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Quantitative structure-activity relationship biodegradability modeling in biofiltration of petroleum volatile organic compounds

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A quantitative structure activity-relationship (QSAR) biodegradability model was developed to predict removal capacity of volatile organic compounds (VOCs) in a compost biofilter. Experimental data for o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene was used to develop the model. Biodegradability rate was correlated with three molecular and five quantum mechanical derived descriptor variables. Regression results showed very strong significance between biodegradability of compounds and their molecular weight, M_w ($r^2 = 0.995$), log octanol-water partition coefficient, pK_{ow} ($r^2 = 0.880$), highest occupied molecular orbital energy, E_{homo} ($r^2 = 0.989$), lowest unoccupied molecular orbital energy, E_{lumo} ($r^2 = 1.000$) and energy gap, ΔE ($r^2 = 0.987$). Model significance with excited state energy, E_{es} ($r^2 = 0.678$) and ground state dipole moments, μ ($r^2 = 0.649$) was strong. Log Henry's Constant, H, had weak significance of $r^2 = 0.461$. The descriptors were screened and a complete biodegradability model developed using molecular weight and logarithm octanol-water partition coefficient. The model was calibrated using toluene, ethylbenzene, benzenepropyl-, decane and undecane VOCs and tested. Results showed high prediction of xylene and trimethylbenzene isomers, toluene, ethylbenzene, benzenepropyl-, decane and undecane biodegradability in the biofilter.

Key words: Modeling; biodegradability; biofiltration; VOCs; significant descriptors.

INTRODUCTION

Air pollution is a global concern. Characteristics of air pollution depend on the source of waste gas emissions, and the type and concentration of existing contaminants in the gas stream. Volatile organic compounds (VOCs) found in waste gases contribute to air pollution (Leahy et al., 2004; Otten et al., 2004; Ondiaka, 2011). Biofiltration is а biological air pollution control for treatment of organic and inorganic technoloav substances found in waste gases that are harmful to human and environmental health (Leson and Winer, 1991).Several researchers (Ottenaraf. 1986: Shareefdeen, et.al., 1993; Shareefdeen and Baltzis, 1994; Hodge and Devinny, 1995; Deshusses et al., 1995a, b; Morgenroth et al., 1995; Cherry and Thompson, 1997; Zarook et al., 1997) developed models to predict biodegradability of organic compounds in biofilters. The models considered steady-state dynamic addressed specific systems. which applications definite prediction applicability with and their

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was either uncertain or possible but difficult due to modeling parameters selected (Devinny et al., 1999). Continuous pollutant flows in dynamic modeling limits their accuracy in predicting actual systems where periodic and transient conditions are experienced. Periodic models developed using linear driving force (LDF) show that pollutant adsorption and biodegradation kinetics described transient behavior in biofilters (Chmiel et al., 2005), and biodegradability of VOCs decreased with increased VOCs concentrations, bed heights and gas velocity (Babu and Raghuvanshi, 2006).

Quantitative structure activity-relationship (QSAR) modeling is a developing technique used by few researchers (Choi et al., 1996; Devinny et al., 1997; Johnson and Deshussess, 1997 and Govind et al., 1997; Deshusses and Johnson, 2000 and Aizpuru et al., 2002) to predict pollutant removal in biofilters. The QSAR-based models showed strong prediction by correlating removal rates and selected multiple physical and chemical descriptors of organic compounds existing in waste gas streams. Limitations of biofilter design using QSARbased models has been the inability to predict elimination capacity of individual compounds and compounds found in dissimilar mixtures (Aizpuru et al., 2002).

This study focused on QSAR-based biodegradability modeling of selected VOCs in petroleum off-gases under unsteady waste gas flow and influent concentrations of pollutants. Most QSAR-based models consider steady state operations. Normal industrial biofilter set-ups would give unique trends in the removal of pollutants because of exceptional processes, emission types and varying concentrations of pollutants. The model compounds were representative of typical industrial emissions.

MATERIALS AND METHODS

Selection and Characterization Of Significant Descriptors For Qsar Modeling

Pollution management requires prior in depth understanding of the type, distribution and guantification of existing contaminants and all interacting factors that affect their fate, transport and biodegradation (US EPA, 2006). Organic compounds exhibit different biodegradation in characteristics that affect their bioreactors. Molecular topology descriptors (Randić, 1975; Kier and Hall, 1976; Kier and Hall, 1986) based on chemical structure and numerical connectivity indices (χ) have been used to assess toxicity and biodegradation of organic compounds in the environment (Niemi et al., 1987). Quantum mechanical calculations that use molecular orbital and guantum-chemical descriptors (Csizmadia, 1976) are closely related to oxidationreduction processes and are used to assess treatment of organic pollutants (Tang, 2003). Molecular weight and partition coefficients, including Henry's constant and octanol-water partition coefficient have been used as descriptor variables to model biofiltration processes (Aizpuru et al., 2002; Johnson and Deshusses, 1997). Molecular weight has steric influence on biodegradability of pollutants (Pitter and Chuddoba, 1990). Henry's constant and octanol-water partition coefficient are gas to aqueous phase and liquid to solid phase transfer descriptors (LaGrega et al., 2001).

