Modelling of the Release of Active Substances from Hydrogel

Miloslav Pekař

Faculty of Chemistry
Brno University of Technology

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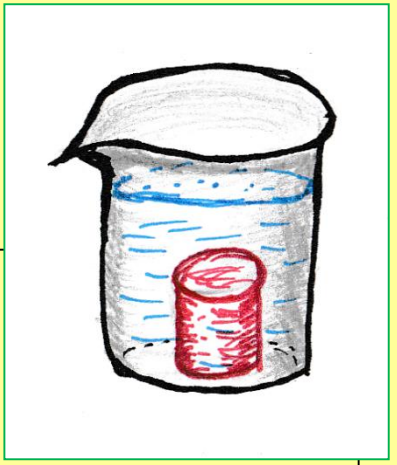
Slow **release** of active substances from carrier; applications, e.g.,

- in medicine – drug release or
- in plant production – release of nutrients (fertilizer).

Hydrogel – one of potential carriers

- soft solid matter full of water
- with network structure,
- prepared from natural or synthetic polymers.

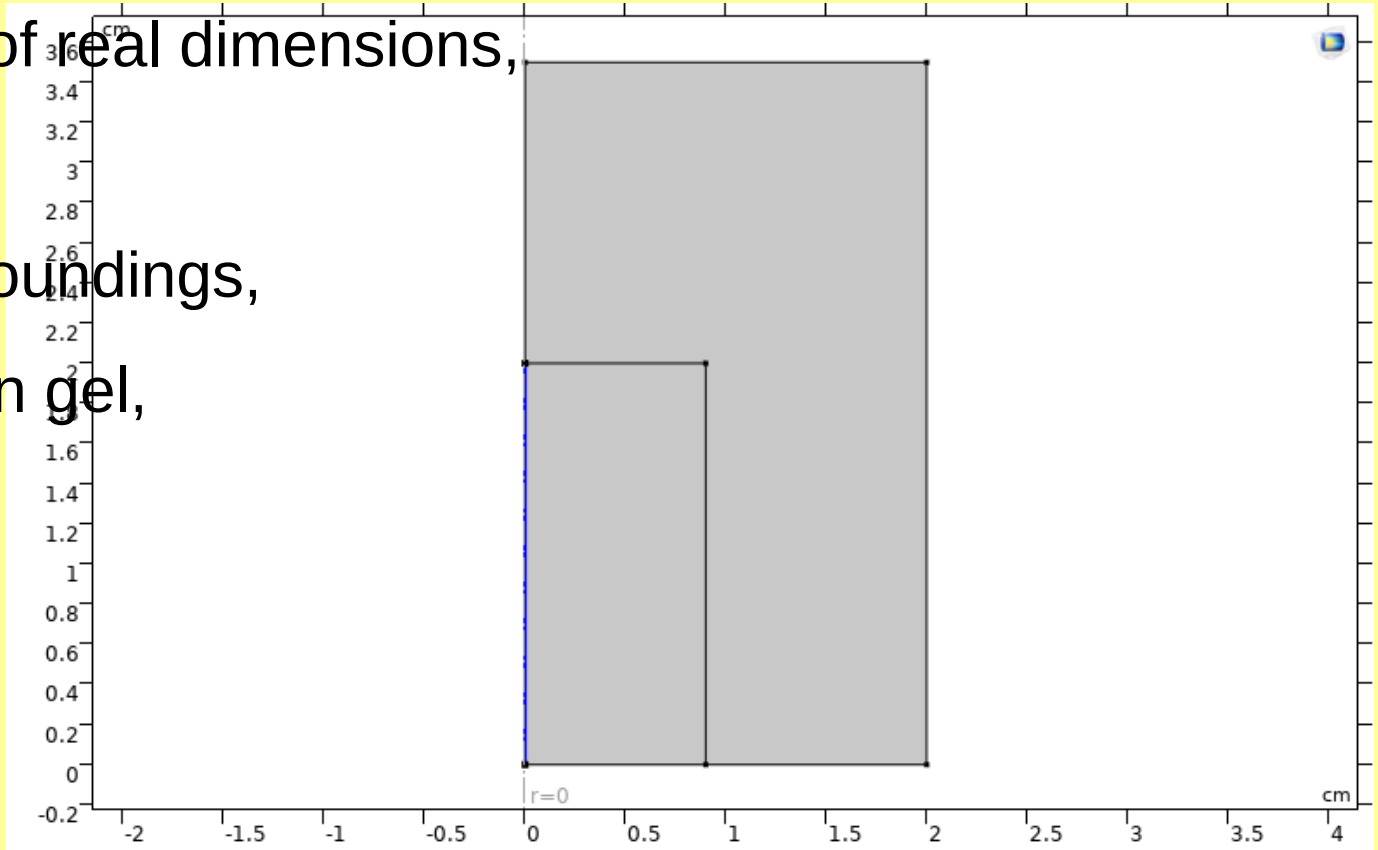


A simple basic **experiment**:

- hydrogel in beaker with aqueous environment,
- detection of active substance concentration in the aqueous phase in time.

Model in COMSOL

- **2D axi-symmetric**,
- gel and environment as rectangles of real dimensions,
- „**Transport of Diluted Species**“,
- diffusion coefficients in gel and surroundings,
- homogeneous initial concentration in gel,
- zero in surroundings.

