UNIVERSITI
PENDIDIKAN
SULTAN IDRIS

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Sijil Penyertaan

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Venue

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UNIVERSITI PENDIDIKAN SULTAN IDRIS

Professor Dr. Mustaffa Ahmad
Dean
Faculty of Science and Mathematics
Universiti Pendidikan Sultan Idris

Scientific Programme

Room 1 (Chemistry)

Session 1
Chairperson: Dr.Eli Rohaeti

Time	Presenter
10.15-10.30	OR-001: Synthesis of Dual Herbicides-Intercalated Layered Double Hydroxide Nanohybrid
10.30-10.45	OR-002: Direct Determination Of Trace Concentration Of Lead In Fresh Water Samples By Adsorptive Cathodic Stripping Voltammetry Of A Lead-Citrate Complex
10.45-11.00	Or-003: Application Of N,N'-Bis[2-Hydroxyacetophenone] Ethylenediamine For Electrochemical Detection Of Transition Metal Cadmium, Copper, Lead And Zinc Ions
11.00-11.15	OR-004: Synthesis of Multifunctional Porphyrins via Condensation Reaction
11.15-11.30	OR-005: Structure-Antioxidant Activities Relationship Analysis Of Benzalacetone's Derivatives
11.30-11.45	OR-006: Aporphine Alkaloids From Leaves Of Alseodaphne Peduncularis
11.45-12.00	OR-007: Voltammetric Measurement Of Copper(Ii) Using Zinc Layered Hydroxide-2(3-Chlorophenoxy) Propionate Nanocomposite Modified Multiwalled Carbon Nanotube Composite Paste Electrode
12.00-12.15	OR-008: Eggshell, Coconut Tree Sawdust, And Sugarcane Bagasse As Low-Cost Adsorbents For Cu(Ii) Removal From Aqueous Solution
12.15-12.30	OR-009:Adsorption Of Pb(Ii) From Aqueous Solutions Using Durian Tree Sawdust, Oil Palm Empty Fruit Bunch And Coconut Coir
12.30-12.45	OR-010: Surface Complexation Model Of The Sorption Of Phosphate Ions By Montmorillonite
	Lunch

Session 2
Chairperson: En. Sheikh Ahmad Izzddin Sheikh Mohd Ghazali

Time	Presenter
14.00-14.15	OR-011: The Effect Of Unsaturated Fatty Acids On The Size And Encapsulation Efficiency Of Nanostructured Lipid Carrier (NLC)
14.15-14.30	OR-012: Factorial Analysis on the Migration of Bisphenol A from Polycarbonate Baby Bottles via Modified European Standard Method
14.30-14.45	OR-013: Indole Alkaloids From The Roots Of Kopsia Singapurensis Ridl. (Apocynaceae)
14.45-15.00	OR-014: Determination of Toxic Heavy Metals in Herbal Medicines of Malaysian Market- A Preliminary Study
15.00-15.15	OR-015: XRF Analysis Of Trace Element In River Bank Soil By The Effect Of Electrokinetic-Assisted Phytoremediation
15.15-15.30	OR-016: Bacterial Cellulose From Rice Waste With Addition Of Chitosan

Room 2 (Chemistry)

Session 1
Chairperson: Dr.Hari Sutrisno

Time	Presenter
10.15-10.30	OR-017: Adsorption Of Technical Direct Red Dye By Tanduk And Kepok Banana Peels
10.30-10.45	OR-018: Hernagine Type Of Aporphine Alkaloids From Alseodaphne Perakensis
10.45-11.00	Or-019: Review Of $LiNiO_2$ System And Their Derivative As Cathode For Lithium Ion Batteries
11.00-11.15	OR-020: Studies On The Hydrogen Evolution Reaction On Fe-Co/S, FeNi/S And Co-Ni/S Electrodes
11.15-11.30	OR-021: Adsorption And Photocatalysis Of Nicotine In Cigarettes Smoke Using Tio_2 Embedded In Activated Carbon From Tobacco (Nicotiana Tabaccum) Stem Waste
11.30-11.45	OR-022: Effect of DOPE-PEG 2000 on Oleic and Linoleic Fatty Acid Liposomes
11.45-12.00	OR-023: Pore Formation and Doping Process on the Sol Gel Synthesis of Nanocrytalline Nitrogen-doped Titania
12.00-12.15	OR-024: Raman spectroscopy Study of carbon nanotube prepared using ferrocene-fermented tapioca-chemical vapour deposition
12.15-12.30	OR-025: Molybdenum Complexes with Amino Acids as Antihyperglicemic Agent : Preparation and Spectroscopic Studies
12.30-12.45	OR-026: DNA Binding Properties of Ruthenium(II) Polypyridyl Complexes.
	Lunch

