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MODELLING MASS TRANSFER DURING CRYOPRESERVATION IN A BIOLOGICAL SAMPLE TREATED AS A HOMOGENEOUS AND POROUS MATERIAL WITH UNCERTAIN PARAMETERS

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Abstract: *Biological tissues are often modelled as homogeneous materials, but their structure can also be treated as a porous medium. In addition, models of biological processes contain uncertain quantities that are introduced as deterministic numbers. The article presents a numerical simulation of the cryopreservation process of articular cartilage, using homogeneous and porous material models (Analyses 1 and 2). Analysis 1 considers the uncertainty of thermophysical parameters by introducing interval set theory. The mathematical model includes a description of coupled heat and mass transfer phenomena, and the diffusion coefficient is estimated using the Einstein-Stokes equation in Analysis 1 and using a relationship that accounts for the porous structure of the sample in Analysis 2. Finally, the simulation results are compared with the experimental data for validation. The maximum relative error equals 15.82% for Analysis 1 and 24.96% for Analysis 2.*

Keywords: Diffusion coefficient, Porous material, Interval numbers, Mass transfer, Heat transfer

1. Introduction

Porous media are materials in which the matrix contains fluid-filled pores. Biological tissues can also be considered porous materials because they consist of dispersed cells between which nutrients are transported, for example (Khaled & Vafai, 2003).

Several transport phenomena occur in biological materials. Heat transfer is induced by heat conduction as well as blood perfusion (blood convection). Thermal phenomena can be described, for example, using Fourier's equation. On the other hand, mass transfer is driven by diffusion and is associated with the transport of nutrients, drugs, and cryoprotectants (CPAs) during cryopreservation (Khaled & Vafai, 2003).

Additionally, modelling biological processes involves an inherent degree of uncertainty. This is because the parameters of biological materials are determined experimentally and depend on their individual characteristics. Uncertain variables in the model can be analysed using probabilistic or non-probabilistic approaches. The latter approach uses the fuzzy numbers and interval numbers. In fuzzy set theory, each element of the set is described by a membership function. Meanwhile, interval numbers are defined by lower and upper bounds, which determine the membership of a given element in the set (Wang & Matthies, 2021).

The article presents a mathematical and numerical model of a cylindrical sample of cryopreserved articular cartilage. As experimental studies indicate, this biological tissue contains pores with sizes ranging from 2 nm to 6 nm or from 11 nm to 14 nm, depending on the testing method (Skorupa & Piasecka-Belkhayat, 2025). Therefore, the study compares the temperature and CPA concentration

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distributions in a two-dimensional computational domain by modelling the tissue as a homogeneous material (Analysis 1) and as a porous medium (Analysis 2). Additionally, in the homogeneous material model, thermophysical parameters are introduced as interval numbers.

2. Methodology

The cryopreservation process can be performed using conventional methods such as slow freezing and vitrification. The article presents an alternative method named the liquidus-tracking (LT) protocol, in which the temperature of the bath solution and the concentration of the cryoprotectant are appropriately regulated. In this study, the CPA is assumed to be a solution of dimethyl sulfoxide (DMSO) and water (Pegg et al., 2006; Yu et al., 2019). Cryoprotectants such as DMSO differ from standard diffusing species due to their temperature-dependent viscosity, which affects the transport process. In the present model, this effect is partially taken into account through the temperature-dependent diffusion coefficient.

2.1. Mathematical model

To determine the distribution of the CPA in the computational domain as interval numbers, the following relation is used (Skorupa & Piasecka-Belkhayat, 2025; Yu et al., 2019):

$$\frac{\partial \bar{c}_d(r,z,t)}{\partial t} = \nabla\left(\bar{D}_{eff}\nabla\bar{c}_d(r,z,t)\right), \tag{1}$$

where $\bar{c}_d$ [%(w/w) or mol m^{-3}] is the interval DMSO concentration in the sample, $\bar{D}_{eff}$ [m^2 s^{-1}] is the interval effective diffusion coefficient, and t, r, and z are the time and the spatial coordinates, respectively. The value of the interval effective diffusion coefficient is estimated using three relationships depending on whether the sample is treated as a homogeneous or porous material.

