

Surface characteristics of TiO₂ in the Alcohol-Water Cosolvent System

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ABSTRACT

Surface complex models(SCMs)은 최근 흡착모델링에 대한 관심이 부각되면서 수질(표면수, 지하수)오염에 대한 영향을 예측하고 흡착결과를 파악하는데 많은 주목을 받고 있다. SCMs의 흡착모델의 하나인 diffuse double layer model(DDL)은 특정조건에서 Gouy-Chapman 이론을 바탕으로 설명하고 있지만, 실제와는 상당한 차이를 보인다. 따라서 본 논문은 기존의 자료를 바탕으로 TiO₂/용매(수용액/ 물-에탄올 (1:1))간의 거리를 추정해 감에 따라, 각 실험적 변수에 따른 electrical double layer(EDL)의 흡착형태의 변화를 알아보았다. 또한, cosolvent가 존재할때, 흡착모델 형태의 변화와 흡착결과에 대한 영향에 대해 알아보았다.

I. Introduction

During the last two decades, concern with the fate and transport of toxic pollutants in surface and ground waters have been shown to be describing adsorption processes onto mineral surfaces by many adsorption models. Because of the importance of ion adsorption on oxide surfaces, both in natural systems and industrial processes, one of the adsorption models, surface complexation models(SCM) have been developed. However, in domestic, recently these SCMs are utilized in determining the mechanism of adsorption reaction by surface reactions and the electrical

properties.

Previous assessment of SCM almost always conservative (low) because few field data exist in the process causing adsorption and the models all rely on distribution coefficients (K_d) or sorption ratios (R_d). Distribution coefficient evaluated for site-specific materials are observed to vary over several orders of magnitude without providing any insight as to why such variability might be expected, and thus predicted. In the an aspect of structure for SCMs, a diffuse-layer model, based on their ability to simulate the acid/base titration behavior of oxide surface. It is a two-plane model since both an adsorption and a diffuse-layer plane are included. However diffuse-layer model using this parameter (K_d) is regarded without the potential in the β -plane and with only the α - and diffuse-layer potentials are indistinguishable. Furthermore, this model is similar in their descriptions of surface reactions, but differ in that of the electrical double layer and the manners in which changes in the background electrolyte concentration are incorporated in model computations. In the field electric double layer theory the use of computer simulation and other accurate theoretical methods has opened up the possibility to make penetrating and detailed studies of double layer structure and interactions.

To evaluate its surface characteristics based on diffuse-layer model simulations for SCMs, various methods have been suggested. However, depending on the electrokinetic method chosen, electric properties of diffuse-layer model and titration data may be obtained. For many years electrophoresis has been one of the electrokinetic techniques most commonly used to obtain the zeta (ζ) potential of dilute dispersions. By means of the zeta potential, the electrical state of liquid/solid interface can be characterized. In relation to the model mentioned above, it can be said that they include other properties, such as κ (κ the reciprocal Debye-Hückel length), ϵ , φ and χ , the dielectric constant, surface potential and distance from solid to bulk solution, respectively, which characterize the solid particles and the liquid properties.

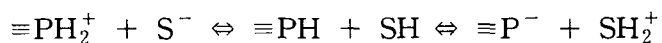
The aim of this paper is to clarify the role that properties of diffuse-layer model can play in order to explain; (1) It is anticipated that with appropriate modification, current experimental work evaluating K_d values could consider with assuming that the o- and diffuse-layer potentials are distinguishable on diffuse-layer model. (2) Defensible experimental data including surface charge density, zeta potential and sharpened understanding of electrical double layer(edl) structure controlling the fate of pollutants in natural system are needed to ensure more reliable model simulation. (3) Presence of cosolvent at the oxide/electrolyte solution interface is investigated to be changed the edl structure. It is visualized using Mathcad.

II. Experimental methods

The some properties of titanium dioxide were obtained by the existing data. The surface potential was calculated from the equation given by the Gouy-Chapman equation. The distance between titanium dioxide and cosolvent computered by using Mathcad.

III. Results

Titanium dioxide, TiO_2 , is the first of the metal oxides that we analyze. In theses cases absorbed ions the surface charge results from surface group dissociation as follows;



Where $\equiv PH$ is the protolitic surface group; SH is the molecule of the solvent. The surface charge is formed on the metal oxide as a result of ionization and complexation reactions of surface hydroxyl groups. Electric charge verse pH dependence is one of the most important characteristics of the surface properties of the metal oxide/electrolyte solutions. The positions of pH_{pzc} depends on the alkali-acid character of surface hydroxly groups.

The point of zero charge for titanium dioxide/aqueous water of the NaCl system occurs at a pH of 6.2 and in the cases for water-ethanol(1:1) of the system is assumed equal to 6.2.

By comparison of the ζ potential-pH relationship for water /mixed water-ethanol solution of NaCl, it can be stated that , for higher ionic strengths, the presence of the alcohol results in a considerable decrease of the ζ potential.

According to the Gouy-Chapman model, the relationship between potential at the distance χ from the surface, (Ψ), and the surface potential (Ψ_0) are

$$K\chi = \left[\frac{\left[\exp\left(\frac{Ze\Psi}{2kT}\right) + 1 \right] \left[\exp\left(\frac{Ze\Psi_0}{2kT}\right) - 1 \right]}{\left[\exp\left(\frac{Ze\Psi}{2kT}\right) + 1 \right] \left[\exp\left(\frac{Ze\Psi_0}{2kT}\right) + 1 \right]} \right]$$

From above equation, it was calculated the distance of zero potential plane at different pH values. The distances of shear plane from the surface of TiO₂ as a function of pH in aqueous solutions on the following each ionic strength, 0.2mole/L, 0.02mole/L are 10Å, 30Å. In mixed solution, the values of the distances on the following each ionic strength, 0.2mole/L, 0.02mole/L are 15Å, 35Å.

IV. Reference

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