The choice of significant descriptors in quantitative structure-activity relationship modeling of biofiltration processes is a very important step. To evaluate biodegradation of organic compounds during biofiltartion, molecular weight (M_w) , Henry's Law constant (H), log octanol-water partition coefficient (pKow), and quantum mechanical derived descriptors including highest occupied molecular energy (E_{homo}), lowest unoccupied molecular energy (E_{lumo}), energy Gap ($\Delta E = E_{lumo} - E_{homo}$), singlet electronic excited state (Ees) and ground state dipole moment (μ) were selected as significant variables for modeling. Model compounds selected were o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene. Henry's Law constant values at 25°C were interpolated to a reference temperature of the soil at 20°C. properties Thermodynamic of o-Xylene, 1.3.5-Trimethylbenzene and 1.2.4-Trimethylbenzene were used to calculate dimensionless *H* values using Clausius-Clapeyron relationship (Lide, 1994) given in Equation 1 and expanded in Equation 2. The Clausius-Clapevron relationship is a correction procedure used to predict actual volatilization of organic compounds from soils at given soil temperatures.

$$H_{Ts} = \frac{\exp\left[\frac{-\Delta h_{Ts}}{R_c}\left(\frac{1}{T_s} - \frac{1}{T_r}\right)\right]}{RT_s}H_{ref}$$
(1)

and:

$$\Delta h_{T_s} = \Delta h_{T_b} \left[\frac{\left(1 - \frac{T_s}{T_c}\right)}{\left(1 - \frac{T_b}{T_c}\right)} \right]^n$$
(2)

Where H_{T_s} = Henry's Law constant at average soil temperature (unit less); Δh_{T_s} = enthalpy of vapourization

VOC	Mw	рК _{оw}	<i>р</i> Н	E _{homo}	E _{lumo}	E _{es}	ΔE	μ
o-Xylene	106.17 ^a	3.12 ^c	5.18E-3 ^d 1.59E-1 [°]	-9.421 [†]	4.426 [†]	6.393 [†]	9.847 [†]	0.463 [†]
1,3,5-TMB	120.19 ^b	3.42 ^c	8.77E-3 ^d 2.62E-1 ^e	-9.280 [†]	0.437 ^f	6.236 ^f	9.717 ^f	0.040 [†]
1,2,4-TMB	120.19 ^b	3.63 ^c	6.16E-3 ^ª 1.84E-1 [°]	-9.286 ^t	0.438 [†]	6.316 [†]	9.724 [†]	0.267 [†]

Table 1. Physical and chemical properties of o-Xylene and trimethylbenzene isomers.

^d O'Neil, (2006); ^b Budavari et al., (1989); ^b US EPA, (1987a); ^c Hansch et al., (1995); ^d Values of Henry's Law Constant @ 25°C: National Institute of Standards and Technology (NIST) (2005); ^e Interpolated dimensionless values of Henry's Law Constant @ 20°C; ^fComputed quantum mechanical values.

at average soil temperature (cal mol-1); T_s = average soil temperature (oK); T_r = Henry's Law constant reference temperature (oK); H_r = Henry's Law constant at the reference temperature (oK); R_c = gas constant (1.9872 cal mol-1oK-1); R = gas constant (8.205 x 10-5 atm-m3 mol-1oK-1); Δh_{Tb} = enthalpy of vaporization at normal boiling temperature (cal mol-1); T_c = critical temperature (oK); T_b = normal boiling temperature (oK) and n = exponent (unit less). Quantum mechanical derived descriptors were computed using approximate Hamiltonian semi-empirical parametric method 3 (PM3) in ArgusLab 4.0.1 Software (Mark A.

Thompson, Planaria Software LLC, Seattle, WA, USA, http://www.arguslab.com). A summary of the selected physical and chemical properties of o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene used as descriptors are given in Table 1.

