COMPUTATIONAL MECHANICS 2018
34th conference with international participation
Srní
October 31 - November 2, 2018

Modeling of mechanical properties of macroporous hydrogel

J. Zavřel [a], T. Vampola [a], M. Dušková-Smrčková [b]

[a] Faculty of Mechanical Engineering,Czech Technical University in Prague, Technická 4, 166 07 Prague 6, Czech Republic
[b] Institute of Macromolecular Chemistry, Czech Academy of Sciences, Heyrovského nám. 2, 162 06 Prague 6, Czech Republic

Macroporous hydrogels with controlled morphology are widely used in biomedical fields, as drug delivery, tissue engineering, analytical and technical separations or responsive constructs. Porosity can be achieved by several methods. In the preparation of physical experiments it is made by salt crystals which are extracted from the hydrogel after polymerization. The salt crystals have different sizes and shapes. The pore sizes and their distribution affects the final mechanical properties. Such polymer structure is designed by simulations. The simulated structure is than transfered into ANSYS environment and its mechanical properties are examined and compared with experiments.

Modelling of the structure: The first step is to prepare the hydrogel structure model. It is based on the real mechanism of its formation. The porosity is achieved by salt crystals which are later extracted. In our case of modelling there are randomly distributed cubes (crystals) subtracted from the initial volume. The milestone is to reach the first through path in the initial volume. Upon further adding of the crystals, the saturation point can be reached. It corresponds to the case when the hydrogel is saturated with crystals and at is not possible to add additional crystals. Such state can be described by volume fraction of connected paths (paths going through the volume) and all paths (including all pats and crystal holes) to the whole volume (Fig. 1). It is described by the experimentally detected value Φ_{exp} and simulated value Φ_{teor}. Behaviour of different materials when using different sizes of salt grains has the same trend.

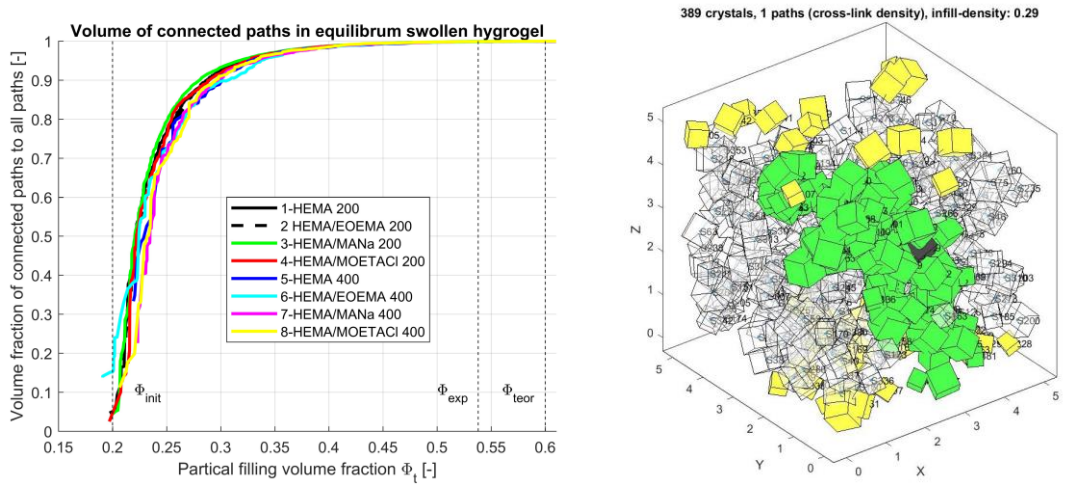

Fig. 1. Partical filling volume fraction of different materials and crystal sizes (left). An example of simulation model creation (right)

Computation of mechanical properties: The previous structure is transferred into the ANSYS environment. The export script is generated. Crystals generated in the previous step are also subtracted from the initial volume and then it is meshed. It is also the inverted structure from the Fig 1 – on the right. The boundary conditions and forces are applied. The stresses and deformation fields were analysed.

Experimental results: Oscillatory shear measurements of swollen gels (Fig. 2) were performed using the rheometer Bohlin Gemini HR Nano (Malvern Instruments, UK) equipped with a Peltier temperature table and a solvent stainless steel dish. All tests were performed using 25 mm diameter stainless steel parallel plate geometry with disc-like samples of a diameter 25 mm and swollen thickness in the range from 1 to 4 mm. During the measurement, the samples were immersed in water or aqueous solution of sodium phosphate buffer (PBS). The distance between the measuring plates – gap size – for each sample was adjusted to a value at which the sliding of samples was avoided and full contact between plates and sample was achieved [1].

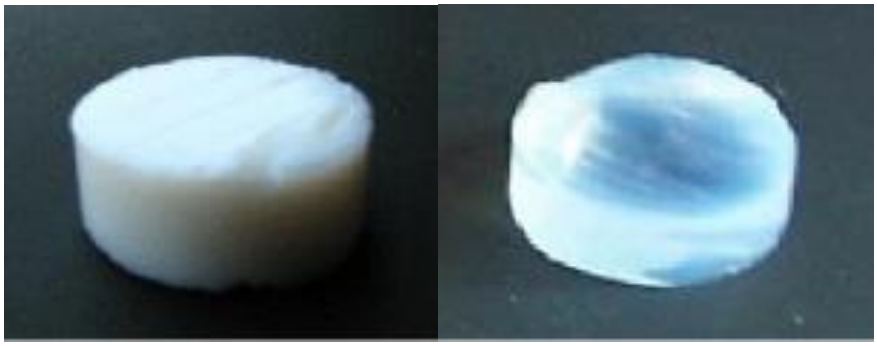

Fig. 2. Swollen macroporous gels – macroscopic appearance of tested sample

Precise sample placement between the upper and lower measuring plates is a crucial condition as the resulting apparent moduli values are very sensitive either to the plate slippage or to normal force acting on the sample excess. The amplitude sweep tests were performed first in the stress-control mode to find the linear viscoelastic range of the stress-strain response and the stress value for subsequent frequency sweep measurement was chosen within that linear range. The measurements were carried out in the range of frequencies from 0.01 Hz to 100 Hz at 25 °C. The apparent storage and loss moduli of the gels were obtained.

Acknowledgements

The research is supported by the Grant Agency of the Czech Republic by project No GA17-08531S – "Computational design of hydrogel cell scaffolds".

References

[1] Karpushkin, E., Dušková-Smrčková, M., Remmler, T., Lapčíková, M., Dušek, K. Rheological properties of homogeneous and heterogeneous poly(2-hydroxyethyl methacrylate) hydrogels, Polymer International 61 (2) (2012) 328–336.