Partitioning model of the adsorption of explosives from soils to determine its environmental fate

Modelo de compartimentación de la absorción de explosivos de suelos para determinar su destino ambiental

Modelo de compartimentação da adsorção dos explosivos dos solos para determinar seu destino ambiental

Fecha de recepción: 2014/09/10 Fecha concepto evaluación: 2014/11/03 Fecha de aprobación: 2014/11/14

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Para citar este artículo / To reference this article / Para citar este artigo: González F., R. (2014). Partitioning model of the adsorption of explosives from soils to determine its environmental fate. *Revista Criminalidad*, 56 (3): 139-152.

Abstract

The purpose of this research was to identify the principal soil characteristics that influence the adsorption of munitions constituents (MC) of explosives in soils, through a partitioning model to determine the fate of the explosives. To do that, batch experiments near 1:1 (w/v) soil to solution ratios reflecting field conditions were conducted using a mixture of HMX, RDX, nitroglycerine (NG), nitroguanidine (NQ), TNT and 2,4-dinitrotoluene as MC, where the mix of MC was adsorbed in twenty-five different soils that varied from 4.0 to 43.2 % clay content and 0.07 to 18.23 % total carbon, in an experiment that involved 2 days of adsorption followed by four consecutive desorption steps. The most important result was that for each MC, even if it was in a mixture, were successfully predicted the partition coefficients using the organic carbon, cation exchange capacity and extractable iron as the principal soil characteristics that determine the fate of these explosives.

Key-words

Munitions, Explosives, Environment (fuente: Tesauro de política criminal latinoamericana - ILANUD).

Resumen

El objeto de esta investigación consistió en identificar las principales características de suelo que influyen en la adsorción de constituyentes de municiones (CM) en suelos, mediante un modelo de compartimentación, para determinar el destino de esos explosivos. Para hacerlo, se llevaron a cabo experimentos de lote ("batch experiments"), de relaciones de cerca de 1:1 (w/v) entre suelo y solución, que reflejaban condiciones de campo, empleando una mezcla de HMX, RDX, nitroglicerina (NG), nitroguanidina (NQ), TNT y 2,4-dinitrotolueno como CM, en donde la mezcla de CM fue adsorbida en veinticinco suelos diferentes, que variaban desde 4,0 a 43,2 % de contenido de arcilla y de 0,07 a 18,23 % de carbono total, en un experimento que implicó dos días de adsorción seguidos por cuatro pasos consecutivos de desorción. El resultado más importante consistió en que para cada CM, incluso en una mezcla, se predijeron exitosamente los coeficientes de partición empleando el carbono orgánico, la capacidad de intercambio catiónico y hierro extraíble, como características principales del suelo que determinan el destino de tales explosivos.

Palabras clave

Municiones, explosivos, ambiente, entorno (fuente: Tesauro de política criminal latinoamericana - ILANUD).

Resumo

A finalidade desta pesquisa era identificar as características principais do solo que influenciam a adsorção dos constituintes de munições (MC) dos explosivos nos solos, através de um modelo de compartimentação para determinar o destino dos explosivos. Para fazer a pesquisa, experimentos em lote perto do solo de 1:1 (w/v) das proporções da solução que refletem condições do campo foram conduzidas usando uma mistura de HMX, de RDX, nitroglicerina (NG), de nitroguanidina (NQ), TNT e 2.4-dinitrotolueno como MC, onde a mistura de MC adsorvida em vinte e cinco solos diferentes que variaram o índice da argila de 4.0 a 43. 2% e o carbono total de 0.07 a 18.23 %, em uma experiência que demandou 2 dias da adsorção seguidos por quatro etapas consecutivas de dessorção. O resultado o mais importante foi que para cada MC, mesmo se estivesse em uma mistura, os coeficientes de partição foram preditos com sucesso usando o carbono orgânico, a capacidade de troca e o ferro extraível como as características principais do solo que determinam o destino destes explosivos.

Palavras-chave

Munições, explosivos, ambiente (fonte: Tesauro de política criminal latinoamericana - ILANUD).