Session 2
Chairperson: Prof. Endang Widjajanti Laksono

Time	Presenter
14.00-14.15	OR-027: Electronic States of Vanadium-doped Anatase TiO_2 by First Principles Calculations
14.15-14.30	OR-028: Effect of Electron Beam Irradiation on the Molecular Weight of Hydrolyzed Collagen
14.30-14.45	OR-029: Conductivity Behaviour Of Polyacrlamide-Methane Sulfonic Acid Gel Polymer Electrolyte In Tin-Air Battery.
14.45-15.00	OR-030: Solar Photocatalytic Degradation Of Azo Dye New Coccine In Solution With Zinc Oxide Sodium Alginate Beads
15.00-15.15	OR-031: Solar-Photocatalytic Degradation of Phenol Using Zinc Oxide Prepared by Precipitation Method
15.15-15.30	OR-032: Effect Of Inconsistent Organic Loading On The Development Of Aerobic Granulation In Sequencing Batch Reactor

OR-010

SURFACE COMPLEXATION MODEL OF THE SORPTION OF PHOSPHATE IONS BY MONTMORILLONITE

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The sorption of phosphate by montmorillonite was investigated at 30 °C. The purpose of this investigation is to determine the adsorption reactions and their equilibrium constants. Data were collected from adsorption edge experiments investigating the effect of pH, adsorption isotherms enabling the effect of sorbate concentration, acid-base titration calculating protons released or taken up by adsorption process, and sorption kinetics studying time needed by the sorption process to reach the equilibrium. The extended constant capacitance surface complexation model (ECCM) was used to determine the adsorption reactions and their constants, which then used as fixed parameters to model adsorption edge and adsorption isotherm data. The ECCM and X-ray Diffraction measurement indicated that the phosphate interacting montmorillonite surface by forming two *outer-sphere* surface complexes through hydrogen bonding. In first complex, $[(XH)^0 - H_2L^-]^{-1}$, the phosphate was held to permanent-charge X^- sites on the tetrahedral siloxane faces. The second complex, $[[(SO^-)(SOH)]^- - [H_2L^-]]^{-2}$, is due to the interaction between the phosphate and variable charge surface hydroxyl groups at the edges of montmorillonite crystals and on the octahedral alumina faces.

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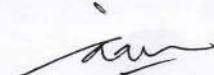
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Keywords: phosphate; montmorillonite; outer-sphere complex; extended constant capacitance surface complexation model (ECCM).

A. INTRODUCTION

As an agronomical region, Indonesia has land and water containing excess phosphate with high concentration. The excess phosphate can be from the use of fertilizer or the waste of industrial activities. The high concentration of phosphate in the natural environment can decrease water quality that results in serious problem to human life.

The excess of phosphate can carry the growth of superfluous plants in water system in Indonesia, which is worrying. For instance, the growth of water plants called *Enceng Gondok* in Indonesian rivers and lakes, which are used to cause serious

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ABSTRACT

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environmental problems, and can disturb the water biota and shallow rivers and lakes insides.

This research investigates the mobility of phosphate in the water so that caring actions can be taken by use of adsorption principles. Sorbents for the purpose of phosphate adsorption can be varied. For example, Kabayama *et al.* (2004) studied the adsorption of phosphate in sea water system using Boehmite (Aluminium oxide-hydroxide)[1]. Kitano *et al.* (1978) used calcium carbonate[2], and Madrid *et al.* (1991) used montmorillonite and goethite to adsorb phosphate and $Zn(II)$ ions[3]. In the principle, adsorption is a chosen method to decrease effectively the waste of ions in environment.

This research investigates reactions occurring on the surface when the adsorption of phosphate onto the clay mineral montmorillonite takes places. The reactions are predicted by Surface Complexation Model using a computer program, GRFIT[4]. The model has been used by previous investigators and produced excellent results to describe adsorption process of metal ions[5] or organic ligands by metal oxide-hydroxide and clay minerals[6,7,8,9,10,11,12]. Fourier Transform Infrared and XRD measurement were also conducted to confirm the surface complexes produced by interaction of the adsorption process.