Evaluation Of Degradation Rates Of Xylene And Trimethylbenzene Isomers

Empirical data used was obtained from a laboratory biofiltration treatment study for the removal of xylene and trimethylbenzene (XTMB) volatile organic compounds (VOCs) in a mixture of petroleum hydrocarbons (Ondiaka, 2011). In the study that was conducted at the International Centre of Insect Physiology and Ecology (ICIPE) in Nairobi, Kenya, a compost bofilter with heterogeneous microorganism population was used to treat petroleum VOCs (Ondiaka, 2011). Natural logarithm and inverse of influent concentrations of o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene were plotted against cumulative time to determine the order of reaction and reaction rate constants, k (LaGrega et al.,

2001). Equation 4 (Ottengraf and Van Den Oever, 1983) and Equation 5 (Ottengraf, 1986) were used to reveal zero order and first order reactions respectively. Influent concentrations of XTMB at retention times of 0 to 156-hours of biofilter operation were used in the computation.

$$\Delta C = -k\Delta t \tag{3}$$

$$\Delta C = -kC\Delta t \tag{4}$$

Where t = retention time; C = concentration of contaminants; k = order reaction rate constant; and $\Delta C/\Delta t$ = rate of change of concentration in the biofilter.

1.3. Qsar-Based Biodegradability Model Development

The QSAR-based model was developed stepwise. Each descriptor was correlated with log biodegradation rate (logk) and treated as a best-fit sub-model. Log-*H* was used (Johnson and Deshusses, 1997). A combination of the descriptors was used to evaluate the significance of sub-models. A theoretical mathematical relationship (Equation 5) was formulated to describe the complete model.

$$\hat{\log k} = \beta_0 + \sum_{i=1}^{i=n} |\beta \times D|_1^n$$
 (5)

Where β = model constants to be determined using experimental data; D = descriptor variables used in model development

Model Analysis

Best-fit descriptor parameters were used to calibrate the

model. Five compounds including toluene, ethylbenzene, benzenepropyl, decane and undecane constituted in the petroleum off-gases but not used in model development were used in calibration. The parameters of m-,p-Xylene, o-Xylene, 1,3,5-Trimethylbenzene, 1,2,4-Trimethylbenzene, toluene, ethylbenzene, benzenepropyl-, decane and undecane were correlated with log biodegradation rate $(\log k)$ and a calibrated model developed. A quassi-steady state system was assumed (Aizpuru et al., 2002) by using constant biodegradability rates at different retention times. Using Equation 6 (LaGrega et al, 2001), model effluent concentrations were computed.

$$C_o = C_I \varepsilon^{-kt} \tag{6}$$

Where C_I = influent pollutant concentration in the biofilter and C_o = effluent pollutant concentration in the biofilter. Model mass loads and elimination capacity data was calculated using Equations 7 and 8 (Devinny et al, 1999) respectively.

$$L = \left(\frac{C_I \times 60}{EBRT}\right)$$
(7)
$$EC = \left(\frac{C_I - C_o}{V}\right) \times Q$$
(8)

Where L = mass load; EBRT = empty bed retention time; EC = elimination capacity; V = empty volume of bioreactor and Q = volumetric gas stream flow rate. The model was tested to predict removal efficiency, mass load and elimination capacity of m-,p-Xylene, o-Xylene, 1,3,5-Trimethylbenzene, 1,2,4-Trimethylbenzene, toluene, ethylbenzene, benzenepropyl-, decane and undecane using Equation 9 (Devinny et al, 1999).

$$RE = \left(\frac{C_I - C_o}{C_I}\right) \times 100\% \tag{9}$$

Where *RE* is the removal efficiency in the biofilter. The removal efficiency and elimination capacity of m-,p-1,2,4-Xylene. o-Xylene, 1,3,5-Trimethylbenzene, Trimethylbenzene, evaluated using was both experimental and model data sets. Model elimination capacity of toluene, ethylbenzene, benzenepropyl-, decane and undecane was tested. Linearity of predicted values at different retention times was established. GenStat and Excel statistical packages were used to

Table 2. Reaction and log-reaction rates of Xylene andTrimethylbenzene isomers.

VOC	k (hr-1)	Log k
m-,p-Xylene	3.60E-2*	-1.444*
o-Xylene	3.12E-2	-1.506
1,3,5-Trimethylbenzene	2.05E-2	-1.688
1,2,4-Trimethylbenzene	1.98E-2	-1.703

analyze data. Statistical linear, general and multiple regression tests were performed to establish significant relationships among response and descriptor variables. Fischer and two-sided Student-T tests were performed at 95% confidence interval to compare variances and means of experimental and predicted values of the model respectively.

RESULTS AND DISCUSSION

First order biodegradability reaction rate was established for m-,p-Xylene, o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene. Reaction rate constants are presented in Table 2.

