UP 5: Measurement Techniques and Simulations

Time: Wednesday 16:00–17:00 Location: MOL/0213

UP 5.1 Wed 16:00 MOL/0213

Concept of a Raman-based microfluidic system for measuring trace substances in the field of wastewater treatment — •Simon Jansen, Jan Berk, Sebastian Mammitzsch, and Martin Reufer — Hochschule Ruhr West, Institut Naturwissenschaften

In wastewater treatment plants, sewage is cleaned in various purification stages. But not all impurities are removed in this process. In particular, easily water-soluble substances and those that are difficult to biodegrade, such as pharmaceutical residues, are present in low but nevertheless environmentally harmful concentrations ($\sim \mu g/l$). To reduce the residual amount of these substances, an additional (fourth) purification stage is currently implemented in the wastewater treatment plants. The efficiency of this purification stage can be determined and controlled on the basis of the so-called lead substances with classical analytical methods like gas chromatography-mass spectrometry or indirectly by proof of a sum parameter. We demonstrate a measurement concept suitable for an inline approach, based on a microfluidic system. This concept provides for a concentration of the lead substances by specific binding to surface-activated magnetic beads and a subsequent determination of the concentration. The approach for concentration measurement is based on Raman spectroscopy, due to the distinguishable fingerprint of the different trace elements. This measurement concept is advantageous because the purification process will be monitored and optimised based on the concentration of the lead substances. First results of the particle concentration in the microfluidic system and the subsequent analysis are presented.

UP 5.2 Wed 16:15 MOL/0213

Optimization of excitation and detection windows for the optical detection of microplastics via photoluminescence — •Stefan Brackmann, Srumika Konde, Katharina Gejer, Marina Gerhard, and Martin Koch — Department of Physics and Material Sciences Center, Philipps-Universität Marburg, Renthof 5, 35032 Marburg, Germany

Current microplastics research utilizes subjective hand-picking of particles to identify plastic particles. Recently the first methods using visible photoluminescence to detect plastic particles have been publicized. Here, we investigate the excitation and detection wavelength range suitable to 12 common virgin polymer types. Based on our findings, we recommend a range from 270 to 320 nm for the excitation and 320-425 nm for the detection window. We further show that plastics have unique UV-PL signatures that may be suitable for identifying microplastic particles. This approach may lead to a low-cost alternative to the established methods.

UP 5.3 Wed 16:30 MOL/0213

Time-resolved simulations of wind speed fluctuations across atmospheric boundary layers using a stochastic forward model — •Marten Klein and Heiko Schmidt — BTU Cottbus-Senftenberg, Cottbus, Germany

Atmospheric boundary layers (ABLs) govern the atmosphere–surface coupling and are therefore of fundamental relevance for Earth's weather and climate system. Time-resolved numerical simulations of ABLs are challenging due to intricate interactions of inertial, Coriolis, buoyancy, and viscous forces on all relevant scales of the turbulent flow. Small-scale processes, albeit potentially nonuniversal, are typically not resolved due to cost constraints but modeled based on physically justified relations with the resolved scales, neglecting expensive backscatter. This lack in modeling is addressed here by utilizing a dimensionally reduced stochastic modeling approach. The model aims to reproduce turbulent cascade phenomenology by a stochastic process, respecting fundamental physical conservation principles. Momentary wind velocity and temperature profiles evolve autonomously in time for an ensemble of initial conditions. By comparison with available high-fidelity reference numerical simulations, reanalysis, and observations, it is shown that the model captures various relevant flow properties, exhibiting limitations mainly in a delayed relaminarization under very stable conditions. Forthcoming research aims to contribute to a better understanding of polar boundary layers, requiring predictive modeling capabilities, high resolution, and numerical efficiency to perform long-time simulations.

UP 5.4 Wed 16:45 MOL/0213

Simulated outdoor efficiency and performance ratio of a III-V-on-Si solar panel for direct solar hydrogen production — •Johannes Grabenstein[1,2], Moritz Kölbach[3], Matthias M May[3], Klaus Pfeilsticker[1], and Kira Rehfeld[1,2] — [1]Institut für Umweltphysik, Universität Heidelberg, Germany — [2]Geo- und Umweltforschungszentrum, Universität Tübingen, Germany — [3]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Germany

Tandem solar cells might play a substantial role in future energy systems and in negative emission technologies, both for electricity- and direct hydrogen generation. In a tandem solar cell, photocurrent mismatch between the absorber layers due to variation in the spectral irradiance distribution induces efficiency losses. Together with the temperature-related efficiency modulation, this effect gives rise to its sensitivity to climatic conditions. Here, the performance of an AlGaAs-on-Si tandem solar cell that is either used for electricity production or directly connected to an anion exchange membrane electrolyzer is evaluated for different locations on earth using numerical modeling. The ratio between the outdoor harvesting efficiency and efficiency at standard conditions [1] lies within 0.86 and 0.95 for electricity- and within 0.91 and 0.95 for hydrogen production. This study allows to improve performance predictions and highlights how tuning the top absorber band gap to the prevailing spectral irradiance composition can enhance the harvesting efficiency, depending on the location. [1] Kölbach et al., Sustainable Energy Fuels, 2022, **6** DOI:10.1039/D2SE00561A