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Statistical Modeling of Surface Complexation of Selenium Onto Iron and Aluminum Oxide Using SAS®

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ABSTRACT

Simulation of chemical element adsorption, release, and transport is possible without the need to perform time consuming, detailed adsorption studies on multiple samples by incorporating prediction equations into chemical speciation–transport models before simulating. Adsorption models also assume that the chemical species in a mixture is at chemical equilibrium which is the state in which the chemical activities or concentrations of the reactants and products have no net change over time. By the second law of thermodynamics, a mixture of chemicals satisfies its chemical equilibrium state (at a constant temperature and pressure) when the free energy of the mixture is reduced to a minimum. In this study a constant capacitance chemical surface complexation model was applied to simulate selenate (Se(IV)) adsorption on iron and aluminum oxides by optimizing monodentate Se(IV) surface complexation constants and surface protonation constants. Samples selected for variation in chemical properties were used. The composition of the chemicals satisfying its chemical equilibrium state was found by minimizing the function of the free energy of the mixture using PROC IML. Non linear least squares optimization was developed using PROC NLP to fit the equilibrium surface complexation constants specifying initial and boundary values. A general non linear multiple regression model was fit ted using PROC NL MIXED to the measured adsorption using easily measured soil parameters. Good fit of the model predicted and the experimental data indicated success of the protocol.

KEYWORDS

Surface Complexation, Least Squares Minimization, Chemical Equilibrium; PROC NLP; PROC NL MIXED; PROC IML

PROBLEM IDENTIFICATION

Selenium is a trace element extremely toxic to animals, including humans, wildlife, and aquatic species in trace amounts. The removal of trace amount of selenium from process water is a challenging problem. The compliance standard for selenium is around 1ppb enforced by EPA and other regulatory agencies. In order to meet the enforced standard it is required to develop a new adsorbant for selenium. Continuous removal of selenium from water bodies is essential and requires careful prediction of selenium in water and careful measurement of selenium adsorption. Currently the best removal technology recommended by EPA for the removal of selenium is adsorption to iron and aluminum oxides minerals. Selenium adsorption is highly pH dependent and dependent on other soil properties such as cation exchange capacity, organic matter content, and soil mineralogy such as surface area available for adsorption. Currently adsorption of selenium is modeled through the generalized composite approach, where it is assumed that the adsorption behavior of selenium in soil can be described by surface complexation reactions written for generic surface functional groups that represent average properties of the soil as a whole rather than of specific mineral phases. On the other hand since selenium is present and adsorbed in trace amounts, measurement of selenium in solution is expensive, tedious and requires stringent methods of measurement such as spectroscopy. This problem can be resolved if predictive equations for adsorption of selenium can be developed considering a wide range of soil properties with easily measured soil parameters. In this study a predictive equation was developed for the adsorption of selenium using easily measured soil parameters that affect adsorption of selenium using SAS®. The speciation of selenium in solution at chemical equilibrium was predicted. Equilibrium constants of selenium adsorption were fitted to the measured adsorption data by least squares minimization using the constant capacitance model equations.

DATA INTEGRITY

A total of 100 samples of adsorption of measurements of selenium as a function of six soil parameters were investigated in this study. The soils samples were collected from five soil types at different depths from utility sites within from the state of California in the United States where ash landfills are presently in use or are planned

(Goldberg et al., 2005). For each site, soils were sampled down gradient from the landfill areas at depths ranging from 0 to 51 cm. Soil surface areas were determined using ethylene glycol monoethyl ether adsorption (Cihacek and Bremner, 1979). Soil pH values were measured in deionized water (1:25 soil/ water ratio) (Goldberg et al., 2005). Cation exchange capacities were measured by Na saturation and Mg extraction. Free Fe and Al were extracted with a Na citrate/citric acid buffer and Na hydrosulphite and measured using inductively coupled plasma (ICP) emission spectrometry (Goldberg et al., 2005). Carbon contents had been determined using a UIC Full Carbon System 150 with a C coulometer1 (UIC, Inc., Joliet, IL) (Goldberg et al., 2005). Mean values of previously determined soil properties such as Cation exchange capacity (CEC), inorganic carbon content (IOC) organic carbon content (OC), pH and aluminum (Al) and iron (Fe) content (Burns et al., 2006; Hyun et al., 2006) along with surface areas (SA) of the five soils are summarized in Table 1.

Table 1: Selected physical and chemical properties of soils used in this study.