Introduction

The fate of contaminants in the environment has been studied intensely since pollution became a public health problem. For this reason, many researchers have devoted their efforts to studying the physicochemical mechanisms of fate and transport phenomena. One group of these contaminants is the munitions constituents (MC). Contamination by MC is the result of incomplete detonation of explosives at operational ranges resulting in the heterogeneous dispersion of particulates. The toxic and mutagenic effects observed for many MC indicate a danger to biological receptors at down gradient sites (Kaplan & Kaplan, 1982; Robidoux et al., 2001, and Sunahara et al., 2009). In this sense, researchers have found that animals that ingest or breathe TNT evidence affections in the immune system (U.S. Department of Health and Human Services, 1995) and 2,4 DNT is toxic to aquatic organisms and cause long-term adverse effects in the aquatic environment (Material Safety Data Sheet OSHA, 2008). Millions of acres of land in the United States are believed to be contaminated by MC with the costs of assessment and remediation estimated to be in the billions of dollars and more than 2000 sites have been identified as potentially contaminated by energetic chemicals (U.S. General Accounting Office, 2003). In Canada training sites are known to be associated with activities involving RDX, HMX, and TNT (Hawari & Halasz, 2002). The contamination degree is extremely varied at these sites and the distribution is heterogeneous (Pennington, 2002). MC are one of the major causes of organic pollution (Travis, Bruce & Rosser, 2008) and some of them such as TNT, inhibit microbial activities in contaminated soil (Gong et al., 1999). In addition, millions of gallons of wastewater containing explosives are generated each year from production facilities (Walsh, Chalk & Merritt, 1973) and the wastewater after treatment still contain MC, becoming a second major source of surface and groundwater contamination. In Colombia this impact is not taking into account knowing that groups as the guerillas used mines in some places in the country. In order to minimize the environmental impact and maintain the balance between the environment, the needs of the military, and human health, it is necessary to understand the physicochemical processes that control the transport and the reactivity of the MC.

To understand the transport of MC one of the mechanisms used is partitioning. It determines how much of the compound is distributed among different environmental phases present in the system (Schwarzenbach, Gschwend & Imboden, 2003). To describe this mechanism the partition coefficient (K_p) is usually used. It is defined as the ratio of the concentration of chemical in the soil to the concentration of chemical in the aqueous phase. The partition coefficient is calculated using the following relationship:

$$K_p = C_s/C_w \quad (1)$$

where K_p is the partition coefficient (L/kg), C_s is the concentration of the compound adsorbed to the soil (mg/kg), and C_w is the concentration in the aqueous solution (mg/L).

The organic matter contained in soil is generally the most important soil constituent responsible for the sorption of organic compounds (Ran et al., 2007, and Zhang, Zhu & Chen, 2009). This has led to the use of the organic carbon normalized partition coefficient, K_{oc} (L/kg) (Schwarzenbach, Gschwend & Imboden, 2003), the octanol-water partition coefficient, K_{ow} (L water/L octanol), and fraction of organic carbon in the soil, f_{oc} (g organic carbon/g soil) based on the following relationships:

$$K_p = K_{oc} f_{oc} \quad (2)$$

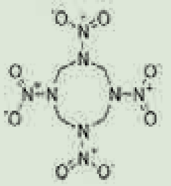
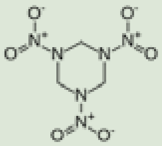
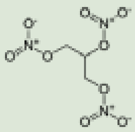
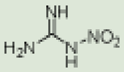
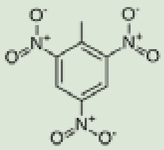
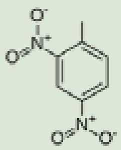
This simplification has been successfully employed to model the partitioning of many hydrophobic organic chemicals like PCBs and PAHs, but their application to MC results in order of magnitude errors (Gotz et al., 1998). Thus, direct measurements of the concentrations of munitions constituents adsorbed on the soil are required. For hydrophilic MC, differences in K_{OC} can be greater than 2 orders of magnitude; therefore, sorption to phases in addition to organic matter is important. Michalkova, Szymczak & Leszczynski (2005) and Dontsova et al. (2009) found that for nitro compounds K_{oc} is not a constant. In addition, many authors have focused their investigations on determining what fraction of the soil is responsible for the majority of adsorption of MC and probing the mechanisms for the adsorption in these fractions. Dontsova et al, (2009), and Michalkova, Szymczak & Leszczynski (2005) are examples of that. These studies identified the main fraction of the soil that is responsible for the adsorption of MC, but to predict partitioning of MC in a realistic way, some other soil characteristics should be studied together with the organic carbon. This is the goals of the present study.

Materials and Methods Proposed

Chemicals

Military grade HMX, RDX, NG, NQ, TNT and 2,4-DNT were used. Properties of MC's are presented in Table 1. Calibration standards (>99% purity) for each of the MC were obtained from AccuStandard Inc. (New Haven, CT). Calcium chloride, sodium azide, ethanol, and HPLC grade methanol and acetonitrile were obtained from Acros Organics through Fisher Scientific and distilled. Deionized water (18mΩ of Resistivity) was provided by an E4GE Osmotic DI Water System, Model: R4 6600DLX on tap at the University of Delaware (Newark, DE).