In Analysis 1, where the articular cartilage is homogeneous material, the Einstein-Stokes equation is applied (Skorupa & Piasecka-Belkhayat, 2025):

$$\bar{D}_{eff} = \frac{k_B\bar{T}(r,z,t)}{6\pi r_s \mu_d}, \tag{2}$$

where k_B [J K^{-1}] is the Boltzmann constant ($k_B = 1.38\times10^{-23}$ J K^{-1}), $\bar{T}$ [K] is the temperature, r_s [m] is the radius of the spherical particle, and μ_d [Pa s] is the dynamic viscosity of DMSO.

Considering the sample as a porous medium (Analysis 2), the effective diffusion coefficient is calculated as a deterministic value using the following relationship (Skorupa & Piasecka-Belkhayat, 2025; Yu et al., 2019):

$$\bar{D}_{eff} = D_{dw}\frac{\varepsilon}{\tau^2}, \tag{3}$$

where D_{dw} [m^2 s^{-1}] is the diffusion coefficient of DMSO in water, ε is the water content in the sample, and τ is the tortuosity factor. A detailed description of the diffusion coefficient calculation in water and other required variables is provided in the literature (Skorupa & Piasecka-Belkhayat, 2025; Yu et al., 2019).

The interval temperature distribution is defined by the Fourier equation (Skorupa & Piasecka-Belkhayat, 2025; Yu et al., 2019):

$$\bar{c}_p\bar{\rho}\frac{\partial \bar{T}(r,z,t)}{\partial t} = \nabla\left(\bar{k}\nabla\bar{T}\right), \tag{4}$$

where $\bar{c}_p$ [J kg^{-1} K^{-1}] is the interval specific heat capacity, $\bar{\rho}$ [kg m^{-3}] is the interval density, and $\bar{k}$ [W m^{-1} K^{-1}] is the interval thermal conductivity.

The mathematical model includes the following initial condition:

$$t = 0:\ \bar{T}(r,z,t) = T_{init}\ \ and\ \ \bar{c}_d(r,z,t) = c_{init}, \tag{5}$$

and boundary conditions:

$$\begin{cases} r = R \text{ and } z = 0: & -\mathbf{n}\bar{k}\cdot\nabla\bar{T} = \alpha[\bar{T}(r,z,t) - T_{bath}] \text{ and } -\mathbf{n}\bar{D}_{eff}\cdot\nabla\bar{c}_d = 0.9c_{bath}, \\ r = 0 \text{ and } z = \dfrac{H}{2}: & -\mathbf{n}\bar{k}\cdot\nabla\bar{T} = 0 \text{ and } -\mathbf{n}\bar{D}_{eff}\cdot\nabla\bar{c}_d = 0, \end{cases} \tag{6}$$

where α is the natural convection heat transfer coefficient, and **n** is the normal vector, T_{bath} and c_{bath} are the temperature and the DMSO concentration of the bath solution, respectively, R and H are the sample dimensions. The axisymmetric cylindrical geometry was selected to simplify the problem and to enable comparison with available experimental data.

2.2. Numerical model

The finite difference method (FDM) is used to perform numerical simulations. A fixed time grid is assumed ($t^0 < t^1 < \cdots < t^{f-1} < t^f < t^{f+1} < \cdots < t^\infty$, where $\Delta t = t^f - t^{f-1}$ is the constant time step) and the geometric mesh is prepared applying the five-point stencil (Skorupa, 2023).

The interval distribution of CPA in the sample for central nodes is estimated using FDM by:

$$(\bar{c}_d)_{i,j}^{f} = (\bar{c}_d)_{i,j}^{f-1} - \Delta t \sum_{a=1}^{4} \frac{\Phi_e}{\bar{W}_e}\left((\bar{c}_d)_e^{f-1} - (\bar{c}_d)_{i,j}^{f-1}\right), \tag{7}$$

where $i = 2, 3, \ldots, n-1$, $j = 2, 3, \ldots, m-1$, with n and m denoting the number of nodes in the z- and r-directions, respectively. The index a corresponds to the set of neighbouring nodes $e = \{(i, j+1); (i, j-1); (i+1, j); (i-1, j)\}$, Φ_e [m^{-1}] is the shape function, and $\bar{W}_e$ [s m^{-1}] is the interval mass resistance. The shape function and the interval mass resistance can be expressed as:

$$\Phi_{i,j-1} = \frac{r_{i,j} - 0.5h_1}{r_{i,j}h_1}, \quad \Phi_{i,j+1} = \frac{r_{i,j} + 0.5h_1}{r_{i,j}h_1}, \quad \Phi_{i-1,j} = \Phi_{i+1,j} = \frac{1}{h_2}, \tag{8}$$

$$\bar{W}_{i,j-1} = \bar{W}_{i,j+1} = \frac{h_1}{\bar{D}_{eff}}, \quad \bar{W}_{i-1,j} = \bar{W}_{i+1,j} = \frac{h_2}{\bar{D}_{eff}} \tag{9}$$

where $r_{i,j}$ [m] is the radial coordinate of the node (i, j), h_1 [m] and h_2 [m] denote the mesh steps in the r- and z-directions, respectively.

The interval temperature distribution in the computational domain for central nodes is given by:

$$\bar{T}_{i,j}^{f} = \bar{T}_{i,j}^{f-1} - \frac{\Delta t}{\bar{c}_p \bar{\rho}} \sum_{a=1}^{4} \frac{\Phi_e}{\bar{R}_e}\left(\bar{T}_e^{f-1} - \bar{T}_{i,j}^{f-1}\right), \tag{10}$$

where $\bar{R}_e$ [m^4 K W^{-1}] represents the thermal resistance given by:

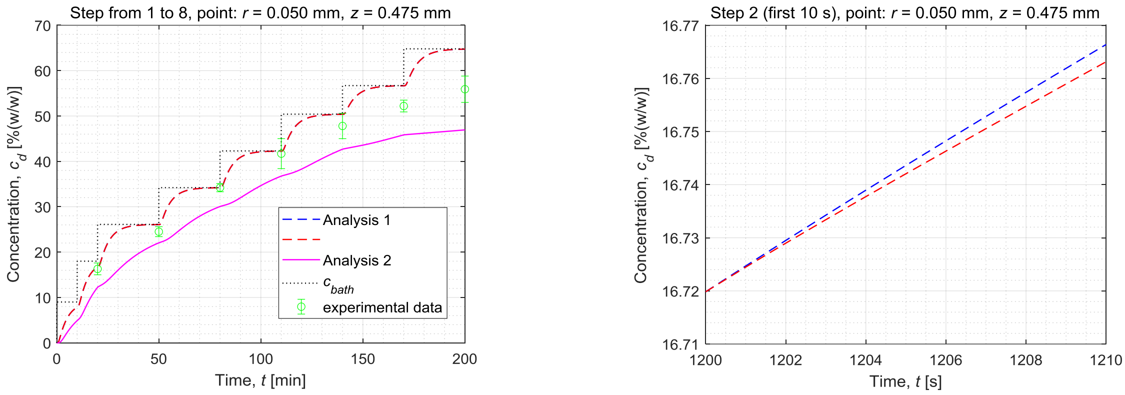
$$\bar{R}_{i,j-1} = \bar{R}_{i,j+1} = \frac{h_1}{\bar{k}}, \quad \bar{R}_{i-1,j} = \bar{R}_{i+1,j} = \frac{h_2}{\bar{k}}. \tag{11}$$

Details about the derivation for boundary nodes and the rules for mathematical operations on interval numbers can be found in the literature (Skorupa, 2023). The adopted time step and mesh resolution were selected based on preliminary numerical tests, ensuring stable and consistent results.