Soil Name	N	Depth	pH	SA	CEC	IOC	OC	FE	AL
		(cm)		(km ² /kg)	(mmol/kg)	(g/kg)	(g/kg)	(g/kg)	(g/kg)
Arlington	17	0-25	6.87	0.0611	107.00	0.30	4.70	8.20	0.48
Pachyappa	16	0-25	6.18	0.0151	39.00	0.03	3.80	7.20	0.67
Sabree	16	0-13	6.09	0.0212	27.00	0.01	2.20	6.00	0.46
Wasco	14	0-5.1	5.49	0.0309	71.00	0.01	4.70	2.40	0.42
Wyo	16	0-5.1	6.18	0.0539	155.00	0.01	19.90	9.50	0.89

The soil samples represented a broad range of chemical characteristics. Ranges of the properties were: pH, 1.4 to 11.9; surface area, 0.02 to 0.1 km²/kg; cation exchange capacity, 27 to 190 mmol/kg; organic carbon content, 1.9 to 19.9 g/kg; inorganic carbon content, 0.01 to 0.3 g/kg; iron content 2.4 to 10.1 g/kg and aluminum content 0.35 to 0.89 g/kg. Selenate adsorption experiments were performed in batch systems to determine adsorption envelopes [amount of Se(IV)]. The selenate adsorption profile for the five soils as a function of the measured soil parameters are shown in Figure 1, Figure 2 and Figure 3. Selenium adsorption (on the z axis) envelopes were plotted in SAS® using PROC g3d (SAS® Code 1A) after creating smooth grids of the x and the y variables in PROC g3grid. Spline interpolation was used to create smooth surface profile (SAS Code 1B). Fine grid spacing was chosen to generate continuous surface profiles.

SAS® CODE 1A

```
proc g3grid data=selenium out=out1;
  grid ph*sa=ads / join spline
  smooth=.1
  axis1=0 to 12 by 0.1
  axis2=0 to 0.2 by 0.001;
run; quit;
```

Adsorption of selenium increase with pH reaching a maximum between pH =5 and pH=7 for most soils and decrease thereafter (Figure 1). Adsorption of selenium also increases with organic carbon content but decrease with cation exchange capacity (Figure 2). Adsorption of selenium increase with aluminum content but decrease with iron content (Figure 3).

SAS® CODE 1B

```
proc g3d data=out1;
  note j=r f=Albany      "Soils Used:  "
      j=r      c=red     "Wasco       "
      j=r      c=red     "Pachyappa  "
      j=r      c=red     "Arlington "
      j=r      c=red     "Wyo       "
      j=r      c=red     "Sabree    " ;
  plot ph*sa=ads/ctext=blue cbottom=red
  ctopy=green rotate=45 zmin=0 zmax=1.0 style=3 grid;
run; quit;
```

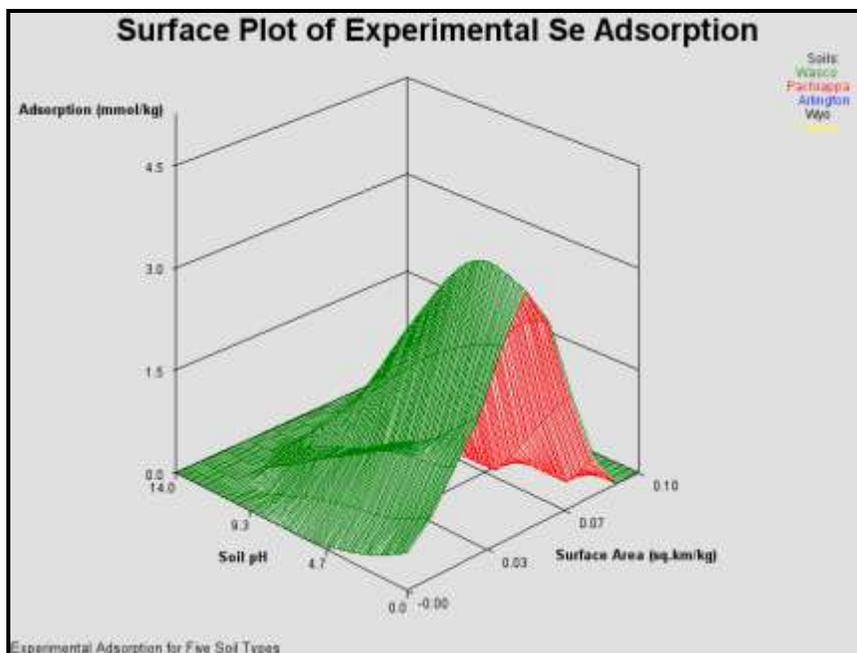


Figure 1: Measured adsorption profile of selenium as a function of pH and surface area for five soils. (240 X 200 grid size with spline interpolation at smooth=0.1 were used to generate smooth grids).