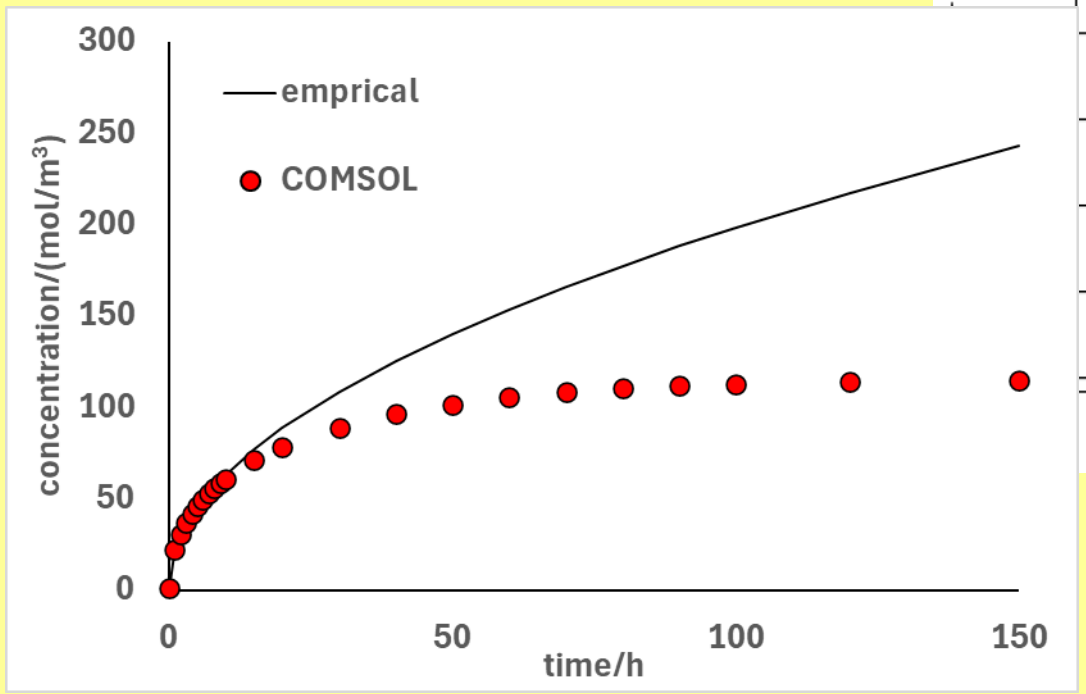


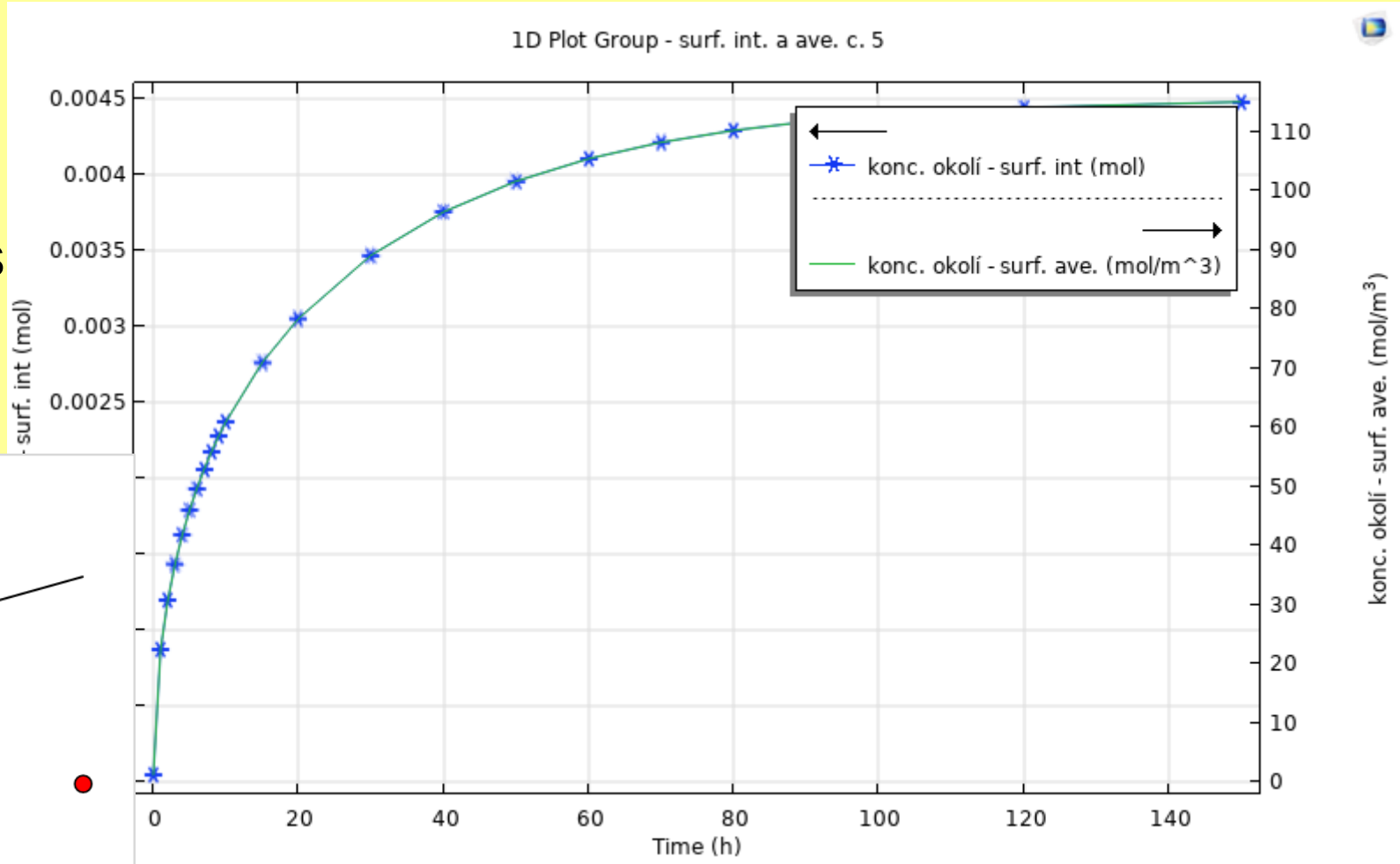
Diffusion coefficients in liquids (water):

orders of 10^{-9} až 10^{-11} m^2/s depending on the size of diffusing (macro)molecule.