Table 1.
Physicochemical Properties of the MC Studied

Physicochemical Properties	HMX	RDX	NG	NQ	TNT	2,4-DNT
						
Molecular Weight (g mol^{-1})	296.16	222.26	227.11	104.07	227.13	182.15
Water Solubility at 25°C (mg L^{-1})	4.5 (4)	56.3 (4)	1800 (2)	4400 (2)	130 (1)	270 (2)^{b}
Octanol/Water Partition Coefficient (Log K_{ow})	0.17 (4)	0.90 (4)	1.62 (2)	0.89 (2)	1.60 (2)	1.98 (2)
Henry's Law Constant at 25°C atm-m^{3} mol^{-1}	2.5 x 10^{-14} (1)^{a}	1.96 x lo^{-11} (3)	3.4 x lo^{-6} (1)^{a}	4.54 x lo^{-16} (2)	2.18 x lo^{-8} (2)	5.40 x 10^{-8} (3)

^{a} At 20 °C, ^{b} At 22 °C, (1) Chemical Properties Database, (2) HSDB Hazardous Substances Data Bank, (3) ChemIDPlus Lite, (4) Monteil-Rivera et al., 2004.

Soil Properties

This study employed 25 soils collected from the U.S., Europe and South America to identify the major influences of soil properties in the adsorption-desorption process. They were obtained from the National Certified Repository of Soils from the University of Delaware in the amount required for each experiment. They have a pH range between 3.4 to 8.0, clay content percent between 4.0 to 43 % and total carbon content of 0.07 to 32 %. Soil properties were determined by the soil laboratory at the Plant and Soil Science Department at University of Delaware.

Tabla 2.
Soil Properties

Soil	pHa	CECb	Clayc	TOCd	Ale	Fee	Mne	Al Ex.f	Fe Ex.f	Mn Ex.f
		(meq/100g)	(%)	(%)	(mg/kg)	(mg/kg)	(mg/kg)	(mg/kg)	(mg/kg)	(mg/kg)
Zegveld	4.8	54.8	21.7	18.23	21414.39	19650.90	389.05	1516.43	11953.71	147.67

Rhydtalog	5.0	35.9	12.5	12.83	2280.59	2786.49	113.13	281.06	1526.02	52.37
Joplin	6.5	43.8	18.7	10.12	10252.02	21475.14	484.18	243.93	3435.68	271.70
Lewis Core	5.6	37.2	6.3	7.59	27618.63	22269.68	590.59	15180.54	7268.73	573.08
Lewis Clean	5.1	31.4	8.3	6.36	27451.48	19410.03	575.24	13010.64	6130.20	559.89
Pokomoke	4.5	13.1	11.1	3.50	5037.33	794.15	16.26	887.91	52.60	6.22
Elliot IE	6.3	20.4	37.0	2.86	10355.82	19167.52	810.80	455.04	2540.86	514.25
Guadalajara	8.0	11.6	18.2	2.33	10629.84	10984.00	151.97	163.35	ND	31.47
Boxtel	5.4	11.0	10.2	2.32	5757.44	11609.40	269.22	111.89	5000.80	158.54
Houthalein	3.9	2.9	4.0	2.31	710.89	1621.95	3.32	111.17	501.66	ND
Anne Messex	6.3	13.2	12.1	2.30	9142.23	11870.38	303.78	343.22	1152.91	255.19
Whippany	5.9	15.5	22.3	1.75	10739.76	11787.92	107.78	413.05	2496.48	39.68
Sassafras 2	4.4	8.5	16.4	1.63	10538.12	13460.71	83.00	275.97	1120.18	9.45
Matapeake	5.7	9.9	22.3	1.54	18068.28	17956.05	373.02	635.46	2303.77	237.88
SSL	4.5	8.8	18.1	1.35	9121.38	12945.38	73.73	421.58	1782.25	18.82
Chile Muestra	6.6	21.0	14.3	1.20	14146.36	25236.74	651.95	712.36	7083.08	452.74
Sassafras	4.4	5.0	18.2	0.97	8924.39	12609.24	715.68	336.00	1363.58	11.85
Washington 2	6.9	20.3	24.2	0.68	13564.61	18899.43	431.86	302.16	1533.17	199.01
Washington 1	6.9	17.8	24.5	0.63	14342.98	20777.15	552.17	334.23	1742.44	217.34
Souli	6.9	16.1	43.2	0.61	14768.49	29961.11	910.44	444.95	1596.09	629.82
Fort McNelan	3.8	11.0	38.6	0.31	14129.83	39878.10	30.73	557.14	104.43	2.63
MMRB	4.3	2.5	16.2	0.24	10324.67	9513.92	85.80	659.17	1471.40	13.26
Utah	3.4	11.2	20.9	0.20	6444.56	34120.48	219.77	778.30	1886.51	212.02
Aberdeen BA	5.5	3.8	16.2	0.16	7271.46	12764.21	88.87	250.70	2209.50	16.70
Aberdeen BT	4.8	1.9	9.1	0.07	7588.48	9391.73	59.20	153.32	1314.48	18.20

[a] 1:1 (w/v) (v/v) soil:water
[b] Ammonium saturation buffered at pH 7.0
[c] Particle size analysis by hydrometer using the modified Bouyoucos Method [24]
[d] Combustion using an Elementar Vario-Cube TOC Analyzer (Elementar Americas, Mt. Holly, NJ).
[e] EPA Method 3051 using a CEM MARs5 microwave digestion system (CEM, Matthews, NC). Digests were analyzed for total sorbed metals by inductively coupled plasma optical emission spectroscopy using Thermo Iris Intrepid II XSP Duo View ICP (Thermo Elemental, Madison, WI).
[f] Ex. = Extractable oxides determined by the Ammonium Oxalate method [25]
ND non detected

Adsorption-Desorption Experiment

The methodology proposed employed a soil to solution ratio near to 1:1 on a mass basis, which was more realistic than the dilute suspensions commonly used by other researchers. Batch experiments were used in this study because of the ease of obtaining partition coefficients.