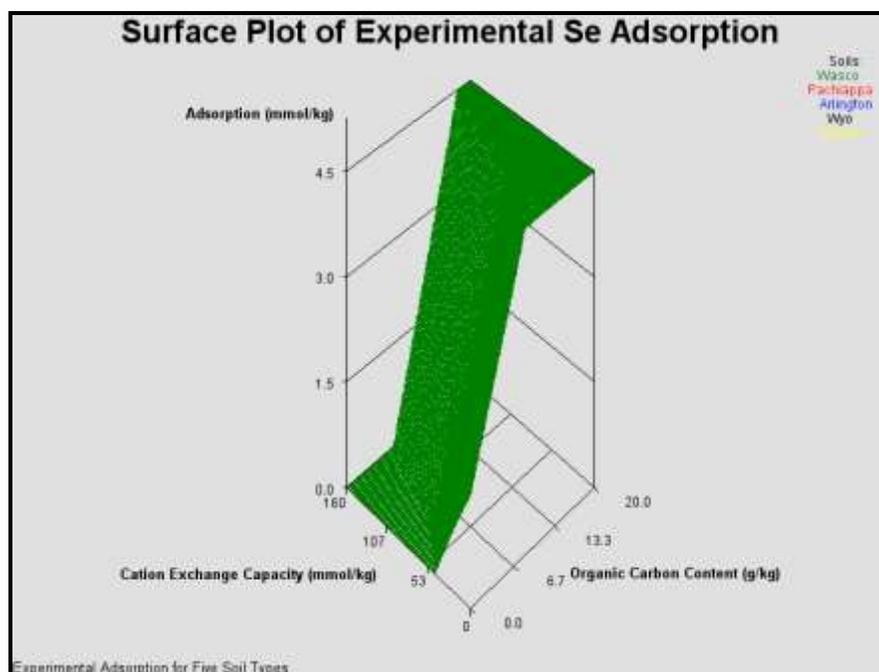


Figure 2: Measured adsorption profile of selenium as a function of CEC and OC of five soils (200 X 200 grid size with spline interpolation at smooth=0.1 were used to generate smooth grids).

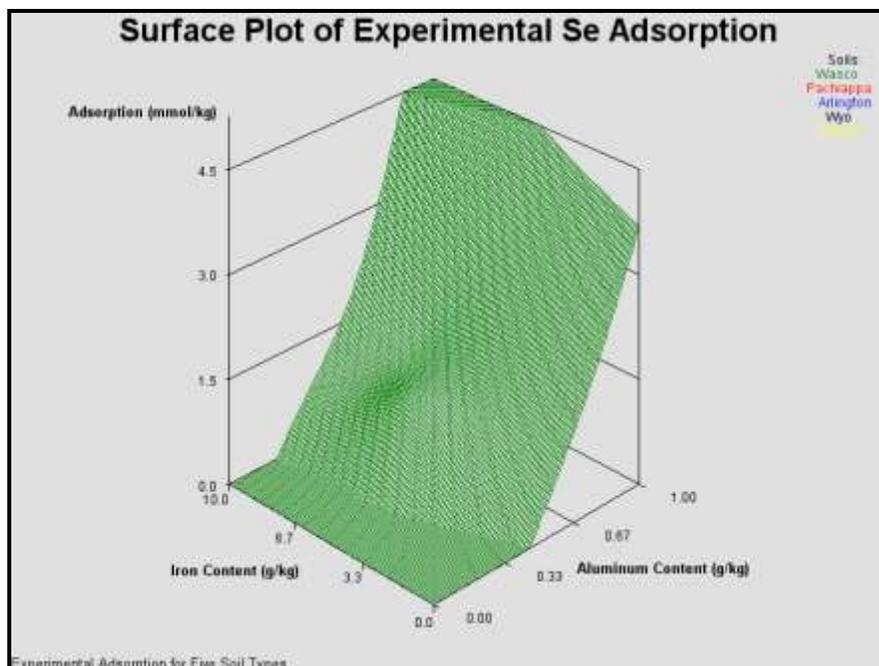


Figure 3: Measured adsorption profile of selenium as a function of iron and aluminum content of five soils (240 X 200 grid size with spline interpolation at smooth=0.1 were used to generate smooth grids).

Line plots of measured selenium adsorption as a function of pH for the five soils by depth is shown in Figure 4. Spline interpolation was used to connect the scatter points. Separate graphs were plotted for each soil type and for the different depths. Soil Wyo (WY) showed the largest adsorption followed by soil Wasco (WS), while soil Arlington (AR) showed the least adsorption (Figure 4). Adsorption of WY and WS remained high for a wide pH range (2 to 9) and decreased from pH=9 to pH=12. PROC SGPLOT was used to obtain Figure 4 (SAS® Code 1C). AR had the largest surface area while WY had the largest organic matter content and Al content with moderate amounts of surface area and iron content.

SAS® CODE 1C

```
proc sgplot data=selenium;
  scatter x=ph y=ads /group=soils markerattrs=(size=10);
  pbspline x=ph y=ads /group=soils lineattrs=(thickness=10);
run;
```

MODELING ADSORPTION

Adsorption of selenium was modeled in the following steps: i) applying the constant capacitance model to fit surface complexation constants for arsenate adsorption using monodentate surface configurations, ii) using non-linear mixed modeling to identify the relationship of the easily measured soil parameters affecting arsenate adsorption such as SA, ph, CEC, OC, IOC Fe and Al to the measured adsorption.

CONSTANT CAPACITANCE MODEL

Constant capacitance model (CCM) (Stumm et al., 1980) is a surface complexation model that is widely used to model trace element adsorption. Surface complexation models, unlike empirical adsorption isotherm equations, are chemical models that define surface species, chemical reactions, mass balances, and charge balance and contain molecular features that can be given thermodynamic significance (Sposito, 1983). With these models, thermodynamic properties such as solid-phase activity coefficients and equilibrium constants are calculated mathematically.

