Physical Chemistry of Organic Compounds in Natural Waters

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Water covers most of the Earth and is critical to life on the planet. While its resources seem endless, deteriorating water quality makes it an increasingly precious commodity. Organic compounds are one of the most important water pollutants. Their number is staggering, and their properties, which determine their fate in aquatic environment, vary widely.

The course will introduce the participants to the physicochemistry of organic pollutants in natural waters and will attempt to explain their fate in this context. It will begin by a brief review of fundamental thermodynamic concepts, including chemical potential, Gibbs free energy, thermodynamic equilibrium, enthalpy and entropy.

Next, selected properties of organic chemicals affecting their environmental fate will be discussed. This section will begin with the discussion of vapour pressure and factors determining its magnitude. This will be followed by a short treatise on aqueous solubility, with a detailed explanation of the fundamental parameters affecting it, viz. the enthalpy and entropy of solution. In addition, the effect of various environmental factors (temperature, inorganic salts, co-solvents and/or co-solutes) on aqueous solubility of organic compounds will be explained. The combined knowledge on vapour pressure and aqueous solubility will be used to explain the phenomenon of air-water partitioning. The concept of Henry's law constant K_H will be introduced, and the effect of various parameters on K_H will be discussed. Selected methods used to estimate the magnitude of Henry's law constant will also be presented. The discussion of air-water partitioning will be followed by organic solvent-water partitioning, with a particular emphasis on octanol-water partitioning coefficient K_{ow}. In this context, linear free energy relationships as tools for K_{ow} estimation will be introduced and discussed. The effect of selected environmental parameters on K_{ow} will be explained.

Acid-base properties of organic chemicals affect their partitioning behaviour, hence will be discussed next, with emphasis on the explanation of the effect of molecular structure on the acidity constant. Methods used to estimate pK_a values of organic compounds, including Hammet's correlations, will be presented.

Sorption is one of the most important phenomena affecting the fate of organic chemicals in natural waters. Its effects manifest themselves for example through the decrease in biological activity of chemicals in water in the presence of suspended particulate matter, or through the retardation of chemicals transported by groundwater. Various sorption mechanisms will be discussed in detail, and the effect of various parameters on sorption will be explained.

The focus of the final section will be transport phenomena. Molecular diffusion of chemicals will be reviewed and its effect compared to that of turbulent diffusion (advection). The concept of eddy diffusion coefficient will be introduced and discussed.

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Course Outline

- Thermodynamics - brief review
- Vapour pressure
- Solubility
- Partitioning (air/water, organic solvent/water)
- Acids and bases in water
- Sorption
- Diffusion

Termin	Dzień tygodnia	Godzina	Miejsce
05.05.2014	**Poniedziałek**	**12.15 – 15.00**	**Minicentrum Konferencyjne (Luwr)**
06.05.2014	**Wtorek**	**12.15 – 15.00**	**Minicentrum Konferencyjne (Luwr)**
07.05.2014	**Środa**	**12.15 – 15.00**	**Minicentrum Konferencyjne (Luwr)**
08.05.2014	**Czwartek**	**12.15 – 15.00**	**Minicentrum Konferencyjne (Luwr)**
09.05.2014	**Piątek**	**12.15 – 15.00**	**Minicentrum Konferencyjne (Luwr)**