In each test, 5 ± 0.001 grams of soil sieved to <0.106 mm was added to 12 mL borosilicate centrifuge tubes with phenolic caps and PTFE liners. Soils were hydrated to maintain a constant volume throughout the adsorption and desorption procedures. A solution containing calcium chloride ($CaCl_2$) and sodium azide (NaN_3) was used. $CaCl_2$ was added to prevent flocculation of soil components and to standardize the soil solution cation concentration. NaN_3 was added as a microbial growth inhibitor. Photodegradation was prevented by wrapping all samples and devices in aluminum foil. The concentrations of the MC in the mix solution was 10.0 mg/L except of HMX that was at 1.5 mg/L because it has a low solubility in water (5 mg/L).

Duplicate samples of the mix solutions were vortex mixed for 15 seconds to suspend the soil, and shaken at 10 rpm in an end-over-end shaker for 2 days. After that time, the tubes were centrifuged for 30 min at 3000 rpm (750 g) and the supernatant was filtered through a 0.45 μm Durapore PVDF filter (Millipore Corp., Bedford, MA). Four consecutive desorptions were then performed after each adsorption time. Five mL of solution containing 0.01 M $CaCl_2$ and 0.01 M NaN_3 were added to samples that have been decanted of the preceding solution, followed by vortex mixing for 15 seconds and mixing in the end-over-end shaker for 1hr. Each supernatant obtained from adsorption and each desorption after each adsorption time was analyzed for MC by HPLC.

Acetonitrile Extraction

The extraction methodology was the Method 8330B (USEPA, 2006) modified. In this modified method five mL of acetonitrile (ACN) was added to each sample. Duplicate samples were vortex mixed for 15 seconds to suspend the soil in solution, and shaken at 10 rpm in an end-over-end shaker for 1 hour. This step was done three times. The tubes were centrifuged for 30 min at 3000 rpm (750 g) and the supernatant is filtered through a 0.45 µm Durapore PVDF filter (Millipore Corp., Bedford, MA). Then this supernatant was analyzed for MC by HPLC.

Analytical Methods

Munitions Constituents HPLC. An Agilent 1200 Series HPLC with a Zorbax SB-C18 reversed phase column (4.6x50 mm; 3.5µm particle size) for the mix of MC was used with: UV detector, Methanol:water and Flow rate was 2 mL/min. For NQ it was necessary to use a different column because with the previous approach the retention time was too short, making it difficult to analyze the MC, because peaks from the dissolved organic matter (DOM) interfered with the NQ peak. A HILIC Plus column (2.1 × 100 mm) was selected for the analysis after results of a preliminary experiment.

Safety

Experiments were conducted with strict adherence to a safety procedure, approved by the Department of Health and Safety at the University of Delaware and US ARMY.

Results and Discussion

As a result of the application of the adsorption-desorption experiment and the analytical method described above, the concentration of each MC in the solution after the contact time of 2 days was determined. In addition the concentration of the MC on the soils was determined by the acetonitrile extraction and the analytical method. With these two parameters the partition coefficient was calculated by equation 1 and the results are in the Appendix 1 for all soils studied.

After that, with the soil analysis obtained by the soil laboratory at the Plant and Soil Science Department at University of Delaware the fraction of some properties on the soils were determined, these values are in Appendix 2.

Multilinear Models

Some multilinear models were proposed to predict the partition coefficients obtained in Appendix 1 to identify the principal soil characteristics that influence the adsorption of munitions constituents (MC) of explosives in soils, and in this way to determine the fate of the explosives.

The first trial used the traditional organic carbon normalized partition coefficient showed in equation 2, then the other soil characteristics were added to the organic carbon and the criteria to select them was the lowest root mean square error RMSE obtained. After this process the best correlation obtained was using organic carbon (OC), cation exchange capacity (CEC) and extractable iron (Fe ext) obtained by the oxalate method.