The CCM was used to describe selenium (Se) adsorption on the soils. SAS® was used to fit, Se surface complexation constants to the adsorption data and to predict adsorption as a function of the easily measured soil parameters. In the CCM model, the protonation and dissociation reactions for the surface functional group, SOH

(where SOH represents a reactive surface hydroxyl bound to a metal ion, S [Al or Fe] in the oxide mineral are defined as:

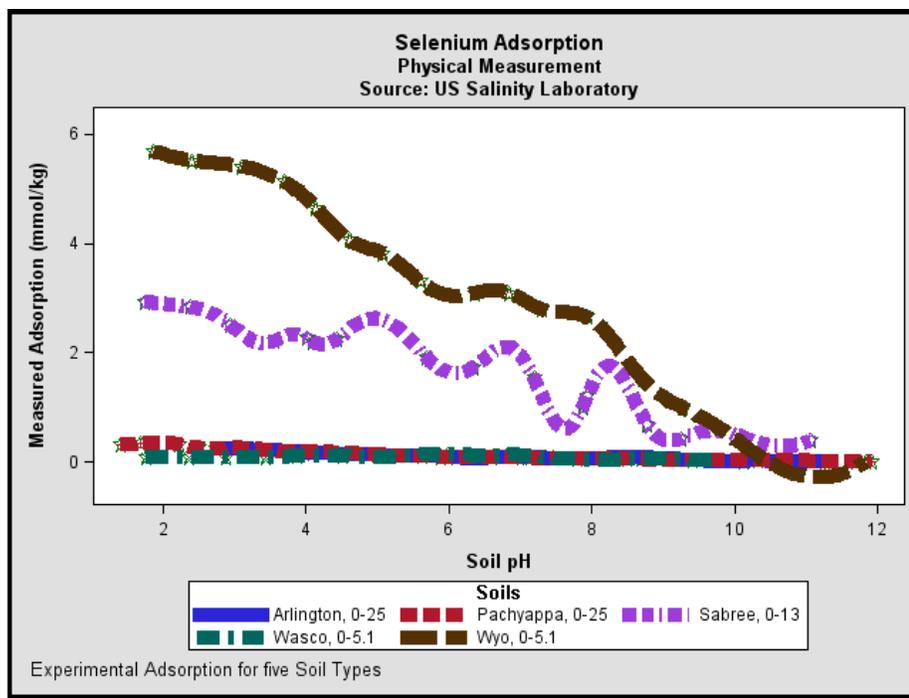
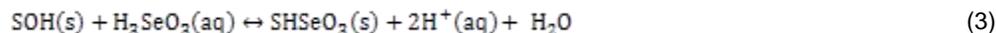
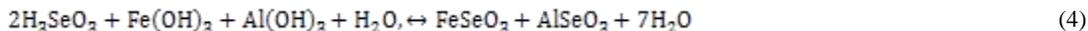


Figure 4: Measured Selenium Adsorption as a Function of pH.

In the CCM model the surface complexation reactions for selenium adsorption are defined as:



The above surface configurations correspond to the dominant As species in solution in the pH ranges investigated. By convention, surface complexation reactions in the CCM model are written starting with completely undissociated acid species; however, the model can contain other aqueous speciation reactions for Se. Other possible surface species include S_2SeO_3 , SSeO_3 , SH_2SeO_3 . At equilibrium the reaction between solid iron- and aluminum-selenates and the dissolved ion can be described as:



However, calculations indicate that other possible solid metal ion species such as $\text{Fe}(\text{OH})_2^-$ and $\text{Al}(\text{OH})_2^-$ can also be present in the solution although not in significant quantities in the pH range studied. Identifying the composition of the solution at equilibrium is important for CCM model application.

EQUILIBRIUM SOLUTION COMPOSITION

The CCM model assumes that the chemical species in a mixture is at chemical equilibrium which is the state in which the chemical activities or concentrations of the reactants and products have no net change over time. In order to meet the thermodynamic condition for equilibrium, the Gibbs energy must be stationary. In other words, to be at equilibrium the rates of the forward and backward (reverse) reactions have to be equal. The problem is to determine the composition of a mixture of the various chemicals added to the system satisfying its chemical equilibrium state. The second law of thermodynamics implies that a mixture of chemicals satisfies its chemical equilibrium state (at a constant temperature and pressure) when the free energy of the mixture is reduced to a minimum. Therefore the composition of the chemicals satisfying its chemical equilibrium state can be found by minimizing the function of the free energy of the mixture. In this study the composition of the chemical mixture at equilibrium was determined through minimizing the free energy of component compounds. The NLPTR subroutine


```

. . . . . 1. 1. . . . 0. 1. ,
. . . . . . . . . 1. 1. 0. 1. ,
. 1. 3. 3. 3. 3. . 1. 1. . 1. 0. 13. };

con[1,1:11] = 1.e-7;
x0 = j(1,11, .1);
optn = {0 3};
call nlpntr(xres,rc,"F_BRACK",x0,optn,con);

```

Table 3: Composition of solution at chemical equilibrium for Equation 4.

