 11].

B. Gayvas et al. further contributed by developing numerical methods to simulate heat and mass transfer in capillary-porous materials, with practical applications in optimizing industrial drying processes for materials like wood and grains. This series of studies emphasized the structural effects of porous media, aiming for accurate predictions of drying rates and energy optimization within these processes [8–10].

The works of Y. Sokolovskyy et al. expanded these foundations by focusing on convection drying processes in anisotropic materials, accounting for phase transition boundaries, which are critical in modeling the complex moisture transport in anisotropic and biophysical materials. Their studies use mathematical models to account for anisotropy in materials, enabling simulations that more accurately reflect moisture distribution and heat transfer in heterogeneous media [17–19].

Concurrently, P. Pukach et al. contributed to modeling mass transfer through their studies on impurity diffusion in layered structures under statistical conditions. By formulating mathematical models incorporating stochastic influences from point mass sources, Pukach’s research provides additional insights into diffusive processes [16].

Recent works by P. Kostrobii, B. Markovych, M. Tokarchuk, and others contribute significantly to the statistical and kinetic modeling of complex systems, including semiconductor structures, catalytic processes, and dense fluids in non-equilibrium conditions. Notably, their studies provide insights into diffusion processes and reaction kinetics within porous and layered materials. These theories support the multiscale approach necessary for modeling moisture distribution in capillary-porous and granular media, as seen in drying applications [14, 15, 20].

B. Gera et al. have contributed to understanding temperature distribution in transport facility metal structures and the application of heat-resistant coatings, which indirectly support research on moisture and temperature management in capillary-porous bodies. These studies emphasize the importance of controlled drying conditions and structural adaptations for minimizing stress and deformation under thermal effects [12].

Research by Tuller and Hansmann on adsorption and capillary condensation in porous media provided additional insights into liquid retention mechanisms and interfacial configurations in angular pores. Their work has been instrumental in understanding moisture retention and movement, particularly relevant to drying processes in porous bodies [13, 21].

By applying a continuum-thermodynamic approach that integrates diffusion, phase transitions, and the effects of capillary-porous structures, our work utilizes the aforementioned thermodynamic principles of mass transfer to model moisture distribution under realistic mixed boundary conditions.

3. Materials and methods

We distinguish between the movement of moisture within the porous bed of the multicomponent material and the movement of moisture within individual particles. This distinction is necessary to consider the influence of all forms of moisture on the drying regime. The influence is associated with the presence of physically different states of moisture particles, which vary in mobility and undergo phase transformations.

A capillary-porous body is considered a solid solution of skeletal particles, moisture, and air. We assume that the equilibrium thermodynamic state of such a body is determined by the values of conjugate macroscopic parameters:

$$T \div S, \quad \sigma^{\alpha\beta} \div \varepsilon_{\alpha\beta}, \quad \mu'_k \div m_k, \quad \alpha, \beta = \overline{1, 3}, \quad k = \overline{0, 1},$$

where T is the absolute temperature, S is entropy, $\sigma^{\alpha\beta}$ are the components of the Cauchy stress tensor, $\varepsilon_{\alpha\beta}$ are the strain tensor components, μ'_k is the chemical potential of component k , and m_k is its mass. The quantities with index $k = 0$ correspond to the skeleton, and $k = 1$ corresponds to the moisture.

We assume the body is divided into representative physically small elements whose states are described by the same conjugate parameters as the entire body:

$$T \div \Delta S, \quad \sigma^{\alpha\beta} \div \varepsilon_{\alpha\beta}, \quad \mu'_k \div \Delta m_k, \quad \alpha, \beta = \overline{1, 3}, \quad k = \overline{0, 1}.$$

When deriving the equations of state, linear approximations are used for small deviations of the independent parameters $\delta T = T - T_0$, $\delta \varepsilon_{\alpha\beta} = \varepsilon_{\alpha\beta}$, and $\delta C_k = C_k - C_k^0$ from their values in the initial thermodynamic state:

$$s = s_0, \quad T = T_0, \quad \sigma^{\alpha\beta} = \tilde{P} \delta^{\alpha\beta}, \quad \varepsilon_{\alpha\beta} = 0, \quad C_k = C_k^0, \quad \mu'_k = \mu_k^0,$$

where \tilde{P} is the pore pressure, and $\delta^{\alpha\beta}$ is the Kronecker delta. Values marked with "0" denote initial state parameters.