Montmorillonite is a sorbent having two active sites, hydroxyl functional group represented by SOH, with S stands for Surface. This site has different charges, depending on the pH, and exists on montmorillonite crystal edges, at the aluminum octahedral surface. Montmorillonite has also another active site who always has negative charges caused by the substitution of Si^{4+} by Al^{3+}, and usually represented by X^-, existing on external sites (at the surface of siloxant tetrahedral) of montmoriilonite, and on internal site (at interlayer regions caused by montmorillonite swelling).

The sorption of phosphate ions by external and internal surfaces can be easily recognized from the sorption kinetics of the adsorbate. The sorption on internal sites take much longer time than that on external sites[13]. Kinetic desorption principles can also be used as theoretical review for further studies. In this case, for example, kinetic desorption can be useful to implement clay minerals as fertilizer that can desorb bonded micro-nutrients with certain amount along with the need of plants. Therefore, this study will also investigate the kinetics of desorption of phosphate ions.

Based on the above mentioned facts, this research investigates the sorption process of phosphate ions by montmorillonite, including the effect of pH and concentration to the adsorption, as well as kinetic of sorption.

B. EXPERIMENTAL SECTION

1. The Determination of Montmorillonite Surface Area

Montmorillonite chosen as the sorbent was saturated by K^+ ions. The surface area of montmorillonite was determined by using *surface area meter* NOVA 1000 which was 20,559475 m^2g^{-1}.

2. Adsorption experiments

The adsorption experiments were conducted at temperature of 30 ^0C and with supporting electrolyte KNO_3 of 5 mM. The experiments included 4 types of experiments: adsorption and desorption kinetics, adsorption edge (adsorption as a function of pH), adsorption isotherm and acid-base titration. The experiment steps as follows.

Adsorption kinetics were done to determine the time needed for the interaction between phosphate ions and active sites of montmorillonite to reach equalibrium. Montmorillonite suspension of 50 m^2L^{-1} with volume of 200 mL was kept to equilibrate by stirring it for 18 – 20 hours. The phosphate stock solution was added to the suspension so that the phosphate ion concentration in the suspension was 0.1 mM. The pH of the suspension was decreased and maintained at pH 4 by adding KOH or HNO_3 solution. At a certain period of time (1 minute, 10 minutes, to 1 day), a sample was taken, centrifuged and its filtrate was analyzed for free concentration of phosphate by using UV-Visible spectrophotometre at wavelength of 390 nm.

Desorption experiments were conducted to determine the equibrium time to release bonded phosphate by surface to solution. Montmorillonite suspension with total volume of 200 mL containing 50 m^2L^{-1} montmorillonite was stirred for about 18 – 24 hours. The pH of the suspension was adjusted to about 4 by addition of HNO_3 solution. Certain amount of phosphate ion stock solution were added into the suspension so that its concentration become 0.1 mM. By maintaining the pH at 4, the suspension was left to

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reach equilibrium time of 2 hours. A sample was taken, centrifuged, and the filtrate was analyzed for free concentration of phosphate ions.

Adsorption edge was conducted to enable the influence of pH on the adsorption. Into suspension which contains 50 m^2L^{-1} montmorillonite which has been equilibrated for 18 – 24 hours, KOH solution was added until the pH of the suspension was about 10. Certain amount of phosphate stock solution was added into the supension, to make concentration of 0.1 mM. The suspension was then stirred for about 30 minutes by using magnetic stirrer, and a sample was taken and put into a well capped-test tube. The pH of the rest of suspension in the reaction vessel was decreased by adding 0.1 M HNO_3 and kept to equilibrate for 30 minutes. A 3 mL sample was taken and transferred into capped test tube. The experiment was repeated until the pH of the suspension was about 3. All samples in the capped test tubes were stirred for at least 1 day (24 hours), the optimal time obtained from adsorption kinetic experiments. Finally, all samples were centrifuged, and the filtrates were measured for free concentration of phosphate ions in the solution.