Optimization Results				
Parameter Estimates				
N	Parameter	Estimate	Gradient	Active
1	H ⁺	1E-7	-112.5649	
2	H ₂ O	6.999995	-375.709987	
3	(SeO ₃) ³⁻	1.99999	-501.214754	
4	(H ₂ SeO ₃) ⁻	1E-7	-719.444874	Lower BC
5	(HSeO ₃) ²⁻	0.000010043	-614.165738	
6	H ₃ SeO ₃	1E-7	-820.184916	Lower BC
7	Fe ³⁺	1	-123.837897	
8	Fe(OH) ²⁺	1E-7	-387.804923	Lower BC
9	O ²⁻	0.000005221	-155.119185	
10	Al ³⁺	1	-95.757893	
11	Al(OH) ²⁺	1E-7	-359.724909	Lower BC

EQUILIBRIUM ADSORPTION CONSTANTS

The equilibrium constants of selenium adsorption were estimated through least squares minimization with the constant capacitance surface complexation reactions. The following system of adsorption equations were written in SAS language and optimized with respect to the adsorption equilibrium constants.

The intrinsic equilibrium constants for the protonation and dissociation reactions are:

$$K_a^1 = \frac{[\text{SOH}_2^+]}{[\text{SOH}][\text{H}^+]} \exp(F\phi/RT) \quad (7)$$

$$K_a^2 = \frac{[\text{SO}^-][\text{H}^+]}{[\text{SOH}]} \exp(-F\phi/RT) \quad (8)$$

where F is the Faraday constant (C mol^{-1}), ϕ is the surface potential (Volts), R is the molar gas constant ($\text{J mol}^{-1} \text{K}^{-1}$), and T is the absolute temperature in Kelvin (K). The square brackets indicate concentrations (mol L^{-1}). The intrinsic equilibrium constants for selenium (Se) adsorption are:

$$K_{\text{Se}}^1 = \frac{[\text{SH}_2\text{SeO}_2]}{[\text{SOH}][\text{H}_2\text{SeO}_2]} \quad (9)$$

$$K_{Se}^2 = \frac{[SHSeO_2^-][H^+]}{[SOH][H_2SeO_3]} \exp(-F\varphi/RT) \quad (10)$$

The mass balance equation for the surface functional groups are gives as:

$$[SOH]_{Tot} = [SOH_2^+] + [SOH] + [SO^-] + [SHSeO_2^-] + [SH_2SeO_3] \quad (11)$$

The charge balance expressions for the surface functional groups are given as:

$$\sigma = [SOH_2^+] - [SO^-] - [SHSeO_2^-] \quad (12)$$

where σ is the surface charge (mol L⁻¹) related to surface area (SA), the solid suspension density (C_p), the capacitance (C), Faraday's constant (F) and φ by the following equation:

$$\sigma = \frac{C SA C_p}{F} \varphi \quad (13)$$

A capacitance of 1.06 F m⁻¹ (Goldberg et al., 2008) was used in the calculation of σ which is a typical value for selenium adsorption on Fe and Al oxides. The protonation (K_a^1) and dissociation (K_a^2) constants and the surface area were fixed at 10^{7.35} and 10^{-8.95}, and 0.3 km²/kg, using equal boundary conditions (upper boundary value=lower boundary value), since these values were averages of a literature compilation for Al and Fe oxides obtained by Goldberg and Sposito (1984) and have been used in prior constant capacitance modeling of As(V) adsorption by soils (Goldberg et al., 2005). Least squares (LSQ) minimization of the adsorption equilibrium constants were performed minimizing both K_{Se}^1 and K_{Se}^2 simultaneously. PROC NLP was used to solve the system of seven equations (equations 7 through 13) with LSQ minimization (SAS® CODE 3). The two equilibrium adsorption constants K_{Se}^1 (k1) and K_{Se}^2 (k2) were minimized simultaneously using the LSQ statement. The parameters and upper and lower boundary values and linear constraints were input into the model using an input data set (indat) specified by the INEST= statement (SAS® CODE 3). The optimization results were output into an output dataset specified with the OUTEST= statement. The system of seven equations was solved simultaneously optimizing k1 and k2 through QUASI NEWTON (QUANEW) optimization technique. The QUANEW optimization was specified in the TECH= statement. Gradient was computed using analytic formulas. Hessian was computed using finite difference approximations using the computed analytic gradient. Cross product Jacobian was computed using finite difference approximations. The ABSGCONV convergence criterion was satisfied and convergence was achieved in 0.81 seconds in real time (equal to 0.1 sec CPU time).

Only monodentate surface species were used in the final optimization (SAS® CODE 3). The results indicated that model fits were superior in quality when monodentate surface species rather than bidentate species were used. Bidentate surface species made the surface complexation constants dependent on the concentration of [SOH] because the [SOH] term is squared. Optimization results including the parameter estimates and function values are shown in Table 4 and Table 5. .

