Determination of soil acid buffer capacity with surface complexation model and the relationship with soil properties

Y. YANG[123], Y. WANG[123], Y.M. PENG[123], T.X. LIU[1*] AND F.B. LI[1]

[1]Guangdong Institute of Eco-Environmental Science & Technology, Guangdong Key Laboratory of Integrated Agro-Environmental Pollution Control and Management, Guangzhou 510650, PR China

[2]Guangzhou Institute of Geochemistry, Chinese Academy of Sciences, Guangzhou 510640, PR China

[3]University of Chinese Academy of Sciences, Beijing 100049, PR China

[*] Correspondence: txliu@soil.gd.cn

Abstract

Although acid buffer properties of soils could be simply evaluated by titration curves, the research of acid buffer mechanism from a molecular perspective is still lacking. The soil acid buffer capacity (soil BC) was determined by titration curves using titration method and continuous potentiometric titration (CTP) method. The results of stepwise regression analysis between soil BC and soil properties show that the cation exchange reaction and the protonation of hydroxyl groups on the surface of amorphous Al oxides are the major acid buffer mechanisms for acid and neutral soils with low carbonate content. The surface complexation model (SCM) was applied to further evaluate the acid buffer properties of the soils by assuming two pK_a values for one proton adsorption site of the soil. The values of point of zero charge (pH_{pzc}) calculated from the model were well matched with those from the titration experiments, indicating that the application of SCM to the soils is feasible. The results of Principal Component Analysis shows that the model-calculated proton adsorption capacity (H_s) was significantly correlated with the buffer properties of the soils, as well as the pH_{pzc} was significantly correlated with the acid-base properties. It suggests that the H_s may well quantify the contributions of major components involved in the acid buffer reactions and the pH_{pzc} may be used to predict the key point from which the soil start to buffer acid. This modeling study provides a new insight into the acid buffer reactions in the complicated soil system from a molecular reaction perspective.

Keywords: acidification; soil buffer capacity; surface complexation model