CEC gives an indirect measure of charge sites. The CEC was tested in the multilinear model because it is the sum of total exchangeable cations that a soil can adsorb (Sparks, 2003) and the cations on the cation exchange sites of the soil particles are easily exchangeable with other cations. The cation exchange capacity is the maximum adsorption of readily exchangeable ions in a diffuse ion swarm and outer-sphere complexes on soil particle surface (De Kimpe, Laverdiere & Martel, 1979). In addition it was selected because the CEC is impacted by the soil texture (amount of clay), clay type (surface areas), soil organic matter, source of charge and pH (Soil Colloids Course, 2007). The extractable iron was selected because according to Keng et al. (Keng & Uehara, 1973) charge sites soils usually contain a high proportion of colloids of metal oxides, especially those of Fe and Al. The oxalate-extractable Fe gives a measure of the "active" forms of the free Fe (Schwertmann et al., 1964), which are ferrihydrite and small amounts of organically bound Fe (Del Campillo & Torrent, 1992). This method is a measure of the quantity of amorphous iron oxides, or more generally as a measure of the "activity" of the iron oxides (Blume & Schwertmann, 1969). Oxalate does not dissolve a major part of the crystalline iron oxides. It attacks most silicate minerals and goethite and hematite only slightly (Schwertmann, 1973). In other words the oxalate extractable Fe provides additional sorption sites that influence the partition coefficient of adsorption of MC. The literature indicates that the presence of Fe in the soil influences the fate of MC in the environment. CEC and extractable Fe are linked to soil/sediment properties. Pennington & Patrick (1990) reported statistically significant correlations among Kd for TNT with oxalate-extractable Fe, CEC, and percent clay, but in their study Kd was not considered with OC. Some researchers have studied the abiotic degradation of the MC due to Fe. Nefso, Burns & McGrath (2005) and Sunahara et al. (2009) are examples of that. In the first case they determined that exchangeable Fe overwhelms any influence of structural ferrous iron in the degradation of TNT. In the second case it was found that Fe reduces TNT and RDX.

The Models proposed are:

Kps,m = Kocm(foc)s (3)
Kps,m = Kocm(foc)s + KCEC m (fCEC)s (4)
Kps,m = Kocm(foc)s + KCEC m (fCEC)s + KFe m (fFe)s (5)

Where Kps,m is the partition coefficient obtained by the model, Kocm = sorption coefficient to organic carbon in the soil KCEC m = sorption coefficient to CEC in the soil, KFe m is the sorption coefficient for Fe in the soil, fOC = fraction of OC in the soil, fCEC = fraction of CEC in the soil, fFe is the fraction of Fe in the soil and s = soil, m = munitions constituents.

The partition coefficient Kp in L Kg-1 was calculated from the data as the relationship between the amount of MC sorbed per mass of soil and the concentration remaining in the solution after equilibration in the adsorption step. The parameters KOC, KCEC and KFe were calculated for all the chemicals and soils. They were obtained by fitting the multilinear model by the minimization of the log residuals square between the Kp calculated from the experimental data and the Kp obtained by the model using the Excel solver tool.

Appendix 3 shows the Kp values calculated by the model of equation 5. Figure 1 shows the relationship of Kp values calculated by the model of equation 5 and measured values of Kp obtained from the adsorption/desorption experiment. This figure shows a good correlation. This observation indicates that the assumption of the importance of the addition of CEC and Fe really influence in the fate of MC and the importance components in the adsorption partition coefficient.

Figure 1.

Relationship between Kp calculated with Equation 5 and measured values of Kp for all MC. The solid line represents the 1:1 ratio, and the dashed lines bracket at 1 log unit above and below the 1:1 line.