Next, we present balance equations based on the solid solution theory model:

$$\begin{aligned} \sigma_{\alpha\beta} &= \left[\left(K - \frac{2}{3}G \right) \varepsilon - K\beta c \right] \delta_{\alpha\beta} + 2G\varepsilon_{\alpha\beta}, \\ \mu &= \mu^0 - \frac{K}{\rho_0} \beta \varepsilon + ac, \\ \nabla \cdot \hat{\sigma} &= 0, \quad \nabla \times (\nabla \times \hat{\varepsilon})^T = 0, \\ \frac{\partial c}{\partial \tau} &= D\Delta c - D_\varepsilon \Delta \varepsilon, \end{aligned}$$

where K is the bulk modulus, G is the shear modulus, β is the volumetric expansion coefficient, a is the chemical potential concentration coefficient, ρ_0 is the initial density, and ε is the first invariant of the strain tensor $\hat{\varepsilon} = [\nabla \otimes \mathbf{u} + (\nabla \otimes \mathbf{u})^T]/2$.

For a wet capillary-porous body, the vapor pressure in the pores \tilde{P} generally does not depend on moisture content and equals the saturation pressure P_{zn} , corresponding to the current temperature. During evaporation, the pore or capillary vapor pressure exceeds the saturated vapor pressure outside the body at the same temperature. This results in an excess pressure, driving vapor movement, primarily through molecular diffusion and convective transport.

4. Formulation of the problem and key equations

In the Cartesian coordinate system, we consider a porous bed of thickness L , composed of identical, moist dispersed particles of radius R , with the Oz -axis perpendicular to the layer surfaces. The flow velocity of the drying agent (air-vapor mixture) is assumed to be constant and equal to v . The particles

in this bed remain stationary, with increasing distances between them as air flows through, expanding the volume of the intergrain environment. The porous bed is defined with boundaries at $z = 0$ and $z = L$.

At the macro level, the moisture concentration in the porous bed, $c_z(z, \tau)$, is governed by a convective-diffusion equation:

$$\frac{\partial c_z}{\partial \tau} + v \frac{\partial c_z}{\partial z} = D_z \frac{\partial^2 c_z}{\partial z^2} + J,$$

where v is the drying agent's velocity, D_z is the diffusion coefficient, and J represents the local moisture source intensity.

To represent the local moisture source term, J , we introduce it in the form:

$$J = \alpha J_R,$$

where α depends on the packing and size of the grains. The term J_R represents the moisture flux from the surface of a single grain, defined by:

$$J_R = -\tilde{D} \frac{\partial c}{\partial r} \Big|_{r=R}.$$

Now, we express J_R as:

$$J_R = -\frac{2\tilde{D}\delta c}{R} \sum_{n=1}^{\infty} \frac{A_n(\tau)}{\mu_n} (\sin \mu_n - \mu_n \cos \mu_n).$$

Substituting back, the local moisture source term $J(\tau)$ becomes:

$$J(\tau) = \alpha J_R = -\alpha \frac{2\tilde{D}\delta c}{R} \sum_{n=1}^{\infty} \frac{A_n(\tau)}{\mu_n} (\sin \mu_n - \mu_n \cos \mu_n).$$

The time change of the moisture flux at the interface of the particle can be found as follows:

$$J(\tau) = c_z J_0(\tau) - c_0 J_0(\tau),$$

where

$$J_0(\tau) = -\alpha \frac{2\tilde{D}}{R} \sum_{n=1}^{\infty} \frac{A_n(\tau)}{\mu_n} (\sin \mu_n - \mu_n \cos \mu_n).$$

This substitution allows us to rewrite the governing equation as follows:

$$\frac{\partial c_z}{\partial \tau} + v \frac{\partial c_z}{\partial z} = D_z \frac{\partial^2 c_z}{\partial z^2} + c_z J_0(\tau) - c_0 J_0(\tau).$$

5. Quasi-stationary approximation

In the quasi-stationary approximation, we neglect the time derivative, which yields:

$$D_z \frac{d^2 c_z}{dz^2} - v \frac{dc_z}{dz} + c_z J_0(\tau) = c_0 J_0(\tau).$$

