Researchers shed light on role of kinetics in fluid transport

February 3 2022

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Remco Hartkamp, Max Döpke and Fenna Westerbaan van der Meij, researchers at the Delft University of Technology department Process & Energy, are shedding new light on the role of surface reaction rates of

liquid in electrokinetic transport. Their research shows that the kinetics (the rate at which reactions occur) of the equilibrium reaction can significantly influence the adsorption and mobility of ions, which in turn influence the electrokinetic behavior. Having a detailed understanding of what actually happens at the interfaces between oxide materials and electrolyte solutions is also vitally important when designing novel energy devices e.g. batteries and osmotic power membranes, or innovative health or ecological applications—for example drug delivery capsules and techniques for reducing environmental pollution. This week they've published their results in *Physical Review Letters*.

Solid-liquid interfaces are found everywhere in the natural world and so the processes that occur at these interfaces have become the focus of countless studies across many areas of scientific research including colloid science, corrosion, battery research, sensing and electro-kinetic transport.

Remco Hartkamp, researcher at Complex Fluid Processing, says, "say you have a very small device at the micro-meter or nano-meter scale, and you want to transport fluid through it. You're not going to use pressure to push fluid through these very small channels because you'd need relatively large pressures. Instead you might use an electric field. But this type of electrokinetic transport depends entirely on how the electrolytes are distributed, and we have now shown that the distribution of electrolytes can be very sensitive to reaction kinetics—how fast reactions occur—which in turn depends on temperature and pH and so on. So with the insights that our study provides, we are in a better position to develop small devices through which we can transport fluids."

Accounting for proton exchange reactions at a solid surface

However, researchers considering the dynamics taking place at these interfaces have traditionally made certain assumptions: "But these assumptions do not take into account the fact that there are always reactions going on, even in equilibrium, because these reactions are assumed to occur at a different timescales," explains Hartkamp. So in collaboration with Benoit Coasne of the National Centre for Scientific Research (CNRS) in Grenoble, Hartkamp, Ph.D. student Max Döpke and Fenna Westerbaan van der Meij developed a molecular dynamics framework that accounts for proton exchange reactions at a solid surface by dynamically evolving the surface charge distribution. "And what we have shown is that if the reactions occur on a timescale that is say comparable to that of ions adsorbing to the surface or ions moving around, then in fact the kinetics of the reactions at the surface do matter and they do affect the distribution of the components near the surface."

This finding has implications for future molecular simulations of solid-electrolyte interfaces and the interpretation of theoretical models predicting ion distributions or electro-kinetic transport. It will also help in the design of for instance lab-on-a-chip devices.

More information: Max F. Döpke et al, Surface Protolysis and Its Kinetics Impact the Electrical Double Layer, *Physical Review Letters* (2022). DOI: 10.1103/PhysRevLett.128.056001

Provided by Delft University of Technology

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