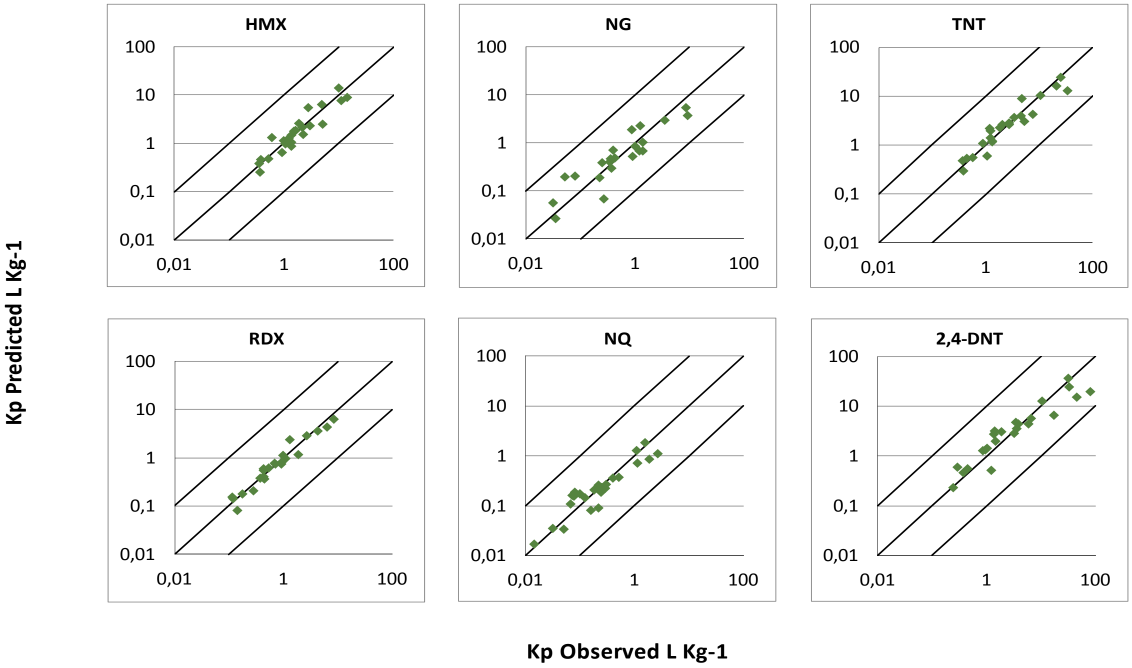
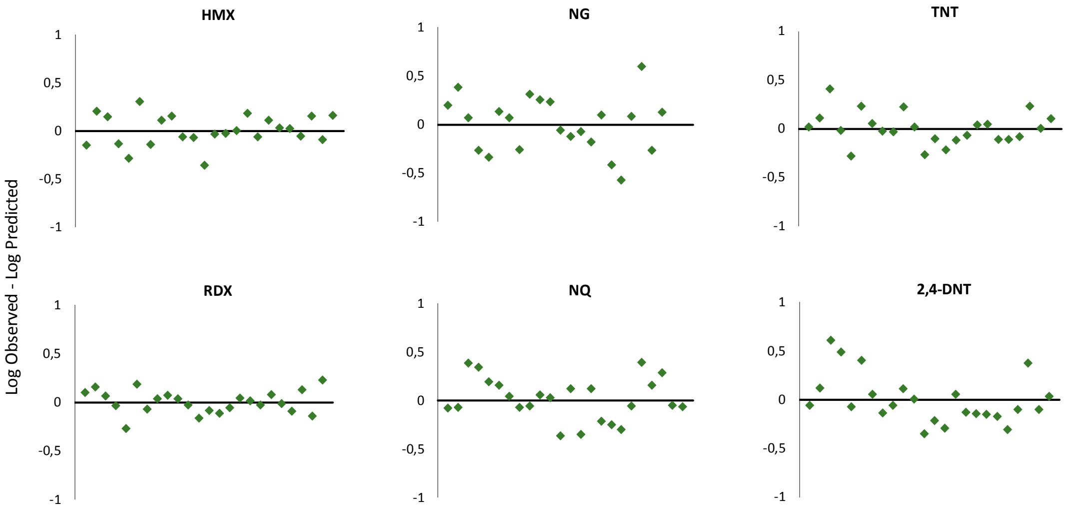


Figure 2.

Residuals (Log Observed – Log Predicted) of Kp calculated with Equation 4.5 and measured values of Kp for all MC. The x-axes is organize in decreasing OC content from 18.23 % from the origin to 0.07 %.



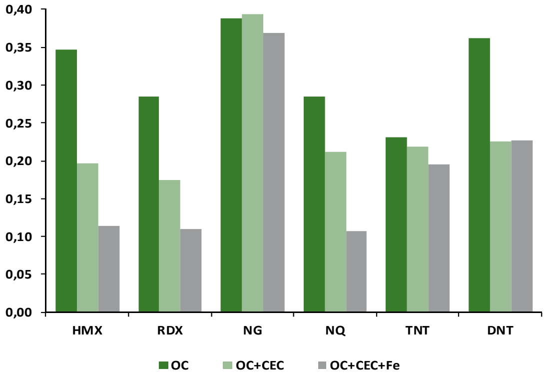
On the other hand, figure 2 shows the residual plot to analyze the fit of model where is observed the good fitting by the use of OC, CEC and Fe ext in the model proposed.

More insights of the previous findings are presented in Figure 3, this figure shows the RSME for the OC model, the CEC model and CEC+ Fe ext models. This figure is evidence of the improvement of the models when the extractable Fe is added; all chemicals showed that improvement especially the NACs and nitramines. This is a confirmation of the Fe influence finding in the literature. For HMX the average of improvement using the trilinear model in comparison to the CEC model was 21 %, for RDX 28 %, for NG 13 %, for TNT 30 %, for DNT 18 % and for NQ 2 %. In soils with low organic carbon the impact of the addition of the clay component was determined.

In addition table 1 presents the empirical parameters obtained of the model for HMX, RDX, NG, NQ, TNT and 2,4-DNT and table 2 shows the RMSE obtained by the OC, CEC and extractable Fe models to low organic carbon content soils (0.07-0.9%). From this table it is observed that for HMX, TNT and 2,4-DNT in these low OC soils the lowest RSME values are obtained by adding the extractable Fe component to the model. For the other MC the values are in the second place of fitting. NG depends mainly on the OC content of the soil based on the results obtained.