Co-linearity among the selected descriptor variables was observed but not reported here. Regression results showed very strong significance between biodegradability of xylene and trimethylbenzene isomers and their molecular weight ($r^2 = 0.995$), log octanol-water partition coefficient ($r^2 = 0.880$), E_{homo} ($r^2 = 0.989$), E_{lumo} ($r^2 = 1.000$) and ΔE ($r^2 = 0.987$). Significance of compound biodegradability with high energy (excited state) and ground state dipole moments was strong at ($r^2 = 0.678$) and ($r^2 = 0.649$) respectively. Log-*H* had weak significance of $r^2 = 0.461$. The findings show that molecular orbital energy and dipole moments of atoms and molecules of VOCs are good correlative descriptors for their biodegradability rates in biofilters.

Statistical sub-models (No.1-5) and best-fit complete QSAR-based biodegradability model (No.6) for xylene and trimethylbenzene isomers developed are presented in Table 3. The complete model was developed using molecular weight and log-octanol-water partition descriptor variables with a statistical accuracy of 99%. Other researchers (Yin and Dan-li, 2007; Okey and Stensel, 1996) developed complete two-variable biodegradability models after testing five and twelve descriptor variables respectively.

The model showed very strong prediction of removal efficiencies, influent and effluent concentrations individual compounds of m - p-Xylene, o - Xylene,

Model No.	Model $(\log k = \beta_0 + \sum_{i=1}^{i=n} \beta \times D _1^n)$	F	Ρ	d.f
1	$-0.071M_{w}-0.0135$	0.044	212.800	2
2	$-0.401 pK_{ow} - 0.272$	7.340	0.225	2
3	$2.88E_{homo} + 30.30$	4.080	0.293	2
4	$5.510E_{lumo} - 16.47$	22137.440	0.004	2
5	$1.490\Delta E - 16.18$	73.230	0.074	2
6	$-0.0119M_{w} - 0.0611pK_{ow} - 0.0517$	96285.740	0.001	7

Table 3. Sub-models and best-fit model developed.



Figure 1. Model removal efficiency, influent and effluent concentration of m-,p-Xylene

1.3.5-Trimethylbenzene and 1.2.4-Trimethylbenzene as presented in Figure 1 and Figure 2. Model mass load and elimination capacity for m-,p-Xylene, o-Xylene, 1,3,5-1,2,4-Trimethylbenzene Trimethylbenzene and are presented in Figure 3. The significance of the model to predict elimination capacity of m-,p-Xylene, o-Xylene, 1.3.5-Trimethylbenzene and 1.2.4-Trimethylbenzene was $(r^2 = 0.846)$ which strongly compared with that of $r^2 =$ 0.892 using experimental data. Comparisons of experimental and model data for m-.p-Xylene, o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene are presented in Figure 4. Mass load data had strong agreement ($r^2 = 0.843$) compared to elimination capacity data ($r^2 = 0.490$). The later phenomenon could be attributed to abiotic losses including sorption and volatilization of xylene and trimethylbenzene isomers in the biofilter that was recorded as biodegradation.

Model data, under null hypothesis of equal means and variances, were higher than those of observed data (Table 4). Large variances could be attributed to the use of m-,p-Xylene, o-Xylene, 1,3,5-Trimethylbenzene and 1,2,4-Trimethylbenzene concentrations at zero time before treatment. Properties that were used to model elimination capacity of toluene, ethylbenzene, benzenepropyl-, decane and undecane are presented in Table 5 and the model statistical significance are presented in Table 6.

Biodegradability profiles for toluene, ethylbenzene, benzenepropyl-, decane and undecane are presented in Figure 5. Removal of benzene-derivative VOCs was exponential while that of non-benzene VOCs was zigzag (Figure 5), indicative of near equal influent and effluent concentrations irrespective of retention times. The results revealed that reaction rates strongly depended on the



Figure 2. Model removal efficiency, influent and effluent concentrations of 1,3,5-Trimethylbenzene (Plate A) and 1,2,4-Trimethylbenzene (Plate B)



Figure 3. Model individual (Plate A) and overall (Plate B) elimination capacity (EC) profiles of Xylene and Trimethylbenzene (XTMB) isomers

pollutant type, molecular weight and structure. Decane and undecane and their isomers are linear alkanes often used as internal standards in hydrocarbon degradation experiments as they are not eliminated easily in biofilters (Zagustina et al., 2010; Solano-Selena et al., 1999). The results revealed that degradation of aromatics was faster than for linear alkanes as demonstrated by other research findings (Ward et al., 2003; Solano-Selena et al., 1999). Both experimental and model data sets of m-,p-Xylene, o-Xylene, 1,3,5-Trimethylbenzene, 1,2,4-Trimethylbenzene and model data of toluene, ethylbenzene, benzenepropyl-, decane and undecane based on retention time produced linear correlations presented in Table 7.