Modeling of experimental profiles

- fully stirred environment,
- evaluation of empirical models

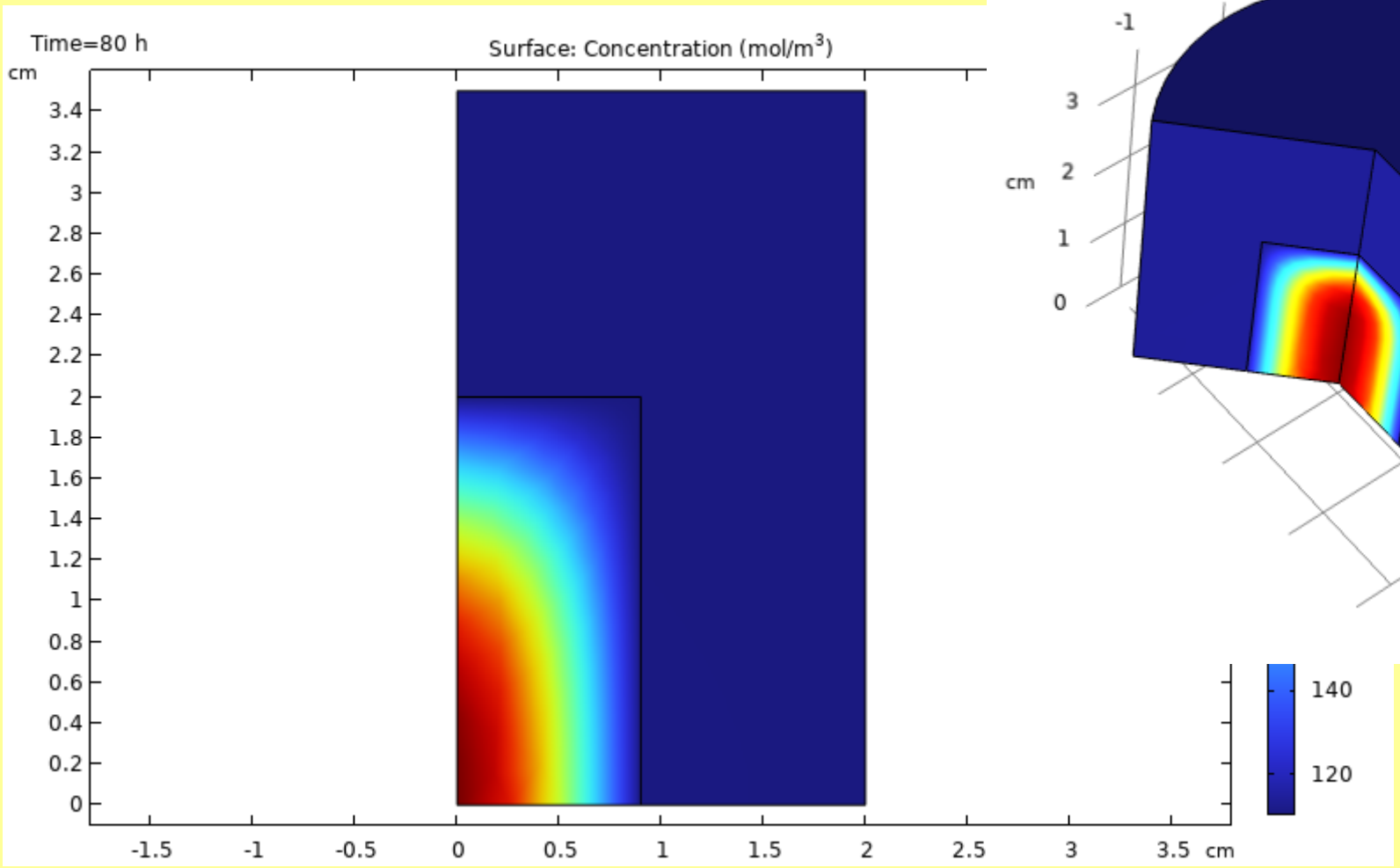


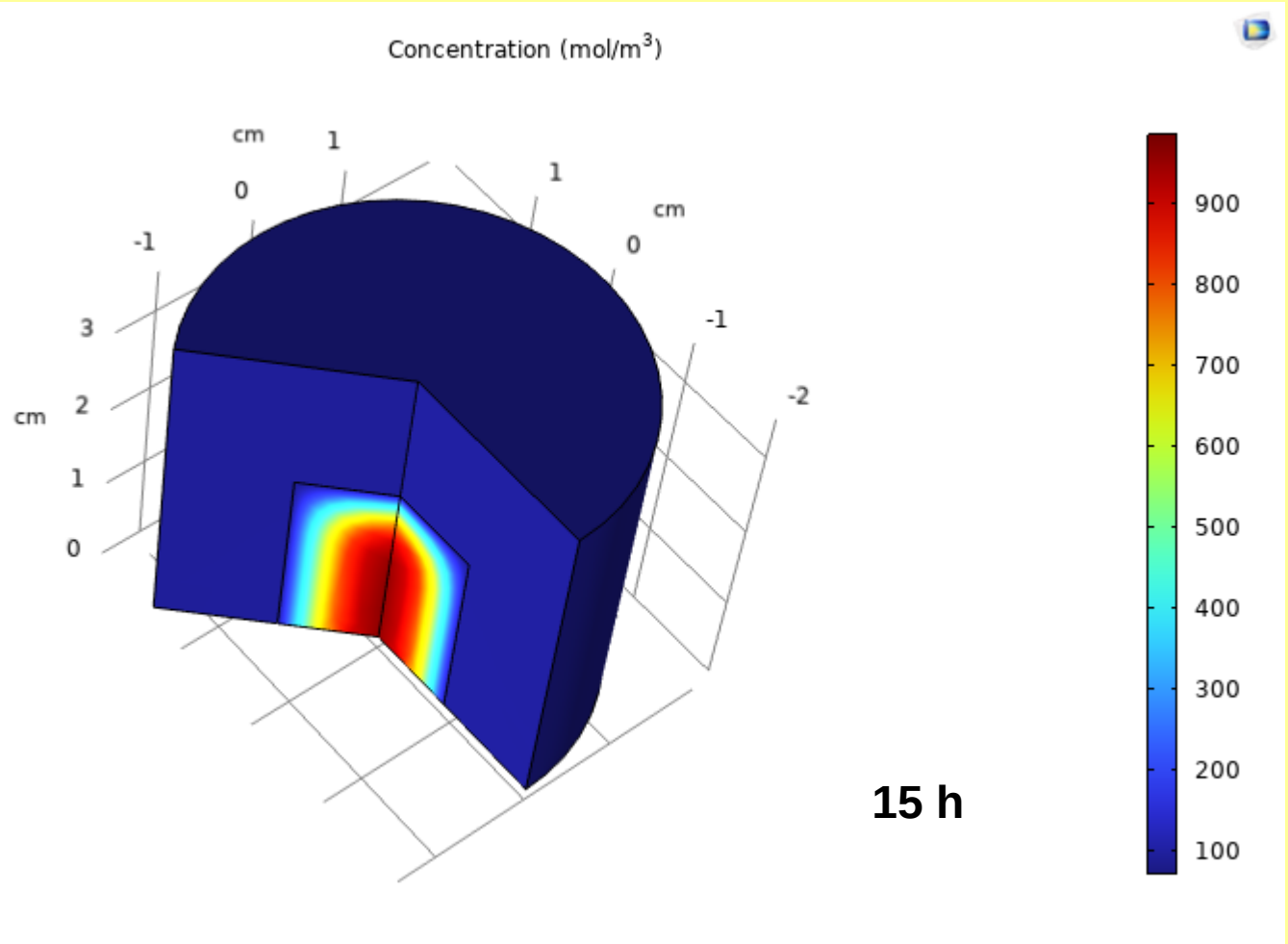


- data fitting,
- partition on the boundary.

