Abstract No: 54 ***Physical Sciences***

MODEL VALIDATION OF Cu(Ⅱ)- KAOLINITE SYSTEMS BY IN-SITU MEASUREMENT OF FREE METAL ION ACTIVITIES

N. Mudannayake[*], K. Heenkenda and R. Weerasooriya

National Institute of Fundamental Studies, Kandy, Sri Lanka.
[*]nalesha63@gmail.com

Surface complexation modelling methods are extensively used to quantify the chemical speciation at the mineral-water interface. However, the input parameters are often not uniquely defined. In 1-pK modelling of metal ions adsorption, the basic Stern layer model (1-pK SLM) calculations require six parameters, viz., specific surface area, site density, inner and outer layer capacitance, and intrinsic acidity/binding constants. The number of input parameters by introducing free Cu^{2+} ions as an observation to determine its binding constants was reduced by 1-pK SLM. The copper selective electrode (Cu-ISE) was calibrated using ethylenediamine/Cu^{2+} metal ions buffer to extend the Nernstian Cu^{2+} detection limit to 10^{-15} M. Spectral data also suggests bidentate complexation of Cu^{2+} with $\equiv AlOH^{-0.5}$ and ion exchange complexes between Cu^{2+} and ≡Si-OH sites as follows, $(\equiv AlOH)_2Cu^+$ pK = -2.8, $(\equiv SiO_2)Cu^0$pK= - 8.4 and $(\equiv X)_2Cu$ pK = -2.02. The ISE measurements of free Cu^{2+} seem to interfere with the presence of $CuOH^{+,}$ particularly when the solution is pH > 7.0. When the analytical data are corrected for $CuOH^+$ interference, the measured $\{Cu^{2+}\}$ of the Cu-kaolinite system is predicted well with 1-pK SLM modelled data. Using this method, the number of input parameters reduced to five while simulating Cu^{2+} - kaolinite interface processes reasonably well is considered a novel method concerning the experiment results. Quantifying chemical speciation at mineral-water interfaces could be done using consistent parameters with reference to the above experiment.

Keywords: Copper, Modeling, Surface complexation