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What NMR can tell us about biodegradation in sediments?

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Subsurface contamination caused by organic compounds is a widespread environmental problem. The main process to reduce the mass of organic contaminants in the groundwater is biodegradation. Often degradation is limited by the supply of organic compounds and electron acceptors for the microbial population and therefore might be influenced by the pore structure and pore connectivity of the aquifer material.

Nuclear magnetic resonance (NMR) allows non-invasive and non-destructive insights into the key processes with sufficient temporal resolution. In our work we applied low field (0.2 T) and high field (3 T) one-dimensional ^{1}H NMR measurements using inversion recovery (IR) and pulsed field gradient (PFG) sequences to analyze the diffusion of water molecules in biomass and water phase and to monitor the concentration changes of electron acceptors. Nuclear spin relaxation times of water molecules reflect their interaction with its porous surroundings as well as the biomass. To localize microbial biomass the mobility of the water molecules can be classified due to different relaxation times corresponding to bound water in the biomass and bulk water. Oxygen is the most important electron acceptor that stimulates the activity and growth of aerobic microbes, and iron(III) is a major one for anaerobes. We show that both, oxygen as well as iron(III) affect the relaxation times by their paramagnetic properties, and thus could be determined by NMR relaxometry in environmentally relevant concentrations. So relaxation time measurements in presence of either oxygen or iron(III) can be used

to detect consumption of these electron acceptors in laboratory systems. This allows assessing the progress of redox reactions and ultimately degradation rates. Furthermore, other important variables of the surrounding porous material, such as porosity and tortuosity, can be determined by methods based on NMR. We present results of porosity, pore size distribution and tortuosity analyses of carbonate rocks and sandstone representing the most common aquifer materials.

Thus, the application of ^{1}H NMR relaxometry and PFG NMR diffusometry provide additional possibilities to study presence, activity and development of microbes quantitatively, and characterize the parameters of their surrounding. Studying key processes non-invasively can contribute to a better understanding of limiting factors for biodegradation and effective degradation rates of organic contaminants in saturated porous systems.