

Modeling of the mechanical behavior of polymer hydrogels

J. Štorkán ^a, T. Vampola ^a, M. Dušková-Smrčková ^b, K. Dušek ^b

^a Faculty of Mechanical Engineering, Czech Technical University in Prague, Technická 4, 160 00 Praha, Czech Republic

^b Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, 162 06 Praha, Czech Republic

Polymeric hydrogels are interesting materials for biomechanics applications. These materials can be used as carriers for the cultivation of different types of biological materials. Hydrogels exist in many species, differing in chemical composition. The chemical composition, together with internal topology and external geometry, defines mechanical properties of the polymer hydrogels. The topology of hydrogels is a porous structure. The shape and size of the pores is affected by their production. It is shown that the mechanical properties of the inner structure significantly affect to cell production. Therefore, there is area for research into the mechanical properties of hydrogels. The goal of the whole research is to be able to design a topology so that the resulting mechanical properties are optimal for biological materials cultivation. This article deals with FEM modeling of hydrogel as homogeneous body without internal topology. This involves problems with the non-standard behavior of the material model over models commonly used in machine practice.

Hydrogels are very soft and flexible materials with a very great strains. Therefore, their material models are hyperelastic. The second significant feature of hydrogels is swelling. During production, they absorb the solvent. Mostly water. When swelling, the volume changes as long as a balance is established between the cohesive forces that hold the solvent in the material and the elastic forces that prevent the volume change of the body. This phenomenon is described by changing Gibbs' free energy, such as Flory-Huggins' formula (2). The overall change in Gibbs' free energy is the sum of the mixing component (2) and the elastic component (3). The elastic component represents any hyperelastic model. The material model based on the Gents' model of material with limited stretchability was used. For simplicity, we do not distinguish between Gibbs' free energy and Helmholtz' free energy.

$$\Delta G = \Delta G_{mix} + \Delta G_{el,n} , \quad (1)$$

$$\Delta G_{mix} = RT \frac{\phi_2^0}{V_{1mol} \phi_2} \phi_1 (\ln \phi_1 + g(\phi_2) \phi_2) - RT \frac{f_e - 2}{f_e} v_e \phi_2^0 \ln \phi_2 , \quad (2)$$

$$\Delta G_{el,n} = -RT v_e \phi_2^0 \left(\ln(\lambda_1 \lambda_2 \lambda_3) + \frac{n-1}{2} \left(\ln \left(1 - \frac{\lambda_1^2}{n-1} \right) + \ln \left(1 - \frac{\lambda_2^2}{n-1} \right) + \ln \left(1 - \frac{\lambda_3^2}{n-1} \right) - 3 \ln \left(1 - \frac{1}{n-1} \right) \right) \right) . \quad (3)$$

Parameters ϕ_1 and ϕ_2 are the volume fractions of solvent and gel. Volume fractions can be expressed by volume ratio. The volume ratio is a deformation function. Parameters λ_i are stretch. Other parameters are constants. Overall, the change of Gibbs' free energy is a function of only the main deformations. With this material model, it is possible to work with conventional continuum mechanics.

When computing, there is a problem with model convergence. Because the description contains a swelling component, the model changes the volume. With free swelling, the volume increases by about 350% and causes a deformation of about 65%. This of course depends on input parameters. Such large deformations must result in the first increment, and this causes numerical instability. The biggest problem is when the body is statically undefined. Another

problem is the shape of the function (1). For some combinations of input parameters it may not be convex. And it may contain more extremes. Such a case is shown in Fig. 1. The solution is not clear and you need to select the correct minimum Gibbs' free energy and avoid the maximum.

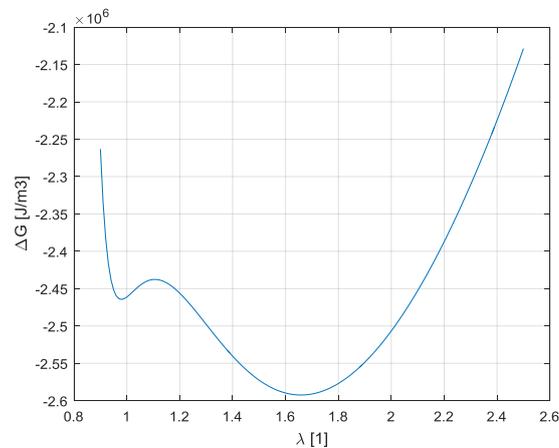


Fig. 1. Change of Gibbs' free energy for free isotropic swelling

The model shown in the figure shows 3 solutions for free isotropic swelling. One is the maximum and is unstable, the other two need to choose one. The easiest way is to choose a solution with lower energy (greater stability), or use the Maxwell construction for choice.

Swelling deformations are large. The calculation may not converge. This can be solved by the correct estimation of nodal displacements in numerical solution. This estimate determines which solution will be found. Nodal displacements estimates are simple for static defined tasks only. For general tasks, it is a very complicated estimate to carry out because it must respect kinematic boundary conditions. Therefore, another method is used. The calculation is made with another material model that does not show swelling. With this model, it is not a problem to calculate the task with all the boundary conditions. After applied boundary conditions, the material model switches to the desired swelling. The switching of the material model can be controlled incrementally. The incremental scheme will ensure convergence. In the case of a model with multiple solutions, the non-swelling model switches to swelling with a clear solution. This solution is consistent with one of the final material model solutions for the isotropic task. This ensures convergence to the chosen solution - choice of solution. And in the last phase it switches to the final material model.

The paper describes the possible procedure of FEM calculation of hydrogel materials. The basis of the calculation is to perform a calculation with a common material model. Only after the application of boundary conditions is the material model incrementally changed to the desired. This procedure reduces the risk of non-convergence. In addition, this allows you to choose a solution to which the model converges, if they exist.

Acknowledgements

The research is supported by Grant Agency of the Czech Republic by project No 17-08531S Computationally designed hydrogel cell supports.

References

- [1] Koningsveld, R., Stockmayer, W.H., Nies, E., Polymer phase diagrams: A textbook, Oxford University Press, 2001.
- [2] Dušek, K., Dušková-Smrčková, M., Šomvářsky, J., Effect of constraints on swelling of polymer networks, Macromol, Symposia 2015, 358, pp. 120–127.