Figure 3.

Comparison of the RMSE for Kp obtained by the OC model, CEC model, and trilinear CEC model which includes extractable Fe in addition to OC and Kp measured data.



ISSN 1794-3108. Rev.crim., Volumen 56, número 3, septiembre-diciembre 2014, Bogotá, D.C., Colombia

Table 1.
Parameters of the trilinear model for HMX, RDX, NG, NQ, TNT and 2,4-DNT

Kp Trilinear Model						
	HMX	RDX	NG	TNT	DNT	NQ
KOC	60.1830	30.9725	29.2773	121.9344	190.1531	8.2683
KCEC	143.8570	40.3709	0.0000	42.5228	0.0008	31.7862
KFe	120.1630	35.0383	4.3567	151.3280	72.7077	0.0000

Table 2.
RMSE obtained by the OC, CEC and extractable Fe models to low organic carbon Table content soils (0.07-0.9%)

Model	HMX	RDX	NG	NQ	TNT	2,4-DNT
OC	0.3469	0.2854	0.3882	0.2849	0.2308	0.3621
OC+CEC	0.1964	0.1746	0.3944	0.2120	0.2193	0.2263
OC+CEC+Fe	0.1143	0.1094	0.3693	0.1073	0.1958	0.2277

Conclusions

This study concluded that the multilinear model which includes OC, extractable Fe and CEC improved the estimation of the partition coefficients and provided good evidence that the use of this properties in the study of partitioning of MC in soils with a wide range of properties is useful to predict partition coefficients and fate and toxicity of explosives in the environment.

An additional conclusion is that the extractable Fe is a soil property that contributes to the adsorption of MC (HMX, RDX, TNT and 2,4-DNT) because the addition of Fe in the model showed small differences between the Kp values obtained experimentally and the Kp values from this model.

By measuring the sorption of MC over a wide range of soils that vary in their physical and chemical characteristics, robust, predictive model was developed to improve understanding of sorption phenomena. Such a large number of soils was necessary to isolate the effects of independent physical and chemical characteristics that affect sorption and to use them as parameters for models.

The multilinear model based on sorption to sites rather than the traditional organic carbon normalization approaches to predict partition coefficients for various soils improved the predictions. For compounds that sorb by mechanisms other than by hydrophobic bonding, or by mechanisms in addition to hydrophobic bonding, binding to soil phases other than organic carbon must be included. MC are among the compounds that may partition to additional soil phases.

Acknowledgements

This study was supported by SERDP (Strategic Environmental Research and Development Program Project ER-1688). The authors thank the U.S. Army Edgewood Chemical Biological Center (ECBC) at the Aberdeen Proving Ground for their support and collaboration.

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Appendix 1.
Experimental Partition Coefficients (Observed Data)

Soil	Kp Observed L Kg-1					
	HMX	RDX	NG	NQ	TNT	2,4-DNT
Zegveld	10.0123	8.2521	8.4411	1.5420	25.4608	31.1901
Rhydtalog	14.3634	6.2470	9.0179	1.0862	20.6978	32.4851
Joplin	10.8421	4.2284	3.4994	2.6428	33.6665	79.9458
Lewis Core	4.8022	2.7022	1.2220	1.8723	10.2857	46.0596
Lewis Clean	2.8022	1.3054	0.8700	1.1157	4.6911	10.6039
Pokomoke	5.0326	1.8275	1.3929	0.5225	7.4942	16.9826
Elliot IE	1.8562	0.9659	0.9982	0.3947	4.5501	6.4532
Boxtel	2.9837	1.0752	0.3883	0.2176	3.4464	3.4989
Houthalein	2.1896	0.8996	1.3938	0.1832	2.7247	3.8694
Anne Messex	1.6468	0.9370	1.2109	0.3037	5.1719	5.8120
Whippany	1.5225	0.7061	0.8998	0.2507	2.7408	3.5689
Sassafras 2	0.5912	0.4244	0.4223	0.0803	1.1972	1.4216
Matapeake	1.3645	0.5223	0.3492	0.2449	1.8148	1.8960
SSL	1.1972	0.4219	0.3395	0.0729	1.2052	1.3769
Chile Muestra	2.1577	0.6840	0.2504	0.2925	2.0423	3.1699
Sassafras	1.3579	0.4285	0.3646	0.0673	1.2276	1.4442
Washington 2	0.9799	0.4321	0.0793	0.0977	1.3363	1.0105
Washington 1	1.3698	0.3671	0.0513	0.0783	1.2925	0.9411
Souli	1.0635	0.4381	0.2229	0.1250	0.8670	0.8558
Fort McNelan	0.5208	0.1776	ND	0.2199	0.3710	0.2957
MMRB	0.3451	0.1187	ND	0.0496	0.4412	0.4448
Utah	0.9175	0.2831	0.2626	0.1577	1.0517	1.2311
Aberdeen BA	0.3786	0.1134	0.0307	0.0314	0.5606	0.3720
Aberdeen BT	0.3660	0.1403	0.0349	0.0146	0.3807	0.2467

ND: No Data

Appendix 2.