Figure 4. Comparison of experimental and model mass loads (Plate A) and elimination capacity (Plate B) of Xylene and Trimethylbenzene (XTMB) isomers

Table 4.	Fisher	and	Student	T-tests	for	experimental	and	model	data	of	Xylene	and
Trimethyl	benzen	e.										

Experimental Vs Model					
•	t	р	d.f(t)	F	d.f(F)
Mass loads	-5.03	0.001	21.03	1345.79	21
Elimination capacity	-7.89	0.001	21.04	1077.80	21

Table 5. Properties of toluene, ethylbenzene, benzenepropyl-, decane and undecane used in model testing.

VOC	Ci	Mw	р К _{оw}	log <i>k</i>	k
Toluene	6573.71	92.14 ^a	2.73 [⊳]	-1.313	4.86E-2
Ethyl benzene	3309.59	106.17 ^a	3.15 [⊳]	-1.502	3.15E-2
Benzenepropyl-	1618.19	120.19 ^a	3.69 ^c	-1.701	1.99E-2
Decane	9014.82	142.28 ^a	5.01 ^d	-2.047	8.97E-3
Undecane	8622.27	156.31 ^a	5.74 ^a	-2.259	5.51E-3

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 6.
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VOC	r²	р	F	d.f(F)
Toluene	0.944	0.001	340.03	21
Ethylbenzene	0.873	0.001	139.28	21
Benzenepropyl-	0.664	0.001	39.56	21
Decane	0.531	0.001	22.67	21
Undecane	0.361	0.060	3.98	21



Figure 5. Model elimination capacity profiles of toluene, ethylbenzene and benzenepropyl- (Plate A) and decane and undecane (Plate B)

	١	Naste gas flow	rate (L hr ⁻¹)	
VOC	11.50	14.50	18.00	23.80
m-,p-Xylene	0.653°	0.759°	0.840°	0.987°
	0.836 ^p	0.999 ^p	1.000 ^p	1.000 ^p
o-Xylene	0.897°	0.923°	0.919°	0.978°
-	0.687 ^p	0.999 ^p	1.000 ^p	1.000 ^p
1,3,5-Trimethylbenzene	0.993°	0.982°	0.432°	0.954°
, , , , ,	0.275 ^p	0.998 ^p	0.999 ^p	0.999 ^p
1.0.4 Trime attaches and and a	0.995°	0.998°	0.918°	0.999°
1,2,4-Inmethylbenzene	0.387 ^p	0.998 ^p	0.999 ^p	0.999 ^p
Toluene	0.951	1.000	1.000	1.000
Ethylbenzene	0.701	0.999	1.000	1.000
Benzenepropyl-	0.372	0.998	.999	0.999
Decane	0.975	0.895	0.997	0.998
Undecane	0.993	0.985	0.729	0.987

Table 7. Linearity of elimintion capacity for Xylene and Trimethylbenzene isomers, toluene, ethylbenzene, benzenepropyl-, decane and undecane data sets at different retention times.

CONCLUSIONS

A QSAR-based model with a statistical accuracy of 99% was developed to predict biodegradability of m-,p-Xylene, oXylene,1,3,5Trimethylbenzene,1,2,4Trimethylbenzene,t oluene,ethylbenzene, benzenepropyl-, decane and undecane volatile organic compounds (VOCs) at different linear significance. The model strongly predicted the serve as a design tool for a biofiltration treatment system. Further research is recommended to include diverse compounds and structural descriptors to develop a

removal efficiency of individual compounds and revealed the characteristic behavior of linear alkane hydrocarbons in a biological treatment system in relation to other volatile organic compounds. The potential to model biodegradability of VOCs in waste gas streams is a key aspect in determining air pollution in the environment. In an industrial application where pollutant concentrations in waste gas emissions are not constant, the model would predictive model. This would guide on the design of biofilters with known pollutant elimination trends and retention times of specific groups of compounds during treatment.

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Endnotes

- ^aO'Neil, (2006)
- ^bBudavari et al., (1989)
- ^b US EPA, (1987a)
- ^cHansch et al., (1995)
- ^dValues of Henry's Law Constant at 25°C: National Institute of Standards and Technology (NIST) (2005)
- ^eInterpolated dimensionless values of Henry's Law Constant at 20°C
- ¹Computed quantum mechanical values.