This equation is a second-order linear differential equation with constant coefficients. Solving it requires first finding the homogeneous part:

$$D_z \lambda^2 - v \lambda + J_0(\tau) = 0,$$

with solutions for λ :

$$\lambda_{1,2} = \frac{v \pm \sqrt{v^2 - 4D_z J_0(\tau)}}{2D_z}.$$

The general solution of the homogeneous equation is as follows:

$$c_{zh}(z) = K_1 e^{\lambda_1 z} + K_2 e^{\lambda_2 z},$$

and we add a particular solution $c_{zp}(z, \tau) = c_0$ to form the complete solution:

$$c_z(z, \tau) = K_1 e^{\lambda_1 z} + K_2 e^{\lambda_2 z} + c_0.$$

6. Application of mixed boundary conditions

Using the mixed boundary conditions at $z = 0$ and $z = L$:

1. At $z = 0$:

$$-D \frac{\partial c_z}{\partial z} = H(c_z - c_{\text{amb}}),$$

Substituting $c_z(0, \tau) = K_1 + K_2 + c_0$:

$$-D\lambda_1 K_1 - D\lambda_2 K_2 = H(K_1 + K_2 + c_0 - c_{\text{amb}}).$$

2. At $z = L$:

$$-D \frac{\partial c_z}{\partial z} = H(c_z - c_z^\infty),$$

Substituting $c_z(L, \tau) = K_1 e^{\lambda_1 L} + K_2 e^{\lambda_2 L} + c_0$:

$$-D\lambda_1 K_1 e^{\lambda_1 L} - D\lambda_2 K_2 e^{\lambda_2 L} = H(K_1 e^{\lambda_1 L} + K_2 e^{\lambda_2 L} + c_0 - c_z^\infty).$$

Solving these simultaneous equations, we find:

$$K_1 = \frac{(c_{\text{amb}} - c_0)e^{\lambda_2 L} + (c_z^\infty - c_0)}{\Delta},$$

$$K_2 = \frac{(c_{\text{amb}} - c_0)e^{\lambda_1 L} + (c_z^\infty - c_0)}{\Delta},$$

where

$$\Delta = e^{\lambda_2 L} - e^{\lambda_1 L}.$$

The final expression for the moisture concentration $c_z(z, \tau)$ with the boundary conditions applied is:

$$c_z(z, \tau) = [(c_{\text{amb}} - c_0)e^{\lambda_2 L} + (c_z^\infty - c_0)] \Delta^{-1} e^{\lambda_1 z} + [(c_{\text{amb}} - c_0)e^{\lambda_1 L} + (c_z^\infty - c_0)] \Delta^{-1} e^{\lambda_2 z} + c_0.$$

7. Numerical experiment

On the basis of the obtained formulae to determine the changes of moisture concentration in time, the numerical experiments were carried out both at the macroscopic (grain bed) and microscopic levels (individual grain).

For the numerical experiment, we investigate the convective drying process of wheat grain ("Tr. durum Desf." cultivar) under controlled ambient conditions to reduce the grain's moisture content from 14% to 10%. The drying occurs at an ambient temperature of 20°C, with a relative humidity of 60%, simulating moderate drying conditions.

The drying process of the wheat grain was simulated using the following key physico-chemical characteristics of the material, the environment, and the drying agent:

The thickness of the bed $L = 1$ m, the average radius of the grain $R = 2.00086 \times 10^{-3}$ m, the initial moisture concentration in the grain $c_0 = 5.5 \times 10^{-5}$ kg H₂O/kg dry matter, the packing coefficient $\alpha_T = 2.5$, the effective moisture diffusion coefficient $\tilde{D} = 1.34 \times 10^{-9}$ m²/s, the mass transfer coefficient $H = 1.0 \times 10^{-7}$, the Fourier number for mass transfer $F_O = 2.00086 \times 10^{-7}$, the volumetric expansion concentration coefficient $\beta = 2.71389 \times 10^{-4}$ m³/kg, the saturated vapor concentration $c_z^n = 1.73 \times 10^{-2}$ kg/m³, the shear modulus $G = 6.833 \times 10^5$ kg/m², the mechanical constant $\xi = 0.5$, the bulk modulus $K = 9.1111 \times 10^{-6}$ kg/m², Poisson's ratio $\nu = 0.2$, and the drying agent velocity through the grain bed $v = 1.0 \times 10^{-1}$ m/s. The time step is 3600 s. The radius step for the grain is 0.002 m, and the step in the bulk of the bed is 0.1 m. The convective air drying was conducted at two airflow velocities ($v = 0.5$ m/s and $v = 2.5$ m/s) to evaluate the impact of flow rate on the drying rate and moisture distribution. Initial moisture concentration in the intergrain air-vapor space was set according to the ambient relative humidity, while the top layer of the grain bed was considered to be in contact with air at a saturated vapor concentration corresponding to the drying temperature of 20°C.