Adsorption isotherm was done to know the effect of sorbate concentration to the adsorption. The pH of 200 mL suspension containing 50 m^2L^{-1} was adjusted into 4 and kept constant by addition of KOH or HNO_3. Stock solution of phosphate ion solution with volume of 3 mL and concentration of 0.01 M whose pH has already been adjusted into pH 4, was added into the suspension and left to equilibrate for the optimum time (obtained from adsorption kinetic). Sample was taken and put in capped test tube. Another amount of stock solution of 5 mL was added into the suspension, and sample was taken again and so on until total volume of stock solution added was about 30 mL. All samples in the capped test tube were stirred for 1 day, then centrifuged and the filtrate were analyzed for free concentration of phosphate ions.

Acid and base titrations were conducted for three separate systems (solutions or suspensions). First, titration was conducted for the system containing phosphate solution to ascertain phosphate dissociation reactions and their equilibrium constants. Second, the titration was toward the system containing montmorillonite suspension for determination of protonation and deprotonation surface reactions and their equilibrium constants. Third, the titration was completed for the systems containing montmorillonite suspension and phosphate to determine adsorption reactions and their adsorption reaction equilibrium

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constants. Firstly, for the phosphate solution titration; 100 mL of 1mM phosphate solution was increased its pH to become 10, and then was titrated with HNO_3 until pH 3.0. Every step of acid addition, the pH was left equilibrate for 30 minutes. Secondly, for the titration toward suspension which contains only montmorillonite mineral, and thirdly toward the phosphate – montmorillonite that was done in the similar experiments. Suspension of montmorillonite substrate was stirred-up for about 18 – 24 hours. Phosphate and montmorillonite with the concentration of 1 mM and 100 m^2L^{-1} respectively were added before the titration.

Determination of Phosphate ion concentration was done by complexation method using molybdenum[1]. Two mL sulphatic acid 10 % and 1 mL of 5% ammonium molibdat were added into sample and stirred-up for 5 minutes. The sample was then measured by using Spectrophotometer UV-Vis at wavelength of 389 nm.

3. Data Analysis

The reactions of adsorption process were determined by Extended constant capacitance complexation (ECCM) model toward the data from the 3 (three) separate experiments. Equilibrium constants for surface adsorption/desorption reactions can be determined by fitting acid-base titration data using computer program GRFIT[4]. The results of model of the titration data was then used for fix parameters to model adsorption edge and adsorption isotherm data, so data from all three sets of experiments can be modelled using the same parameters. The parameters consist of reactions and the equilibrium constants at the adsorption process, as well as density and capacity of adsorbent's surface area.

At the modeling, Schindler *et al.* (1997) suggests that active sites of clay mineral surface are grouped into two: edge site (pH-dependent charged SOH sites) and face site (negative permanently charged X^- sites)[14]. Specific reactions which may occur are:

- Protonation and deprotonation reactions of SOH (represented by equation 1 and 2).

  At low pH : $SOH + H^+ \rightleftharpoons SOH_2^+$ .... (1)

  At high pH : $SOH + OH^- \rightleftharpoons SO^- + H_2O$. .... (2)

- X^- assumed to be bound with K^+ ion from background electrolyte KNO_3 or K^+-saturated surface through cation exchange, with reaction 3 below:

$$(X^- \text{-} K^+) + H^+ \rightleftharpoons (X^- \text{-} H^+) + K^+ \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \quad (3)$$
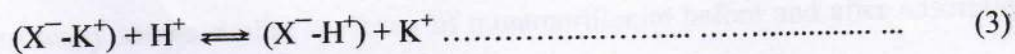
- Phosphate can bind montmorillonite surface in the form of neutral or anion, by binding SOH sites (that is unchargeed, protonated or deprotonated) or X^-.

- Surface complex which was formed can be *outer-sphere* or *inner-sphere*.

Analysis for FTIR spectra and X-ray diffractogram (XRD) was also conducted to support the results of surface complexation model.

