B9: Physico-chemical Investigation of the Swelling Behavior of Enzyme-based Hydrogels for Better System Models

Motivation:

Functionalized and enzyme-based hydrogels can be used in piezoresistive sensors for the detection of numerous inorganic and organic analytes. The hydrogel synthesis, free swelling, and swelling of the enclosed hydrogel in the cavity of the piezoresistive sensor are processes that need to be analyzed and optimized for specific parameters to optimize sensor response. Important parameters are the mesh size, which is decisive for the swelling behavior and the diffusion of the analyte, the network occupation by enzymes, the enzyme kinetics, and the swelling pressure of the hydrogel.
To get a better understanding between the chemical and engineering aspects of hydrogels, experimental physico-chemical results will be connected with the parameters required for the modeling of the hydrogels and the simulation of the swelling process. In addition, the results of the work provide the opportunity to significantly reduce the number of experiments required for the development of new hydrogels in the future.

State of research and own preliminary work:

There are numerous studies on enzyme-based hydrogels and hydrogel-based sensors whose synthesis parameters and manufacturing techniques have been chosen arbitrarily. Therefore, in order to achieve an optimal response of the sensor, extensive parameter studies are required, which, however, only result in an empirical optimization of the specific sensor and hardly allow generally valid conclusions. However, the latter are needed for the modeling and simulation of hydrogels and hydrogel-based sensors.
In previous work of the Research Training Group, functionalized hydrogels were prepared with glucose oxidase and urease and studied with respect to their functioning in piezoresistive sensors.

Scientific questions and project goals:

The investigation of the swelling behavior of hydrogels should be carried out depending on computationally and experimentally given synthesis parameters. For this purpose, hydrogels with a given mesh size and optimal enzyme concentration (from Michaelis-Menten theory, extinction measurements) are to be synthesized. The subsequent investigation of the diffusivity of the hydrogels using diffusion laws and free-swelling measurements allow conclusions to be drawn about the diffusion coefficient and the optimal mesh size for the transport of the analyte. The comparison of the free-swelling behavior with the swelling behavior in the cavity of the piezoresistive sensor leads to the assessment of the influence of the sensor structure on the swelling process. The final aim of the thesis is the determination of suitable parameters for the modeling of the hydrogel and the simulation of the swelling behavior with respect to physico-chemical experimental methods.

Literature:

- D. Caccavo, S. Cascone, G. Lamberti, A.A. Barba, *Chem. Soc. Rev. 47* **(2018)** 2357-2373
- U. Schmidt, C. Jorsch, M. Guenther, G. Gerlach, *J. Sens. Sens. Syst. 5* **(2016)** 409-417
- J. Erfkamp, M. Guenther, G. Gerlach, *Sensors 19* **(2019)** 971