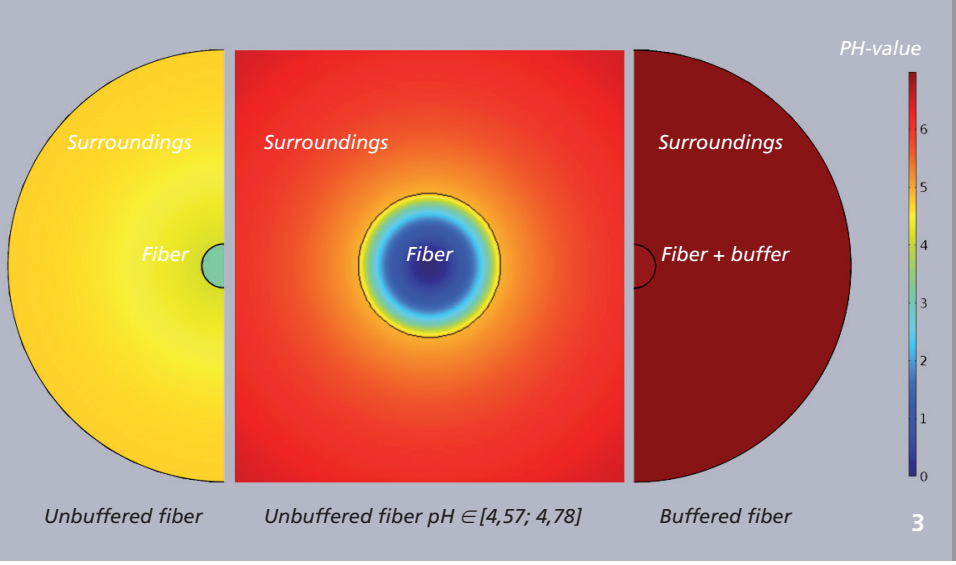

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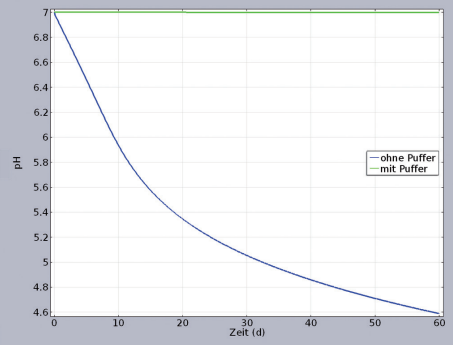

4

SIMULATION OF PH-BUFFERED BIODEGRADATION

Task

Biodegradable polymers play an important role in medicine for implants, sutures or support structures, since, among other things, their use can make secondary surgery – to remove the foreign body from the body – unnecessary. When pure polymers are used, their decomposition leads to a large drop in pH in the vicinity of the polymer, which means difficulties for complication-free healing and should be prevented by the addition of chemical pH buffers. Modeling and simulation of the processes is a promising tool to reduce the large number of necessary experiments and, thus, to minimize animal testing.

Method

The decomposition of the polymers can be described by a system of rate equations in which the temporal evolution of their concentration is given for each molecule size traversing the polymers in their decomposition. In the course of degradation, the concentration of the molecules with a small size increases, those which have a higher mobility and diffuse into the environment. Due to the cleavage of positively charged hydrogen, these short-chain molecules cause the pH levels to drop. The binding of the positively charged hydrogen in the pH buffer molecules occurs on a small time scale. Therefore, the equilibrium state of the reaction buffer can be calculated at any time during the degradation.

Result

The result indicates the pH value as a spatially two-dimensional distributed quantity for a polymer fiber with pH buffer content and its surroundings as a function of time. The simulation tool is available to assess the impact of concentration and distribution of the pH buffer in the fiber on the pH value in the vicinity of the fiber.

Applications

In the project (pH)aser, funded by the Exploratory Research Space at the RWTH Aachen University, pH-neutral degradable support structures are being examined for use in cardiovascular vessels (stents). Other applications include the optimization of implants, sutures or support structures in tissue engineering processes.

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2 Distribution of the pH value in the fiber and its surroundings after 60 days of degradation.
3 pH value in the surroundings of the fiber in elapsed time.