C. RESULTS AND DISCUSSION

1. Phosphate ion Sorption by montmorillonite

The decrease of phosphate concentration when it was dissolved in montmorillonite shows phosphate binding by montmorillonite occured very fast. The XRD diffractrograph also supports the binding represented by the shift of $d(001)$ space of montmorillonite. However, comparison of montmorillonite FTIR spectrum before and after adsorption did not show significant difference. In both figures, there was water adsorption at wavelength of 3610.5 cm^{-1} which was free OH vibration, and at 3394.5 cm^{-1} there was broad band that showed the OH octahedral vibration. As listed in Table 1, montmorillonite contains aluminium and silicate so that there was an adsorption at wavelength of 1031.8, 788.8 and 459.0 cm^{-1} which each indicates O-Al-OH, Si-O-Al and Si-O. It also contains phosphate as shown by adsorbent at wavelength of 831.3 and 916.1 cm^{-1} which shows the characteristics of H_2PO_4, and therefore both similar two spectra were caused by the existence of anion organic mixtures, containing phosphate[15]. Phosphate adsorbent in clay mineral is known as phosphate retention and phosphate implantation. Phosphate retention is adsorbed phosphate in clay surface on which Al^{3+} as a bridge that can be released, and so possibly be readsorbed at certain pH condition. Phosphate implantation is adsorption occuring between phosphate and hydrous Al-oxide. Phosphate ion can react faster to Al octahedral by replacing OH on the mineral surface and forming phosphate hydroxyl and tend to be difficult to dissolve. This results from strong binding between phosphate ions and Al octahedral[15]. Due to strong phosphate bonding and insoluble of phosphate implementation, qualitative analysis using IR

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spectroscopy shows similar spectrum of montmorillonite before and after adsorption of phosphate.

IR Spectrograph can also be used to identify surface complexes either *inner-sphere* or *outer-sphere*. *Inner-sphere* complex has been proved to shift active vibration wavelengths of functional groups, as mentioned by Persson *et al* (1998) finding that adsorption of phtalate by goethite can shift adsorption wavelenghts from 1300 cm^{-1} to 1700 cm^{-1}[16].

XRD diffractogram shows a significant decrease in d(001)-space of montmorillonite as a result of adsorbed phosphate by the clay. It indicates the importance of interlayer regions (also known as internal sites) in the adsorption of phosphate. This indication has also been found by Akyuz *et al*. (1999)[17] and Ikhsan *et al*. (2005)[18] which stated that aminopyridinium ion can affect d-space of clay mineral. Slow kinetic adsorption from which the reaction equilibria was reached after one day, even there was still a continuing adsorption in the following day (although in a small amount) (Figure 1), indicated that montmorillonite's interlayer regions have a crucial role to phosphate adsorption. Phosphate desorption by montmorillonite was also very slow at which 40% of adsorbed phosphate was not desorbed for 2 days (Figure 2).

Some researches showed that kinetic adsorption and desorption in the interlayer region of clay minerals are generally very slow[17,19,21]. From the kinetics experiments results, it is obvious that phosphate is bound in the interlayer region of montmroillonite. Intercalation of phosphate in the interlayer region decreased the interlayer space. It was an interesting phenomenon, as generally organic intercalation causes the increase of interlayer space of clay minerals[17,22]. Smaller space of interlayer region of montmroillonite might result from cation exchange reactions between the phosphate and silicate, or between phosphate and water molecules coordinated by the cations. Insolvated Phosphate ion ($H_2PO_4^-$) which is bound in thin and flat structures can also decrease the gap of interlayer spaces. Similar phenomenon has also been reported by Morillo *et al*. (1991) for 3-aminotriazole adsorption[19] and by Ikhsan *et. al*. (2005) for 2-aminopyridinium ion intercalation[13].

At first, kinetic adsorption (Figure 1) and desorption (Figure 2) lasted fast, although later kinetics lasted slowly. Fast kinetic adsorption indicated the importance of

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external montmorillonite site for phosphate adsorption. However, it needed careful observation to find out which external site had a crucial role in adsorption because external sites consist of 2 active sites; negative permanent charge site at siloxant tetrahedral (X^-) faces, and pH-dependently charged sites at the alumina octahedral (SOH). This phenomenon cannot be seen clearly by infrared spectrum because of similarities as shown by montmorillonite spectra before and after adsorbing phosphate. Therefore, specific comparison is needed, for example, sorbent adsorption that has only dependently-charged external sites, such as goethite.

The fact that isotherm adsorption at pH 4 did not involve many protons shows that adsorption reaction in acid pH values occur without uptaking or releasing protons. From these facts, modeling to adsorption data has to consider (1) the importance of X^- internal site (interlayer regions) in the adsorption, (2) external site, X^- and/or SOH might be important in adsorption, (3) reaction in acid pH values does not involve many protons, (4) the surface complexes are most possibly *outer-sphere* complexes.