There are considered two cases of velocity of the drying agent: $v = 0.5$ m/s, $v = 2.5$ m/s.

The value of c_{amb} , the initial moisture concentration in the intergrain air-vapor space, was chosen based on the ambient relative humidity and the saturation vapor concentration at the drying temperature of 20°C. This choice reflects the equilibrium moisture content that drying agent would have at 60% relative humidity, which is a standard reference condition for ambient air in many drying processes. At 20°C, the saturated vapor concentration of water vapor (100% relative humidity) is approximately 0.0173 kg/m³. Since the relative humidity in the drying environment was set to 60%, the moisture concentration in the intergrain space is ≈ 0.0104 kg/m³. This value of $c_{amb} = 0.0104$ kg/m³ ensures that the drying conditions reflect ambient moisture content, allowing the grains to dry gradually in response to the lower moisture concentration of the intergrain air-vapor mixture. The choice of 60% relative humidity provides a moderate drying environment without extreme desiccation, helping to simulate a common air drying process.

The results of the numerical experiment demonstrate the dependencies of moisture concentration distribution within an individual grain and across the grain bed on the macroscopic and microscopic levels.

In Figures 1 and 2, it is shown the time variations of the moisture concentration $c(r, z, \tau)$ in the grain bed. These figures demonstrate the distribution of moisture concentration across the grain bed for different velocities of the drying agent. Figure 1 corresponds to the drying agent velocity $v = 0.5$ m/s, and Figure 2 corresponds to the velocity $v = 2.5$ m/s.

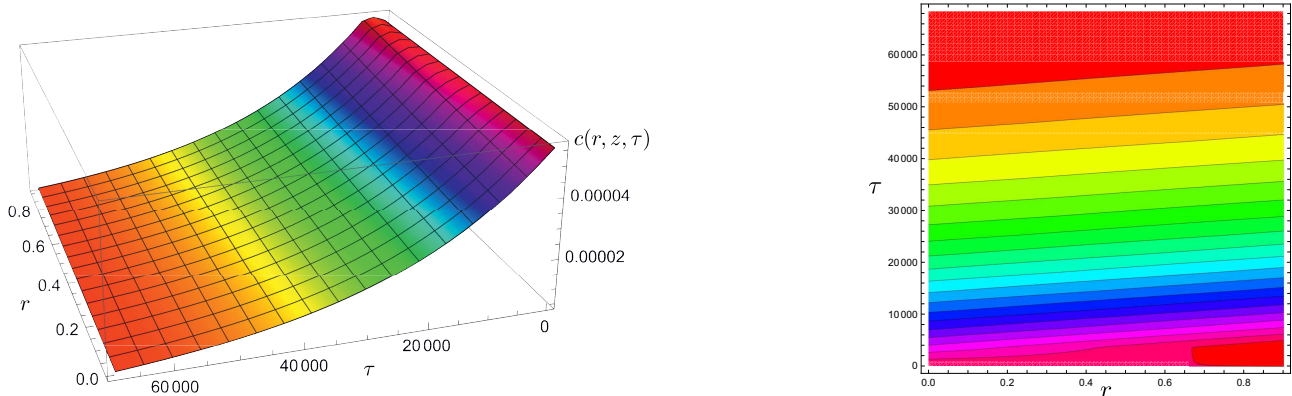


Fig. 1. Moisture concentration distribution $c(r, z, \tau)$ in the grain bed at different depths over time with the drying agent velocity $v = 0.5$.

