2d/P012 - Removal of a model naturally-occurring organic material by aluminium from aqueous solution; the influence of silicic acid

Taylor H., C. Exley Birchall Centre for Inorganic Chemistry and Materials Science, Department of Chemistry, Keele University, Keele, Staffordshire, ST5 5BG, UK. Aluminium salts are highly effective coagulants used by the water industry to remove contaminants from potable and waste waters. In dilute aqueous solutions aluminium interacts with inorganic ligands such as hydroxide and silicic acid ($Si(OH)_4$), and naturally occurring organic materials (NOM), complex, highly heterogeneous materials of high molecular weight. Humic and fulvic acids, common components of NOM in natural waters, impart colour to finished drinking water and may contribute to disinfecting by-product formation; levels of residual organic carbon in finished drinking water are expected to be subject to legislation in the near future. Although effective in inducing the removal of NOM from drinking water, neither the speciation of aluminium, nor the mechanisms by which NOM removal occurs, are well understood. A 'model' NOM was prepared by simple pre-treatment of a commercial humic acid and its spectroscopic behaviour characterised. This material was used in synthetic aqueous solutions to study the interactions leading to the removal of NOM by aluminium across the approximate pH range 3.0 to 8.0. UV-Visible, fluorescence and atomic absorption spectroscopy showed that aluminium-induced removal of humic acid was pH dependent, with optimal removal occurring between pH 5.5 and 6.0. The results of HPLC fractionation of NOM which remained in solution after coagulation by aluminium will be described, along with selected rheological properties of humic acid in aqueous solutions with aluminium present or absent. These results will be compared to those of solutions in which silicon was present as silicic acid.

2d/P013 - The role of soot in desorption kinetics of 1,2,4-trichlorobenzene

ten Hulscher Th.E.M., H. Christiansen and B.A. Vrind. RIZA, Lelystad, the Netherlands. Desorption kinetics of organic micropollutants from sediments is often interpreted with a fast and a slowly desorbing fraction. Recently the presence of a very slowly desorbing fraction has been observed for Ketelmeer sediment. The presence of soot in sediments may be an explanation for the observed slow and very slow desorption: soot has been shown to have a high affinity for organic compounds. In the present study the desorption kinetics of spiked 1,2,4-TCB was studied using Ketelmeer sediment. Part of the sediment was combusted at 275 C to obtain sediment that contains only soot carbon. The desorption experiments show that in combusted sediments a larger fraction of the spiked TCB desorbs slowly. These results will be compared to results from experiments with a NIST Diesel soot.

2d/P014 - Toxicity testing of non-volatile organic pollutants in groundwater

Baun A., L. Kløft, P.L. Bjerg and N. Nyholm. Department of Environmental Science and Engineering/Groundwater Research Centre, Technical University of Denmark, Lyngby, Denmark. A method for assessment of toxicity of non-volatile organic chemical contaminants in groundwater polluted with landfill leachate has been evaluated. The biotests utilised were comprised of an algal growth inhibition test (*Selenastrum capricornutum*), a daphnia immobilisation test (Daphnia magna), and a bacterial genotoxicity test (umuC, Salmonella typhimurium). The feasibility of the selected biotests was investigated for a series of groundwater samples collected along pollution gradients downstream of two landfills in Jutland, Denmark. Two different approaches were used: 1) Direct toxicity testing of whole groundwater samples, 2) Toxicity testing of concentrates obtained by solid phase extraction (SPE). Direct testing of whole groundwater samples produced toxic responses, but the complex sample matrix masked the toxicity of the organic chemical contaminants of interest. SPE was used successfully as an on-site method, which eliminated ion toxicity and which produced biotest responses that reflected the toxicity of the non-volatile organic chemical contaminants in the groundwater.

2d/P015 - Influence of mineral-bound humic substances on the sorption of atrazine on kaolinite

Perminova I.V., N.A. Kulikova, G.Ph. Lebedeva, Dept. of Chemistry, Moscow State University, Russia. Sorption of herbicide atrazine was investigated on kaolinite that had been coated with 11 natural humic substances isolated from soil, peat, and brown coal. Mass percent carbon in coated samples ranged from 0.06 to 0.18%. Distribution coefficient for sorption of atrazine on kaolinite and kaolinite coated with humic substances was determined. Increasing content of sorbed humic substances increased the sorption of atrazine. However, not only quantity of organic carbon, but also properties of humic substances that were used for coating of mineral substrate influenced the atrazine sorption. Desorption isotherms of atrazine showed that sorption was reversible.

2e/P001 - Slow-Stir water solubility measurements for phthalate ester plasticizers

Letinski D.J., M.J. Connelly and T.F. Parkerton, Exxon Biomedical Sciences, Inc., East Millstone, NJ, USA. Water solubility is a key chemical property needed for environmental assessment. Dialkyl phthalate esters with alkyl chains of six or more carbons represent an important class of commercial plasticizers used to impart flexibility to polyvinyl chloride products. Accurate determination of water solubility poses a unique challenge for these chemicals due to their hydrophobic liquid nature and similar density to that of water. Past application of conventional shake flask tests have yielded reported solubilities that are suspect since observations are orders of magnitude higher than theoretical predictions. To overcome the experimental limitations of previous work, a slow-stir shake flask procedure was used to obtain reliable water solubility measurements for selected C_6 to C_{10} single and mixed isomer dialkyl phthalate esters. Aqueous concentrations were quantified using a liquid or solid-phase extraction method followed by GC-MS-SIM detection. Results indicated that water solubility declines with increasing alkyl chain length from 70 micrograms per liter for branched C_6 isomers to below one microgram per liter for C_9 to C_{10} isomers. These findings indicate that conventional experimental methods overestimate the water solubility of these products.