SAS® CODE 3

```
data indat (type=est);
  keep _type_ k1 k2 hc sa soht soh so sseot shseot si ka1 ka2 sig CT;

  _type_ = 'parms';
  ka1= 10**7.35; ka2= 10**-8.95; si=0.6825; sig=10**-5; CT=10**-5;
  SOht=10**-5; SOH =10**-5; SO=-(10**-5); SSeOt=(10**-5);
  SHSeOt=-10**-5; hc = 10**-4; sa=0.3; output;

  _type_ = 'lb';
  SOht=10**-30; SOH =10**-30; SO=-(10**-30); SSeOt=(10**-30);
  SHSeOt=-10**-30; hc = 10**-14; si=-30; sa=0.3; sig=10**-5;
  k1=10**-30; k2=10**-30; ka1= 10**7.35; ka2= 10**-8.95;
  CT=10**-30; output;

  _type_ = 'ub';
  si=100; SOht=10**-3; SOH =10**-3; SO=-(10**-3); SSeOt=(10**-3);
  SHSeOt=-(10**-3); hc=10**-1; sa=0.3; sig=10**-5; k1=10**30;
  k2=10**30; ka1= 10**7.35; ka2= 10**-8.95; CT=10**0; output;

  _type_ = 'LINCON'; ka1= 10**7.35; ka2= 10**-8.95; sig=10**-5;
  sa=0.3; output; run;
```

```

PROC NLP PALL tech=quanew inest=indat outest=outdat phes;
  lsq k1 k2;
  PARMs ka1 ka2 si sa CT;
  BOUNDS 0 < CT < 1.0;
  SOH=(SOHt/(ka1*hc))*(exp(36.72*si));
  SO=(SOH*ka2/hc)*(exp(-36.72*si));
  sig=1.1*(10**(-5))*si;
  SOH2=(sig-SO-SSeO3);
  k1=SHSeO3/(SOH*CT);
  k2=((SSeO3*hc)/(SOH*CT))*(exp(36.72*si));
  SOH2+SOH+SO+SSeO3+SHSeO3=sa;
RUN;

```

The low values of gradient objective function indicated that, the optimization was superior. Reasonable values were obtained for the adsorption constants for the soils used (Table 5). The estimated objective function was equal to 2.548684×10^{-16} . Determinant of the Hessian matrix was equal to 1.54568×10^{-18} .

Table 4: Values fitted of As adsorption constants

Optimization Results		
Function Values		
N	Function	Value
1	k1	-2.923966E-9
2	k2	2.2387211E-8

Table 5: Estimates of parameters at optimization of selenium adsorption constants (ka1 and ka2 are protonation and dissociation constants, SI is the surface potential, SA is the surface area and CT is the concentration of selenium added)

Optimization Results				
Parameter Estimates				
N	Parameter	Estimate	Gradient Objective Function	Active Bound Constraint
1	ka1	22387211	2.276911E-23	Equal BC
2	ka2	1.1220185E-9	0	Equal BC
3	SI	0.682500	-3.1394E-16	
4	SA	0.300000	0	Equal BC
5	CT	0.000010000	-5.09737E-11	

PREDICTING SELENIUM ADSORPTION

A non linear mixed model was fitted to predict the adsorption of selenium as a function of 7 independent variables (SA, CEC, OC, IOC, pH, Fe, Al) using PROC NLMIXED (SAS® CODE 4). The model solution to parameter

estimates with probabilities, upper and lower confidence limits and gradient are shown in Table 6. The predicted selenium adsorption envelop as a function of pH and surface area is shown in Figure 5.