2. Surface Complexation Model

Modelling was conducted step by step toward titration data (Figure 3) of phosphate solution, montmorillonite suspension, and binaries system containing montmorrillonite and phosphate. The results of modelling was adsorption reactions and their equilibrium constants (Table 2), which were then used as fixed parameters to model adsorption edge (Figure 4) and isotherm adsorption data (Figure 5).

Parameters results calculated by the model can fit well to experimental data, although some models did not fit to adsorption isotherm data very well that may be due to some weaknesses, such as: availability of contaminants in montmorillonite. The sample montmorillonite used as sample may contain also organic cation contaminant. These contaminants might not be replaced by K^+ cation in saturated montmorillonite because it is bonded strongly to montmorillonite surface. Therefore, it was not surprising when phosphate functional group was also identified in the FTIR in montmroillonite samples.

3. The process of phosphate ion adsorption by montmorillonite

Figure 3 shows the comparison of H^+ concentration needed in the adsorption process. There is significant difference between 100 m^2L^{-1} montmorillonite titration before and after adsorption of 1 mM phosphate, where $[H^+]$ that has to be added into montmorillonite suspension with 1 mM phosphate was much smaller. This indicates that 1 mM phosphate was continuously deprotonated, releasing H^+ ions to the suspension in the range of experimental pH values. However, in higher pH values (above 7.5), $[H^+]$ ions that has to be added to the suspension was much smaller than the phosphate. Unfortunately, isotherm adsorption in high pH was not conducted, so the proton stoichiometry in higher pH values cannot be determined as that at pH 4, in which there are not many protons involved in complex formation at pH 4. This indicates that in high pH, surface complex reaction occur by releasing protons. Possible surface sites that have a role is SOH because at the pH ranges, X^- site was saturated by K^+ not H^+. Therefore, both active sites of Montmorillonite play an important role for phosphate ion adsorption, e.i. X^- in low pH and SOH in high pH values.

Surface complexation model toward the experimental data suggested that *outer-sphere* complex was formed, $[(XH)^0 - H_2L^-]^{-1}$ and $[[(SO^-)(SOH)]^- - [H_2L]^-]^{-2}$. Distribution of the species of surface complexes is shown in Figure 4. First surface complexes were formed between deprotonated phosphate ions and saturated external sites of X^- in low pH values through hydrogen binding, represented by following reaction, and their reaction equilibrium constants are depicted in Table 2.

$$[X^- - H^+]^0 + H_2L^- \rightleftarrows [(XH)^0 - H_2L^-]^{-1}$$

With H_2L^- represents $H_2PO_4^-$. This complex may be illustrated in Figure 6.

Second surface complex was formed between deprotonized phosphate ions with SOH sites on the edge sites of montmorillonite in alumina octahedral surfaces through hydrogen bounding with reaction as depicted below. Reaction equilibrium constants are shown in Table 2.

$$2SOH + H_2L^- \rightleftarrows [[(SO^-)(SOH)]^- - [H_2L]^-]^{-2} + 2H^+$$
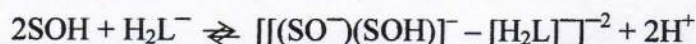
The complex formed in alumina octahedral sites is given by Figure 7.

D. CONCLUSION

Based on the calculation using Extended Constant Capacitance Surface Complexation Model, it can be concluded that phosphate ion adsorption by montmorillonite occur through the formation of two *outer-sphere* surface complexes. Both *outer-sphere* complexes occur are formed via hydrogen binding with the reactions are as follows.
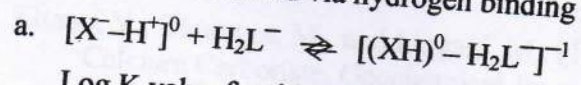
a. $[X^--H^+]^0 + H_2L^- \rightleftharpoons [(XH)^0 - H_2L]^{-1}$
   Log K value for this reaction is −0.425.
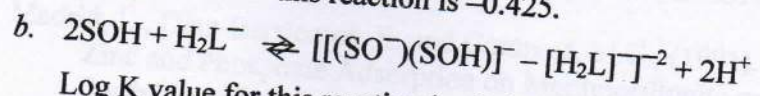
b. $2SOH + H_2L^- \rightleftharpoons [[(SO^-)(SOH)]^- - [H_2L]]^{-2} + 2H^+$
   Log K value for this reaction is −3.624.