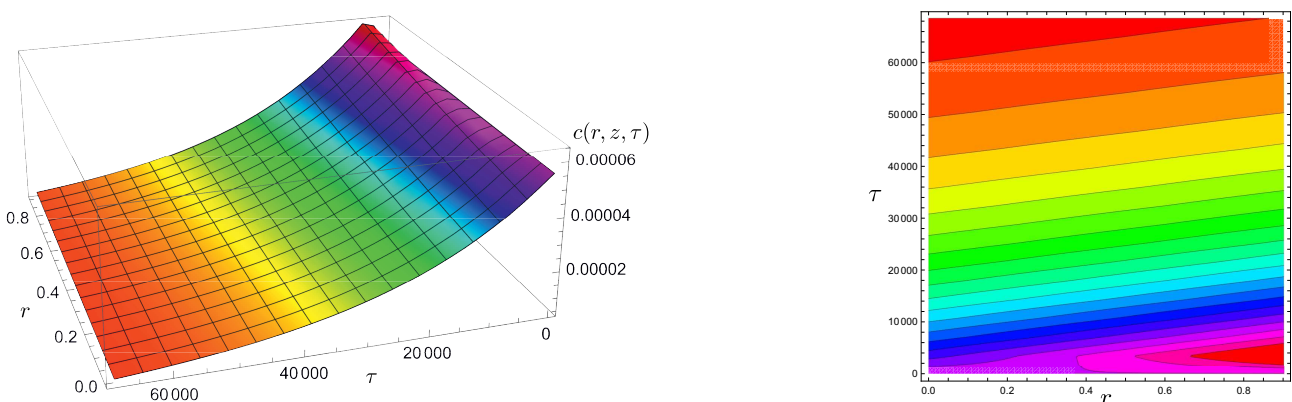


Fig. 2. Moisture concentration distribution $c(r, z, \tau)$ in the grain bed at different depths over time with the drying agent velocity $v = 2.5$.

In Figures 3 and 4, the time variations of the moisture concentration $c(r, z, \tau)$ along the radius of an individual grain are presented for different time moments. Specifically, Figure 3 shows the distribution at $\tau = 3600$ seconds, illustrating the moisture profile after one hour of drying. Figure 4 displays the

distribution at $\tau = 18000$ seconds, corresponding to five hours of drying. These figures highlight how the moisture concentration decreases from the center to the outer surface of the grain over time, reflecting the drying process as influenced by the diffusion of moisture and mass transfer at the grain boundary.

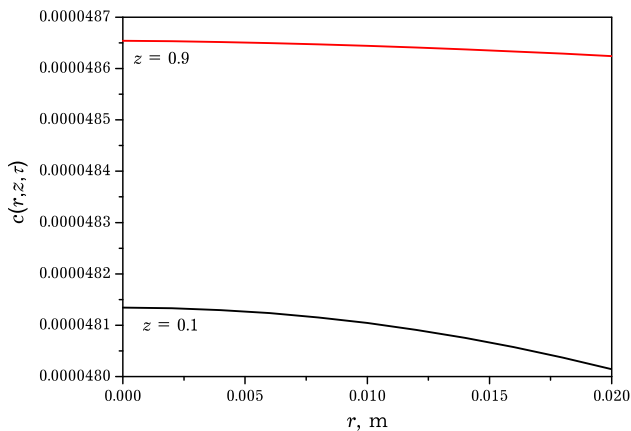


Fig. 3. Moisture concentration distribution $c(r, z, \tau)$ along the radius of an individual grain at depths $z = 0.1$ and $z = 0.9$ for $\tau = 3600$ s.

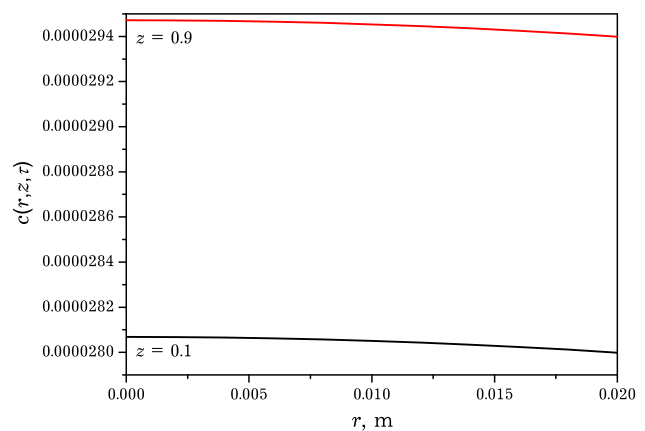


Fig. 4. Moisture concentration distribution $c(r, z, \tau)$ along the radius of an individual grain at depths $z = 0.1$ and $z = 0.9$ for $\tau = 18000$ s.