3. Results of computation

The study modelled the cryopreservation process based on the LT protocol proposed by Pegg et al., which consisted of eight steps in the cooling phase, during which the following values were adopted: $T_{bath} \in \{22; 22; -5; -8.5; -16; -23; -35; -48.5\}$ °C, $c_{bath} \in \{10; 20; 29; 38; 47; 56; 63; 72\}$ %(w/w) and each step lasts: $t_{bath} \in \{10; 10; 30; 30; 30; 30; 30; 30\}$ s (Pegg et al., 2006). The simulation assumed the initial condition T_{init} = 22 °C, c_{init} = 0%(w/w), the natural convection heat transfer coefficient α = 525 W·m^{-2}·K^{-1} and the dimensions of the computational domain are R = 3 mm and H = 1 mm. The following parameter values are applied: the specific heat capacity c_p = 3567.5 J kg^{-1} K^{-1}, the density ρ = 1100 kg m^{-3}, the thermal conductivity k = 0.518 W m^{-1} K^{-1}, the dynamic viscosity of DMSO $\mu_d = 1.996\times10^{-3}$ Pa s, the radius of the spherical particle $r_s = 2.541\times10^{-10}$ m, the water content in the sample ε = 0.78, the tortuosity τ = 1.4. The step of the time grid equals Δt = 0.005 s, the mesh steps are h_1 = 0.1 mm and h_2 = 0.05 mm. In Analysis 1, thermophysical parameters were introduced as interval numbers, where $\bar{c}_p = [c_p - 0.05c_p, c_p + 0.05c_p]$, $\bar{\rho} = [\rho - 0.05\rho, \rho + 0.05\rho]$, $\bar{k} = [k - 0.05k, k + 0.05k]$.

Fig. 1 shows (a) a graph of the DMSO concentration in the sample as a function of time and (b) a graph of the first 10 seconds of step 2 of the LT protocol, which confirms that the values obtained are in the form of intervals. The diagrams represent the results for the point r = 0.050 mm, z = 0.475 mm. The plot also contains the concentration of the bath solution (black dotted line) and the experimental results (green points). One can see that the simulation results differ from the experimental values, mainly in the last steps of the protocol. Based on the experimental results (Pegg et al., 2006), the relative error was calculated, which for Analysis 1 varied between 1.38% and 15.82%, while for Analysis 2 it ranged from 10.05% to 24.96%.



(a) (b)

Fig. 1: Concentration of DMSO as a function of time: (a) the entire simulation time and (b) the first 10 s of the second step of the protocol.

4. Conclusions

The aim of the article was to perform a numerical simulation of cryopreservation in a cylindrical sample of articular cartilage modelled as a homogeneous material (Analysis 1) and a porous material (Analysis 2). The obtained DMSO concentration values were validated with the experimental results. On this basis, the results from Analysis 1 are closer to the experimental data. The higher relative error observed in Analysis 2 may result from several factors, for example, by the sensitivity of the model to tissue parameters, such as porosity, tortuosity, and pore size distribution. These parameters may vary significantly between biological specimens and are difficult to determine accurately. It should also be noted that the thermophysical parameters used in the numerical simulations were not measured directly on the experimentally tested sample. In summary, interval set theory works well for describing uncertain parameters occurring in the model. The novelty of the study lies in the application of interval arithmetic to the modelling of coupled heat and mass transfer and in the comparison between homogeneous and porous material models.

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References

Khaled, A.-R. A., & Vafai, K. (2003). The role of porous media in modeling flow and heat transfer in biological tissues. *International Journal of Heat and Mass Transfer*, *46*(26), 4989-5003. https://doi.org/10.1016/S0017-9310(03)00301-6

Pegg, D. E., Wang, L., & Vaughan, D. (2006). Cryopreservation of articular cartilage. Part 3: The liquidus-tracking method. *Cryobiology*, *52*(3), 360-368. https://doi.org/10.1016/j.cryobiol.2006.01.004

Skorupa, A. (2023). *Multi-scale modelling of heat and mass transfer in tissues and cells during cryopreservation including interval methods* [Doctoral thesis, Politechnika Śląska].

Skorupa, A., & Piasecka-Belkhayat, A. (2025). Analysis of Cryoprotectant Concentration During Cryopreservation in Articular Cartilage Sample Using Homogeneous and Porous Material Models. *Annals of Biomedical Engineering*. https://doi.org/10.1007/s10439-025-03925-6

Wang, C., & Matthies, H. G. (2021). Coupled fuzzy-interval model and method for structural response analysis with non-probabilistic hybrid uncertainties. *Fuzzy Sets and Systems, Fuzzy Intervals and Their Applications*, *417*, 171–189. https://doi.org/10.1016/j.fss.2020.06.002

Yu, X., Zhang, S., & Chen, G. (2019). Modeling the addition/removal of dimethyl sulfoxide into/from articular cartilage treated with the liquidus-tracking method. *International Journal of Heat and Mass Transfer*, *141*, 719–730. https://doi.org/10.1016/j.ijheatmasstransfer.2019.07.032