Thanks and gratitude

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Table 1.

No	Before Adsorption		After Adsorption	
	Number waves (cm^{-1})	Vibration	Number Waves (cm^{-1})	Vibration
1	459,0	Si-O	462	Si-O
2	788,8	Si-O-Al	794,6	Si-O-Al
3	831,3		831,3	
4	916,1	H$_2$PO$_4$	918,1	H$_2$PO$_4$
5	1031,8	O-Al-OH	1029,9	O-Al-OH
6	1633,6	OH from H$_2$O	1633,6	OH from H$_2$O
7	3394,25	OH octahedral	339,1	OH octahedral
8	3610,5	OH free	3606,6	OH free

Table 2.

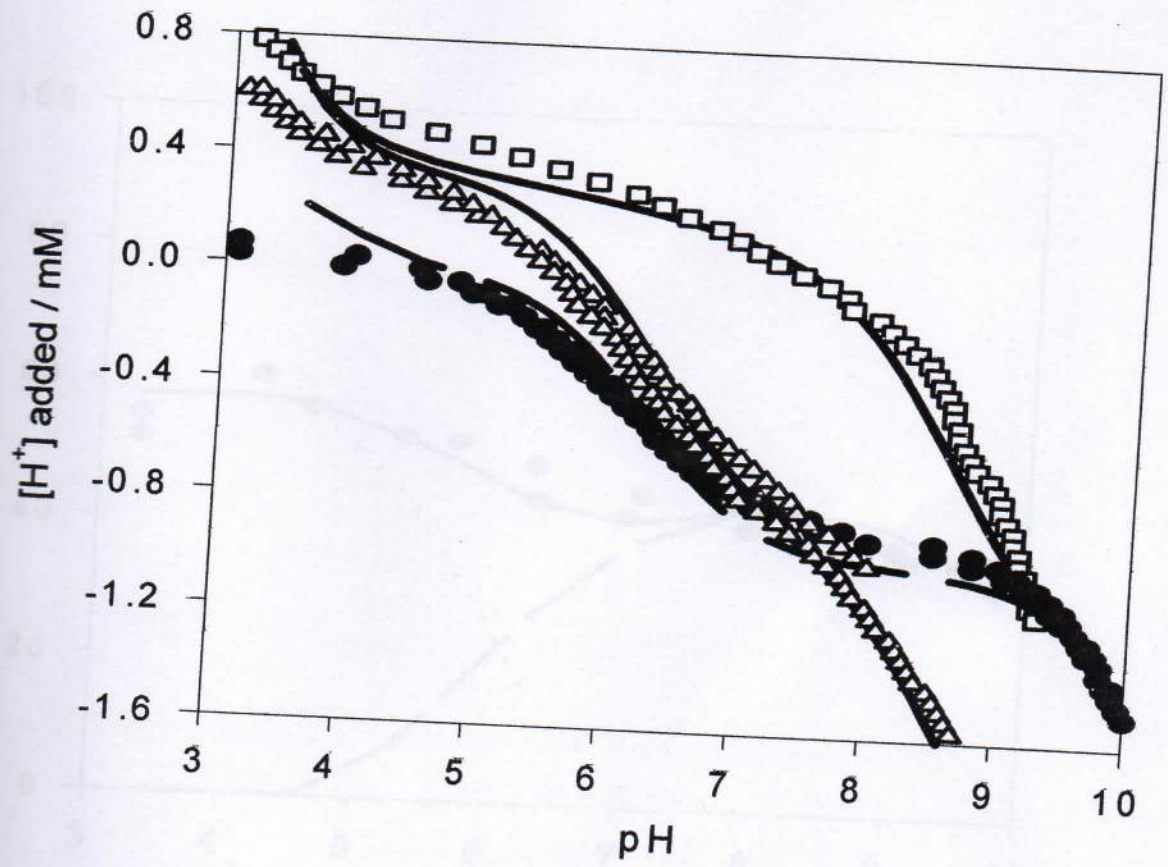| Equilibrium constants, Dissociation of Phosphate, $\log_{10} K$	
$H_3L \rightleftharpoons H_2L^- + H^+$	
	-2.00
$H_2L^- \rightleftharpoons HL^{-2} + H^+$	
	-6.26
$HL^{-2} \rightleftharpoons L^{-3} + H^+$	
	-16.63
Site Concentration	
SOH / mmol m^{-2}	
	0.00376
X^- / mmol m^{-2}	
	0.0125
Inner capacitance (F m^{-2})	
	7
Outer capacitance (F m^{-2})	
	3
Equilibrium conctants of Protonation-deprotonation surface, $\log_{10} K$	
$[X^- - H^+]^0 + K^+ \rightleftharpoons [X^- - K^+]^0 + H^+$	
	-6,25
$SOH + H^+ \rightleftharpoons SOH_2^+$	
	5,46
$SOH \rightleftharpoons SO^- + H^+$	
	-6,50
Equilibrium constants of phosphate adsorption, $\log_{10} K$	
$[X^- - H^+]^0 + H_2L^- \rightleftharpoons [(XH)^0 - H_2L^-]^{-1}$	
	-0.43
$2SOH + H_2L^- \rightleftharpoons [[(SO^-)(SOH)]^- - [H_2L]]^{-2} + 2H^+$	
	-3.62

