Multiphysics modeling of swelling gels

Alessandro Lucantonio

Dipartimento di Ingegneria Strutturale e Geotecnica
Sapienza Università di Roma

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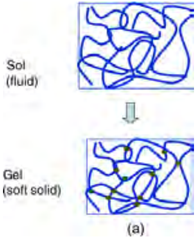
Polymer gels

Gel is a soft elastic material swollen with a fluid.

Polymer gels are made of long–chain polymers which are **cross–linked** into a 3D network. The cross–linking can be *chemical* (irreversible) or *physical* (reversible).

Gels can be made by *gelation* of a polymer solution or by immersing a dry elastomer into a solvent.



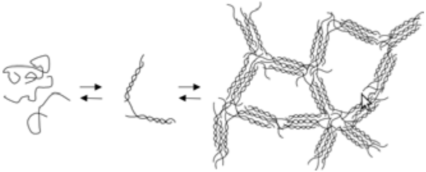


Figure: Gelation with physical cross–linking

L.R.G. Treloar. The physics of rubber elasticity, 2005.
M. Doi. Introduction to polymer physics, 1996.
E. H. Schacht. Polymer chemistry and hydrogel systems, Journal of Physics: Conference Series 3, 2004.

Applications of gels

Figure: Contact lenses

Figure: Bio-inspired soft robots

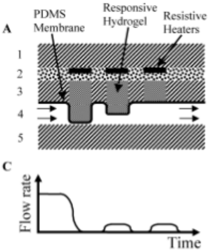


Figure: Microfluidic devices

Figure: Drug delivery systems

Non–linear multiphysics modeling: weak form

- Balance of forces

$$-\int_{\mathcal{B}} (\mathbf{S} \cdot \nabla \tilde{\mathbf{u}}) + \int_{\partial_t \mathcal{B}} (\mathbf{t} \cdot \tilde{\mathbf{u}}) = 0$$

- Conservation of solvent mass

$$\int_{\mathcal{B}} \dot{c}\tilde{c} = \int_{\mathcal{B}} (\mathbf{h} \cdot \nabla \tilde{c}) + \int_{\partial_q \mathcal{B}} q\tilde{c}$$

- Volumetric constraint

$$\int_{\mathcal{B}} (J - 1/J_o - \Omega c)\tilde{p} = 0$$

- Constitutive equations

$$\mathbf{S} = \mathbf{S}(\mathbf{F}, p)$$
$$\mu = \mu(c, p)$$
$$\mathbf{h} = -\mathbf{M}(\mathbf{F}, c)\nabla \mu$$

- Boundary conditions

$$\begin{aligned} \mathbf{S}\mathbf{m} &= \mathbf{t} && \text{on} && \partial_t \mathcal{B} \\ \mathbf{u} &= \bar{\mathbf{u}} && \text{on} && \partial_u \mathcal{B} \\ -\mathbf{h} \cdot \mathbf{m} &= q && \text{on} && \partial_q \mathcal{B} \\ c &= c_b && \text{on} && \partial_c \mathcal{B} \end{aligned}$$

Assigned chemical potential

Non-linear BC implicit in c_b solved through Weak form - Boundary

$$\int_{\partial_c \mathcal{B}} (\mu(c_b, p) - \mu_{ext})\tilde{c}_b = 0$$

A.L., P. Nardinocchi, L. Teresi. Multiphysics Modeling of Swelling Gels, European COMSOL Conference Proceedings, 2012.

Discretization and solver settings

- To avoid *negative concentrations*: change of variable $c \to \log c$;
- to avoid *locking*: Lagrange **discontinuous** linear elements and continuous quadratic elements for all the other fields;

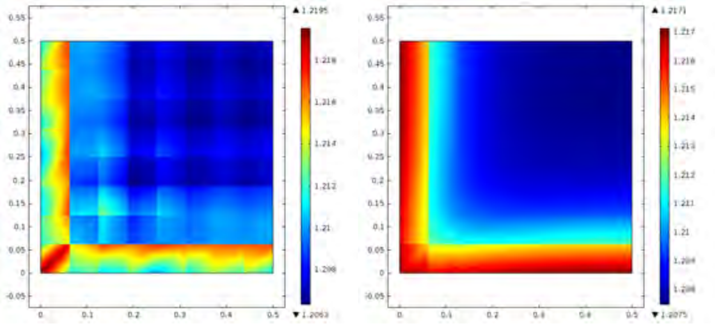
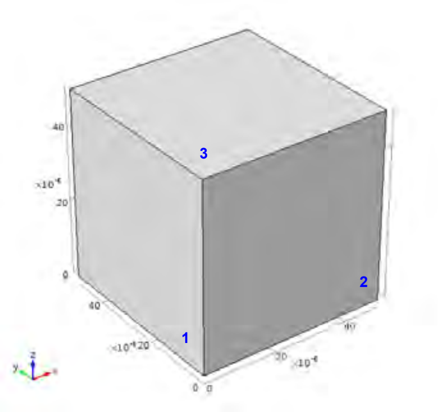


Figure: Volume ratio in a free swelling cube. Continuous (left) vs discontinuous (right) linear pressure elements.

- BDF time-dependent solver with strict option, MUMPS direct solver with automatic damping.

Free swelling of a cubic gel



One-eighth of a free (no forces) cube immersed in a solvent bath at constant chemical potential is modeled.

The chemical potential is assigned on 1-2-3 (chemical equilibrium with external solvent), symmetry conditions are imposed on the other faces.

Free swelling of a cubic gel: results

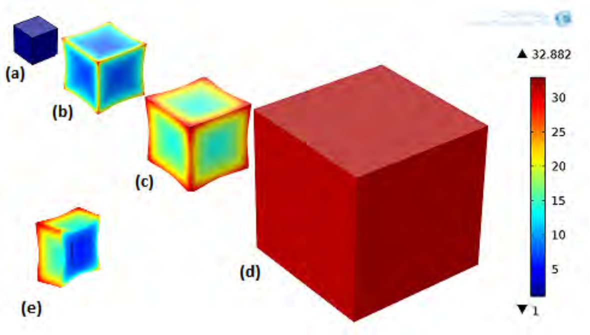


Figure: Several frames of the free swelling of a cubic gel immersed in a solvent bath. Color map shows the volume ratio J at different dimensionless times: (a) 0, (b) 1, (c) 10, (d) ∞. The cut view (e) is taken at the dimensionless time 10.

Conclusions

1. A *non-linear multiphysics* theory that allows to analyze swelling phenomena taking place in gels has been set.
2. The theory has been implemented in COMSOL Multiphysics 4.2a using the *Weak Form PDE mode*.
3. A boundary Physical Interface has been employed to prescribe a *non-linear implicit boundary condition*.
4. The validity of the numerical model through a benchmark problem has been proven.

Acknowledgements

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Thanks for your attention!