What more?

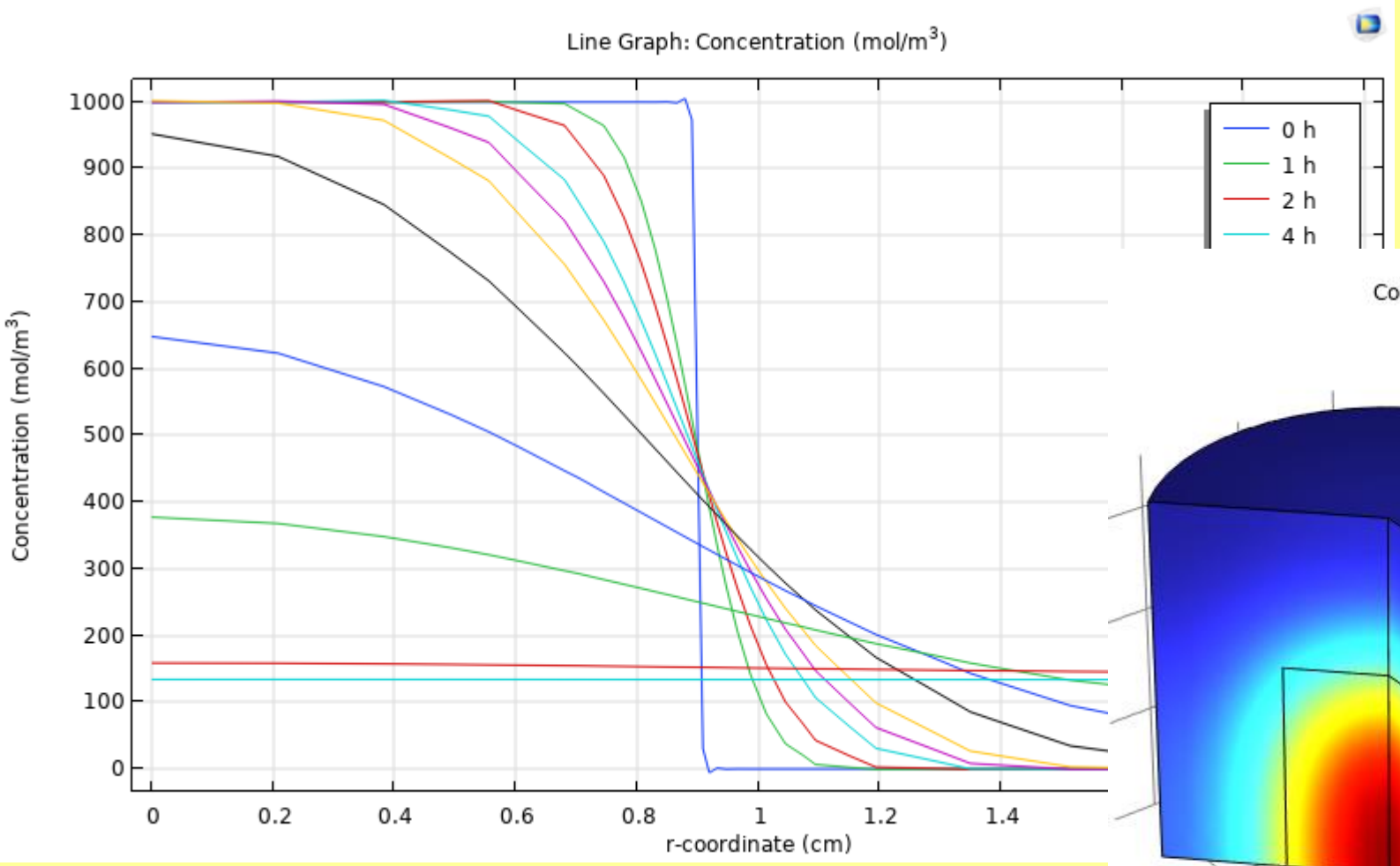
- space profiles in gel,
- 3D view.

