

The Study of Cadmium Accumulation by Floating Macrophytes using Natural Modeling Approach

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It is known that phytoremediation technology became an effective method of environment clearing after it has been found the plant's ability to accumulate the contaminants at high concentration level. The floating macrophytes (*FM*) *Eichhornia crassipes* (*EC*) and *Pistia stratiotes* (*PS*) are applied most often to waste waters purification.

The goal of this investigation was to study the efficiency of the metal's bioaccumulation by *EC* and *PS* when exposed to cadmium with an emphasis on the mechanism of transport and transformation of pollutant within the plant and its fate during accumulation act.

To estimate hit consequences of pollutant on ecosystem an experiment was carried out in the conditions close to the natural using an approach of natural modeling consisting in a statement of natural experiments with the use of mesocosms, established directly in a reservoir into which one enters the set portion of pollutant and then supervises the dynamics of its concentration.

As a result it was found that the degree of cadmium extraction by *FM* from contaminated natural water while maintaining the viability of the plants depends on the way of pollutant introducing and the maximum is observed in the case of its gradual entry. Herewith at the first stage of cadmium uptake the sorption of the metal on the surface of the roots takes place where cadmium mainly localized in rhizodermis, and then the pollutant penetrates into the tissues of the stem according to its translocation factor

In contrast to the traditional black-box approach, detailed investigations of pollutant transport and distribution in plant tissues have given sound understanding of the phytoremediation phenomenon. Such advancements could provide a basis for future improving the efficacy of the biological remediation processes.

Modelling fluid-mineral equilibria in two-phase fluid systems

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There is a demand for modeling fluid-rock interaction in geological systems that contain two fluid phases (e.g., liquid + gas) or experience a transition from supercritical to subcritical state of fluids. The relevant problems include CO₂ sequestration into geological formations; exploitation of gas-rich geothermal systems; quantification of metal transport by low-density fluids in porphyry, epithermal, and lode-gold mineral systems. Modelling of geochemical processes in these systems requires software that allows simultaneous prediction of the accurate phase composition of the fluid part of the system and "conventional" water-rock or gas-rock equilibria. Recent experimental and theoretical studies start to provide thermodynamic models to expand these calculations into the realm of metal bearing fluids [1].

To address these challenges, we employ the HCh software package [2] that uses the Gibbs Free Energy minimization approach for equilibrium calculations. To calculate fluid-fluid equilibria, we have incorporated a customised version of the PRSV equation-of-state [3], where thermodynamic properties of *pure water* at a given temperature and pressure are calculated according to the comprehensive Haar-Gallagher-Kell model [4]. The incorporated algorithms were calibrated and tested against available experimental and theoretical data for the binary H₂O-CO₂ and H₂O-CH₄ systems, and the ternary H₂O-CO₂-CH₄ system.

A practical application of the software to economic geology problems is illustrated by calculation of H₂S concentrations in a supercritical fluid and subcritical gas and liquid phases in equilibrium with mineral assemblages containing iron sulfides and oxides. An equilibrium between pyrite-pyrrhotite mineral pair and the H₂O-CO₂-CH₄-H₂O-H₂S-H₂ fluid offers a plausible explanation of the H₂S concentrations measured in the vapor-rich inclusions from the Missouri lode gold deposit.

- [1] Migdisov & Williams-Jones (2013) *GCA* **104**, 123-135. [2] Shvarov (2008) *Geochem. Int* **46**, 834-839. [3] Stryjek & Vera (1986) *Can. J. Chem. Eng* **64**, 323-333. [4] Kestin *et al.* (1984) *J. Phys. Chem. Ref. Data* **13**, 175-183.