Adsorption of organic components from fluid mixtures on functionalized mesoporous materials: Experiment and Simulation

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Research idea

The research project presented (funded by German Research Foundation program "Processes in Natural and Technical Particle Fluid Systems") focuses on physicochemical interactions between biopolymer aerogels and different fluids in Supercritical Fluid Chromatography (SFC). Experimental and theoretical studies will be performed to explain fluid and particle dynamics and the influence of different fluids on the adsorption processes on biopolymer aerogel surfaces.

Introduction

Supercritical liquid chromatography is an established separation technique in analytical chemistry. Complex mixtures can be investigated with regard to their composition. In SFC, a supercritical fluid above its critical pressure (often carbon dioxide, CO_2) is used as the mobile phase. By injecting a mixture of substances into the flow of the mobile high-pressure phase, the sample is flushed into a column filled with fine particles, the so-called stationary phase. The separation of the sample mixture takes place on the surface of the stationary phase due to adsorptive interactions of the particle types and depends on the migration velocity of the contained components in the mobile phase along the separation path. This retention difference is quantified as the retention time. Retention time and shape of the peak signal of molecules in the sample can be used to explain physicochemical interactions between stationary phase and sample and to determine thermodynamic quantities such as enthalpy and entropy of the adsorption surface energy as well as surface heterogeneity. For the analysis of polar test substances using SFC, polar solvents (i.e. modifiers), are added to the mobile phase.

Material

SFC is used to characterize the surface of bio-aerogels (e.g. alginate and cellulose and proteins) using retention data. Commercial stainless-steel columns are filled with bio-aerogel particles using the dry vibration method. The small particle size (< 50 µm) is achieved by emulsion gelation. After filling, the measurements are performed in an SFC device from Waters (Aquity UPC2). The mobile phase mainly consists of CO_2, a flavor is used as solute (vanillin among others), a variable modifier concentration (EtOH, 5-20 vol%) is employed.

Concept and outlook

The interactions between sample liquid and biopolymer aerogels will be determined with quantitative models according to a previously developed concept for the characterization of silica-based materials. The calculation of the thermodynamic parameters of the used components in the mobile and stationary phase is done by the retention factor k' considering the retention time and the residence time. A modified van't-Hoff equation is established to estimate enthalpy and entropy values of the adsorption process for the dissolved target substance on the biopolymer surface. A cellular automaton model is used to describe the diffusion dynamics and adsorption of solutes and the flow properties of the supercritical liquid phase.

Acknowledgement

This research project is supported by the German Research Foundation (DFG, GRK 2462: Prozesse in natürlichen und technischen Partikel-Fluid-Systemen (PintPFS).

Literature

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