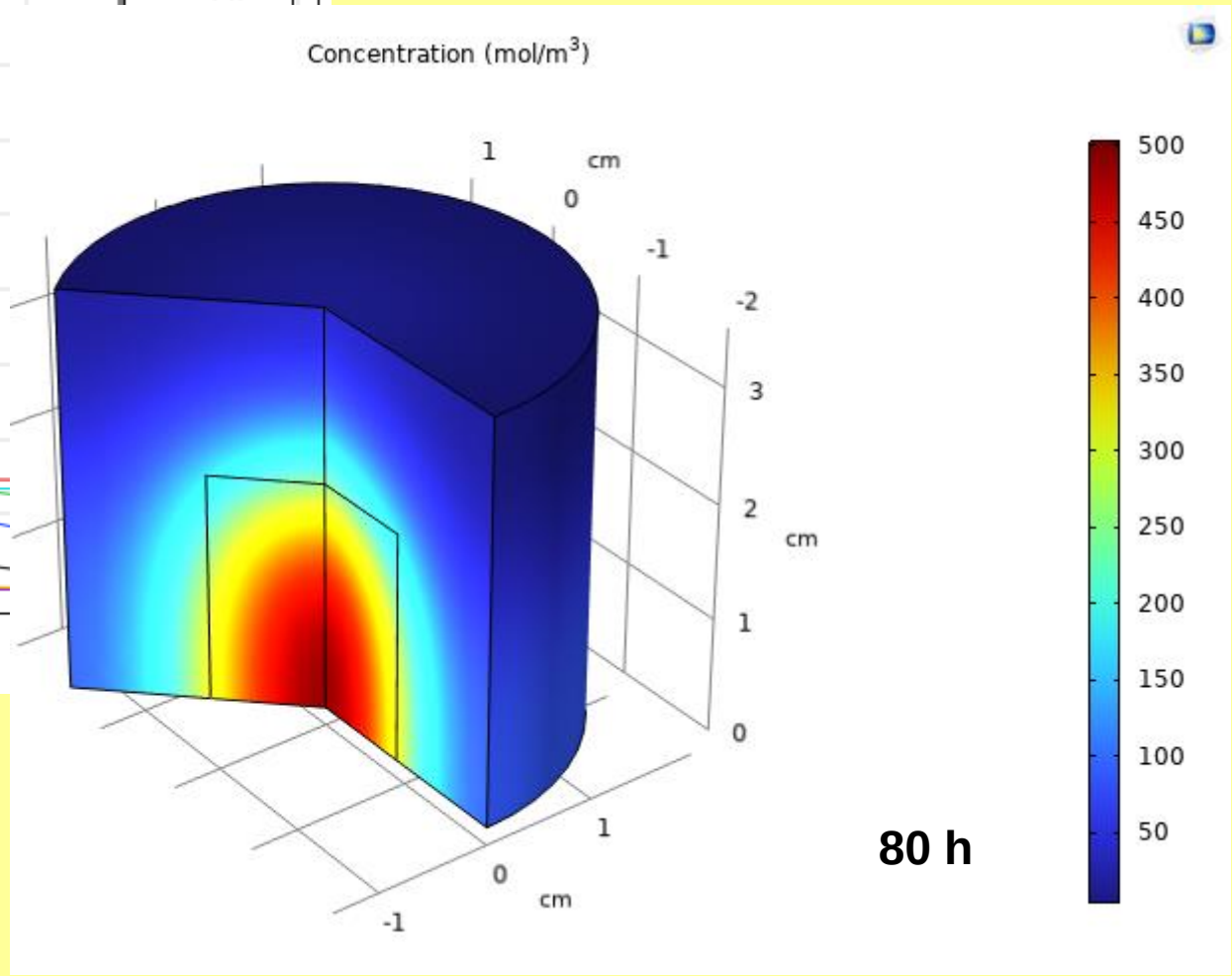




15 h

Non-stirred environment





cut lines in the middle of the gel

80 h