Figure 1
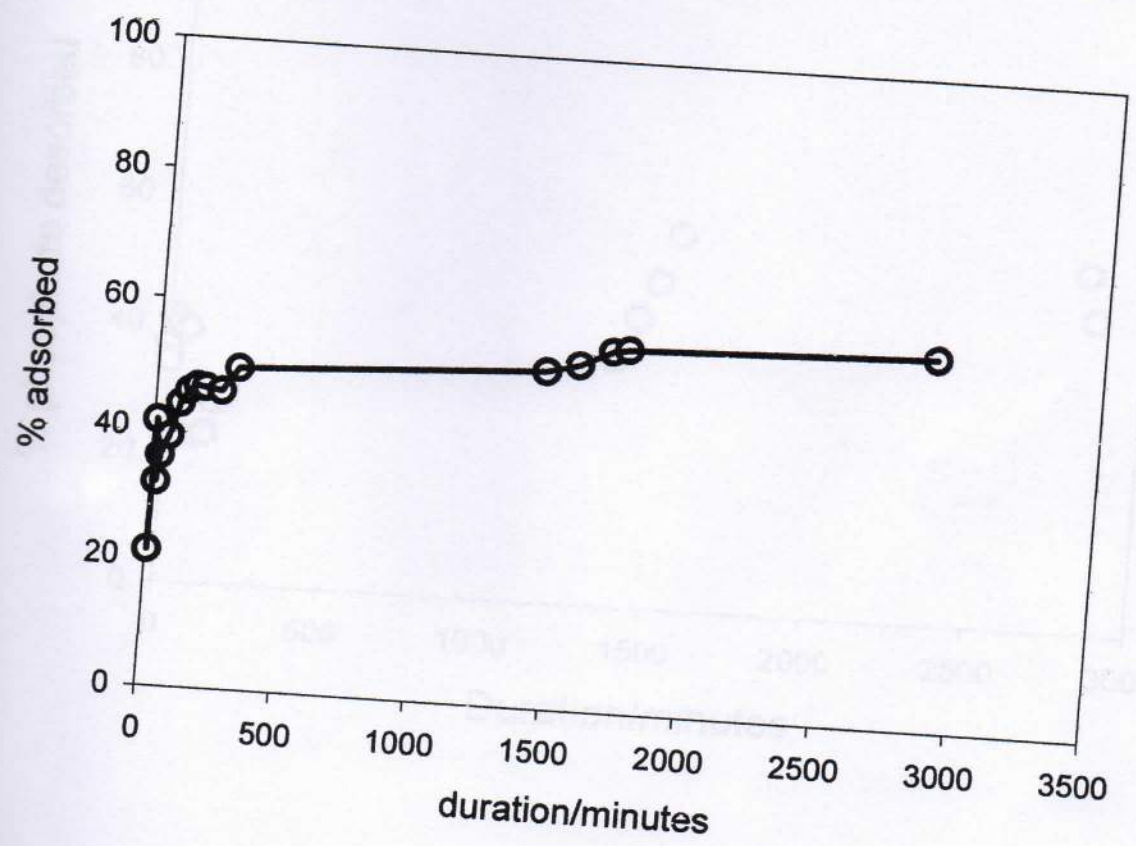
Figure 2

Figure 3

Figure 4

Figure 5

Figure 6

Figure 7