To analyze and compare the results obtained from the simulations with different velocities of the drying agent (0.5 m/s and 2.5 m/s) in the grain bed, we can focus on several aspects: moisture concentration distribution in time. At each depth level z in the grain bed, the concentration profiles in the two simulations reveal different rates of moisture reduction over time. A higher velocity of 2.5 m/s results in faster moisture reduction across the grain bed compared to the 0.5 m/s case. This effect is due to the enhanced air flow, which removes moisture more effectively. The following aspect is the spatial gradient in concentration. At higher depths (near $z = 0.9$), the concentration in the 2.5 m/s case is lower compared to the 0.5 m/s simulation at equivalent time steps. This suggests that the drying process reaches deeper layers more effectively with increased drying agent velocity, which could improve the uniformity of moisture removal.

With the comparison of radial moisture concentration distribution in a grain at different time moments (3600 s and 18000 s) across two different depths, $z = 0.1$ and $z = 0.9$, we observe the following: moisture gradient across radius. At 3600 seconds, the moisture concentration at $z = 0.1$ attains its maximum at the center ($r = 0$) and decreases slightly toward the outer shell. For $z = 0.9$, the moisture levels are slightly higher, but also the maximum is at the center. This indicates a slight moisture gradient, where moisture near the outer surface is slightly lower, especially at the deeper grain bed level. Moisture decrease over time 18000 seconds is notable. For $z = 0.1$, moisture levels reduce significantly to around $2.807 \cdot 10^{-5}$ kg H₂O/kg dry matter at the center. At $z = 0.9$, moisture values remain somewhat higher, showing that deeper layers retain more moisture, slowing the drying process in the bed's interior regions.

The concentration difference between $z = 0.1$ and $z = 0.9$ becomes more prominent over time. At 3600 seconds, the moisture concentrations are close across z values, indicating uniform drying. By 18000 seconds, deeper layers at $z = 0.9$ maintain higher moisture levels than shallower ones, suggesting that drying is more effective near the outer grain bed layers due to higher exposure to the drying agent.

8. Conclusion

In the paper, a model for convective drying of a multicomponent system, considering the process at both micro and macro levels, is presented. The model accounts for phase transitions during drying, as well as the effects of the material structure on moisture transfer. The mass transfer problems under mixed boundary conditions are formulated for both the grain bed and an individual grain. A method-

ology for the simultaneous solving of these problems is developed. Using the obtained solutions, a numerical experiment is performed. The results provide clear regularities in the moisture concentration distribution at both levels. The novelty of this approach lies in the simultaneous consideration of the grain bed and individual grains and explicitly modeling the moisture exchange between them. This dual-level approach allows for a more accurate simulation of real-world drying processes, making it potentially novel in comparison to the majority of existing models.

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Моделювання процесів масопереносу у багатокомпонентних тілах капілярно-пористої структури за змішаних граничних умов

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У роботі представлено фізико-математичну модель конвективного сушіння багатокомпонентного тіла капілярно-пористої структури з урахуванням динаміки вологоперенесення як на макро-, так і на мікрорівнях. Визначаючи вплив локальної структури матеріалу на процеси сушіння, зокрема у фазових перетвореннях, модель інтегрує континуально-термодинамічний підхід, започаткований Я. Бураком, Є. Чаплею та Б. Гайвась. Цей підхід стосується взаємопов’язаних механічних, теплових і дифузійних процесів, що відбуваються в гетерогенних, нерівноважних системах, де припущення про локальну термодинамічну рівновагу дозволяють описувати стан рівноваги за допомогою спряжених фізичних параметрів. Унікальний дворівневий підхід, застосований при моделюванні, описує обмін вологи між окремим зерном і шаром зерна за граничних умов третього роду, що дозволяє реалістично моделювати процес сушіння шляхом прямого врахування фазових перетворень і впливу капілярної структури матеріалу. Представлена методологія дозволяє одночасно розв’язувати рівняння масопереносу для шару зерна та окремих зерен за змішаних граничних умов, що підтверджується чисельним експериментом. Результати показують чіткі закономірності розподілу вологи в зерновому шарі та всередині окремих зерен із змінами, залежними від швидкості сушильного агента. Новизна цього підходу полягає в одночасному розгляді перенесення вологи в області зернини та в шарі шару, що забезпечує детальну перспективу динаміки вологи. Ця модель має потенційне застосування для оптимізації промислових процесів сушіння капілярно-пористих матеріалів, підвищення ефективності та економічності.

Ключові слова: *сушіння; капілярно-пористий; концентрація вологи; дифузія вологи; змішані граничні умови; фазовий перехід; континуально-термодинамічний підхід; масоперенос.*