Fractions of Organic Carbon (OC), Cation Exchange Capacity (CEC) and Extractable Iron (Fe Ext)

Soil	fOC	fCEC	Fe Ext
Zegveld	0.1823	0.00986	0.01195
Rhydtalog	0.1283	0.00646	0.00153
Joplin	0.1012	0.00788	0.00344
Lewis Core	0.0759	0.00670	0.00727
Lewis Clean	0.0636	0.00565	0.00613
Pokomoke	0.0350	0.00236	0.00005
Elliot IE	0.0286	0.00367	0.00254
Boxtel	0.0232	0.00198	0.00500
Houthalein	0.0231	0.00052	0.00050
Anne Messex	0.0230	0.00238	0.00115
Whippany	0.0175	0.00279	0.00250
Sassafras 2	0.0163	0.00153	0.00112
Matapeake	0.0154	0.00178	0.00230
SSL	0.0135	0.00158	0.00178
Chile Muestra	0.0120	0.00378	0.00708
Sassafras	0.0097	0.00090	0.00136
Washington 2	0.0068	0.00365	0.00153
Washington 1	0.0063	0.00320	0.00174
Souli	0.0061	0.00290	0.00160
Fort McNelan	0.0031	0.00198	0.00010
MMRB	0.0024	0.00045	0.00147
Utah	0.0020	0.00202	0.00189
Aberdeen BA	0.0016	0.00068	0.00221
Aberdeen BT	0.0007	0.00034	0.00131

Appendix 3.
Kp Obtained by the Model (Equation 5)

Kp Predicted by the Trilinear Model L Kg-1, Equation 5									
Soil	fOC	fCEC	Fe Ext	HMX	RDX	NG	NQ	TNT	2,4-DNT
Zegveld	0.1823	0.00986	0.01195	13.827	6.463	5.389	24.46	35.534	1.8208
Rhydtalog	0.1283	0.00646	0.00153	8.8345	4.288	3.763	16.15	24.508	1.2662
Joplin	0.1012	0.00788	0.00344	7.6375	3.573	2.978	13.19	19.493	1.0874
Lewis Core	0.0759	0.00670	0.00727	6.4046	2.876	2.254	10.64	14.961	0.8404
Lewis Clean	0.0636	0.00565	0.00613	5.3773	2.413	1.889	8.923	12.539	0.7055
Pokomoke	0.0350	0.00236	0.00005	2.4519	1.181	1.025	4.376	6.6592	0.3643
Elliot IE	0.0286	0.00367	0.00254	2.5548	1.123	0.848	4.028	5.6231	0.3532
Boxtel	0.0232	0.00198	0.00500	2.282	0.974	0.701	3.67	4.7751	0.2548
Houthalein	0.0231	0.00052	0.00050	1.5256	0.754	0.678	2.915	4.429	0.2076
Anne Messex	0.0230	0.00238	0.00115	1.8646	0.849	0.678	3.08	4.4573	0.2657
Whippany	0.0175	0.00279	0.00250	1.7545	0.742	0.523	2.63	3.5092	0.2334
Sassafras 2	0.0163	0.00153	0.00112	1.3357	0.606	0.482	2.222	3.1809	0.1834
Matapeake	0.0154	0.00178	0.00230	1.46	0.63	0.461	2.302	3.0959	0.184
SSL	0.0135	0.00158	0.00178	1.2545	0.545	0.403	1.983	2.6967	0.162
Chile Muestra	0.0120	0.00378	0.00708	2.1171	0.772	0.382	2.696	2.7968	0.2194
Sassafras	0.0097	0.00090	0.00136	0.8771	0.385	0.29	1.427	1.9436	0.1088
Washington 2	0.0068	0.00365	0.00153	1.1191	0.412	0.206	1.217	1.4045	0.1724
Washington 1	0.0063	0.00320	0.00174	1.0494	0.386	0.192	1.168	1.3247	0.1539
Souli	0.0061	0.00290	0.00160	0.9758	0.362	0.186	1.109	1.276	0.1426
Fort McNelan	0.0031	0.00198	0.00010	0.484	0.18	ND	0.478	0.5971	0.0886
MMRB	0.0024	0.00045	0.00147	0.386	0.144	ND	0.534	0.5633	0.0341
Utah	0.0020	0.00202	0.00189	0.6371	0.209	0.067	0.615	0.5175	0.0806
Aberdeen BA	0.0016	0.00068	0.00221	0.4602	0.155	0.056	0.559	0.4649	0.035
Aberdeen BT	0.0007	0.00034	0.00131	0.2493	0.082	0.026	0.299	0.2287	0.0167
ND: No Data									