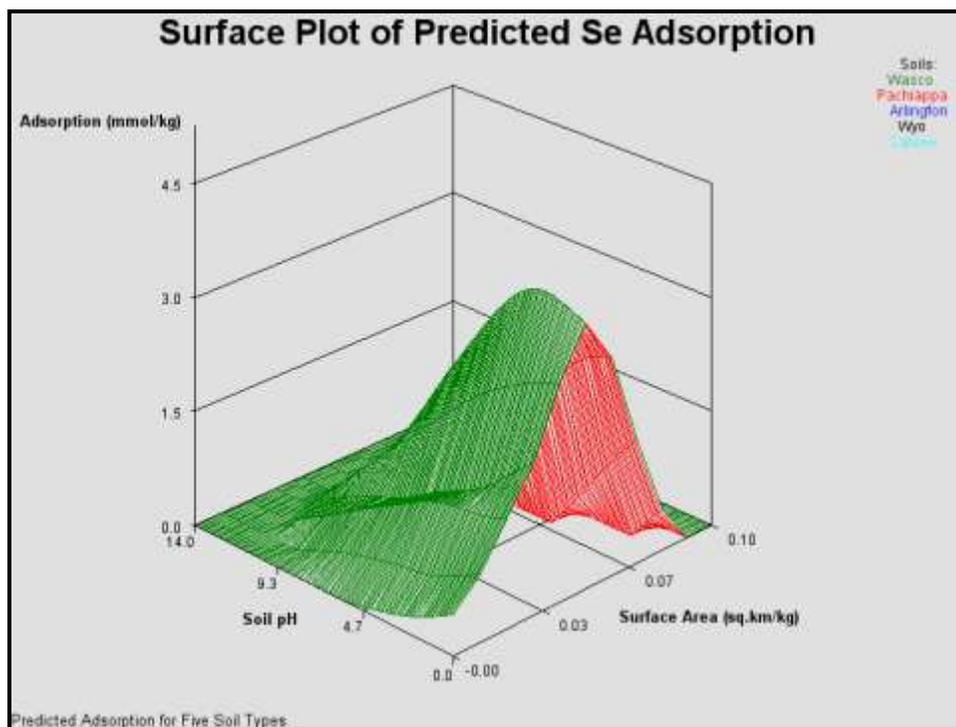


Figure 5: Predicted adsorption profile of selenium as a function of pH and surface area for five soils. (240 X 200 grid size with spline interpolation at smooth=0.1 were used to generate smooth grids).

SAS® CODE 4

```
PROC NLMIXED DATA=selenium QPOINTS=10 ALPHA=0.05 TECH=QUANEW; UPDATE=DDFP;
PARMS
int=-0.4511 bsa=61.2071 bcec=-0.02981 boc=0.08887
bioc=-0.9154 bph=-0.01822 bfe=-0.1619 bal=2.7650
g11=-0.001428 to 0.02 by 0.001 g12=-0.001 to 0.01 by 0.001;
eta = int1+ bsa*sa + bcec*cec + boc*oc + bioc*ioc + bph*ph
+ bfe*fe + bal*al + g12*b1;
num = eta; mu= num;
MODEL ads ~ NORMAL(mu,g12); RANDOM b1 ~ NORMAL(0,g11) SUBJECT=soil;
PREDICT mu OUT=cdf;
RUN;
```

All studied variables significantly influenced selenium adsorption ($p < 0.05$, Table 6). Cation exchange capacity, pH, inorganic carbon content and iron concentration showed negative influence on adsorption while surface area, organic carbon content and aluminum ion concentration showed positive influence (Table 7). Small values of AIC (-130.5), AICC(-127.5) and BIC (-134.8) indicated superior fit of the model. The initial values for the parameters were obtained from an initial linear fit of the measured data using PROC MIXED. Predicted adsorption of selenium increased with surface area but decreased with pH with a maximum between pH=5 and pH=7. Predicted adsorption of selenium increase with aluminum content but decrease with iron content (Figure 6). Predicted adsorption also increased with OC but decreased with CEC (Figure 7). The predicted selenium showed good agreement with the measured selenium content indicating adequacy of the fitted model.

Table 6: Solution for non linear mixed model fixed effects of selenium adsorption.
(the regression coefficients of each variable are shown with a 'b' in front of the variable name; eg., bSA indicates regression coefficient of the variable SA and bpH indicates the regression coefficient of variable pH)

Parameter Estimates									
Parameter	Estimate	Standard Error	DF	t Value	Pr > t	Alpha	Lower	Upper	Gradient
Intercept	-0.4511	0.1811	4	-2.49	0.0674	0.05	-0.9538	0.05158	-0.05488
bSA	61.2071	11.0772	4	5.53	0.0052	0.05	30.4518	91.9624	-0.00904
bCEC	-0.02981	0.005464	4	-5.46	0.0055	0.05	-0.04498	-0.01464	-25.2003
bOC	0.08887	0.01065	4	8.35	0.0011	0.05	0.05931	0.1184	-1.38943
bIOC	-0.9154	0.1498	4	-6.11	0.0036	0.05	-1.3313	-0.4995	-0.00733
bpH	-0.01825	0.004448	4	-4.10	0.0148	0.05	-0.03060	-0.00589	-2.05599
bFe	-0.1618	0.02975	4	-5.44	0.0055	0.05	-0.2444	-0.07922	0.557083
bAl	2.7650	0.5778	4	4.79	0.0087	0.05	1.1607	4.3693	-0.03042
g11	-932E-15	.	4	.	.	0.05	.	.	0.636714
g12	0.01273	0.001759	4	7.24	0.0019	0.05	0.007849	0.01762	-0.94305
DDFP	1.0000	7.515E-6	4	133065	<.0001	0.05	1.0000	1.0000	0

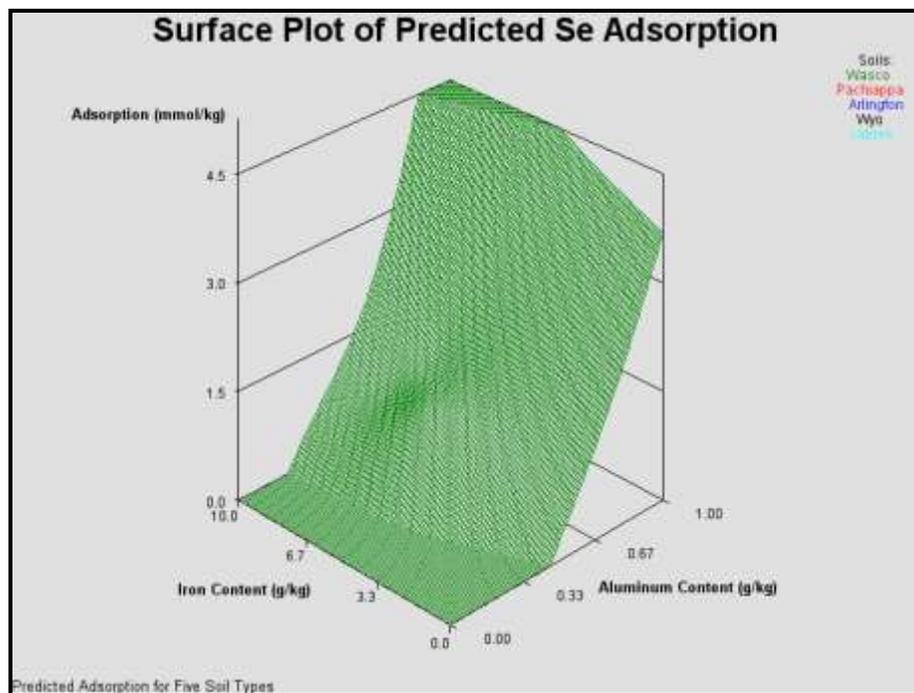


Figure 6: Predicted adsorption profile of selenium as a function of iron and aluminum content of five soils (240 X 200 grid size with spline interpolation at smooth=0.1 were used to generate smooth grids).

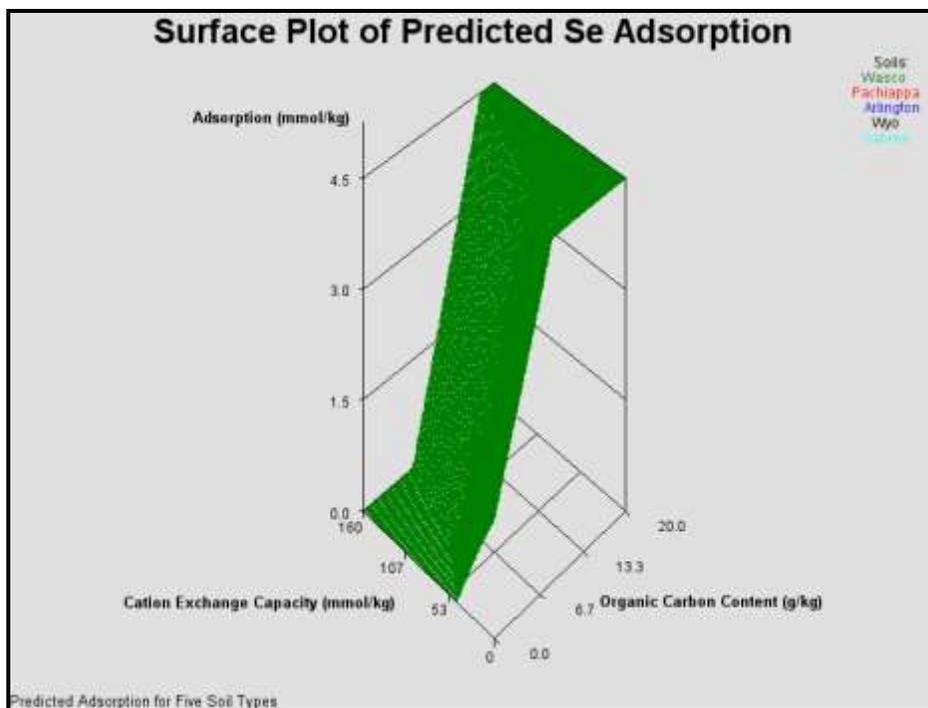


Figure 7: Predicted adsorption profile of selenium as a function of CEC and OC of five soils (200 X 200 grid size with spline interpolation at smooth=0.1 were used to generate smooth grids).

CONCLUSIONS

Adsorption of selenium is significantly influenced by pH, and other chemical and mineralogical properties of soil such as cation exchange capacity, organic carbon content, inorganic carbon content, aluminum and iron content of the soil and the surface area of the soil mineral. Selenium adsorption increases as surface area, organic carbon content and aluminum content are increased but decreases with cation exchange capacity, and iron content. Predictive equation explained adsorption of selenium adequately with easily measured soil parameters reducing the need for time consuming and expensive selenium adsorption measurement experiments. The chemical speciation and composition of mixture at equilibrium were easily predicted through optimization. Through Least squares minimization with SAS® the two monodentate equilibrium selenium adsorption complexation constants were easily fit for the measured adsorption data. The several complicated steps involved in constant capacitance surface complexation modeling of adsorption of selenium were simply performed in SAS®.

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