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SUBJECT: USING ENVIRONMENTAL FATE DATA TO PREDICT PESTICIDE GROUND WATER CONTAMINATION PROBABILITIES

SUMMARY

Several logistic regression models were developed and tested for their ability to predict the probability that a pesticide is a ground water contaminant. The models' explanatory variables were various combinations of log-transformed environmental fate properties: organic-carbon normalized soil sorption coefficient, octanol-water partition coefficient, field dissipation half-life, aerobic soil half-life, anaerobic soil half-life, vapor pressure, and Henry's law constant. The latter two volatility variables displayed little ability to predict ground water contamination, yielding insignificant logistic coefficients for 17 of the 18 models that contained one of the volatility variables. Although pesticide movement to ground water is governed by numerous factors beyond fate characteristics, several of the models were successful in predicting contaminant status for a range of pesticides that have been used and subsequently monitored for in California. Model performance was compared using misclassification percentages based on (a) cross-validated probabilities for the model development set and (b) contaminant probabilities calculated for a "semi-independent" validation data set consisting of pesticides with a California monitoring history. Forty six percent of pesticides in the validation data set were also in the original development data. Consequently, the validation misclassification percentages may be low-biased. Nonetheless, the four best-fit models correctly predicted the contaminant status of all nonpoint source California pesticide ground water contaminants in the validation set. In conjunction with pesticide use data, detection history outside California, and knowledge of pesticide use practices, these models will be useful for prioritizing monitoring of California's ground water protection list pesticides.

INTRODUCTION

California's Food and Agriculture Code (FAC) requires the Department of Pesticide Regulation (DPR) to develop specific numerical values (SNVs) for water solubility, organic carbon normalized soil partition coefficient, aerobic soil half-life, anaerobic soil half-life, hydrolysis half-life and field half-life in FAC section 13144(a). SNVs are used to classify pesticide active ingredients as to whether or not they are "potential ground water contaminants." Pesticides that are classified as potential ground water contaminants comprise the Groundwater Protection List (GWPL). Finally, the law further requires DPR to conduct monitoring for pesticides on GWPL.

The GWPL changes from year to year as new pesticides are registered and products containing old pesticides are retired. There are currently 69 active ingredients on GWPL. DPR monitors for approximately one to three pesticides each year depending on resources. Consequently DPR prioritizes GWPL pesticides periodically (typically every year) to determine which pesticides should be monitored. In prioritizing pesticides for monitoring, DPR considers several factors including (Troiano, 1997):

A. occurrence of the pesticide in ground water due to nonpoint source contamination anywhere in the U.S.
B. physicochemical properties
C. pounds of pesticide applied in California, especially in areas known or suspected to be vulnerable to ground water pollution
D. agricultural production practices for crops treated with the pesticide
E. other pertinent factors

The prioritization process is necessarily somewhat subjective because a variety of factors influence a pesticide's potential to move to ground water. However, one area where improvement to the selection process is needed is in the relative ranking of pesticides based on their physicochemical properties (B, above). While SNVs are used to classify pesticides as to whether they are potential ground water contaminants, that univariate procedure does not consider any interaction between persistence and mobility variables, and does not provide any quantitative numerical ranking of pesticides as to their potential to move to ground water.

The objective of this study was to develop and compare different models for ranking the ground water contamination potential of pesticides based on their physical-chemical properties. These models are not intended to be used alone for the purpose of setting monitoring priorities, rather, in combination with additional information listed under A, C, D, and E above. However, the modeling procedure is attractive because the resulting numerical scores constitute a ranking of pesticides as to their likelihood to move to ground water based on their properties. As such, the models provide an additional tool for prioritizing candidate pesticides for monitoring.

MATERIALS AND METHODS

General Approach

The general approach was to use binary logistic regression to develop models for predicting the probability that a given pesticide belonged to one of two categories: "contaminant" or "noncontaminant." One form of the logistic regression, or logit model is:

[1] $$\log_e\left[\frac{p_i}{1-p_i}\right] = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + ... + \beta_k x_{ik}$$

where i represents the individual pesticide, x_{ik} are the k independent (explanatory) variables consisting of environmental fate properties, p_i is the probability that the ith pesticide is a ground water contaminant, and the β_k are fitted regression coefficients. The quantity $[p_i/(1-p_i)]$ is known as the odds ratio. For the purpose of this study, a pesticide was predicted to be a ground water contaminant if $p_i \geq 0.5$ (i.e., odds ratio ≥ 1). The explanatory variables (x_{ik}) consisted of selected $\log_{10}$-transformed fate properties as explained below.

When the β_k are known, a practical form of the logistic model for computing individual probabilities p_i is:

[2] $$p_i = \frac{1}{1 + e^{(-\beta_0 - \beta_1 x_{i1} - \beta_2 x_{i2} - ..... - \beta_k x_{ik})}}$$

For this study the general tasks were:

1. Determine best fit β_k in Equation 1 and fitting statistics for 27 different models using different combinations of explanatory variables and a single development data set consisting of known contaminants and noncontaminants.
2. Select the top three models based on statistics that describe the predictive ability of the model. Use each of the models to predict contaminant probabilities for a validation data set constructed entirely from California groundwater data.
3. Evaluate relative performance of the models by comparing their predicted classifications for the pesticides to their actual contaminant/noncontaminant status. These comparisons were done using misclassification rates based on (a) cross-validated probabilities for the model development data and (b) predicted probabilities for the validation data.

When the same observations are used to both fit a model and estimate its classification error, that estimate of error will be biased. The purpose of cross validation is to reduce the bias in that situation. The statistical package (SAS) logistic procedure estimated cross-validated probabilities based on the "leave one out principal" during fitting of the model development data set (SAS, 2007). This means that the program estimated the contaminant probability that each pesticide would have had if the pesticide's probability was calculated from model fitted to development data lacking that pesticide. A cutoff of $\alpha = 0.05$ was used to test significance of the regression coefficients, and models with any fitted regression coefficients that were not significantly different than zero were eliminated from further consideration.

Environmental Fate Data

Most of the pesticide environmental fate data used in both the development and validation datasets were obtained from a recent data compilation (Spurlock, 2008). Approximately 90% of data in that compilation were median property values from DPR's pesticide chemistry database. Before aggregating the data and calculating medians, the PESTCHEM data were vetted by (a) removing any data that had not been reviewed and approved by DPR's registration chemists, (b) removing duplicate data, (c) correcting or eliminating data inconsistencies obviously attributable to improper units or half-lives reported as rate constants (and vice-versa), (d) removing solution phase partitioning data collected in systems outside the neutral pH range of 6 to 8, (e) removing any degradation half-life data obtained via regression with correlation coefficients < 0.65, (f) removing any data conducted in systems containing high concentrations of potentially interfering cosolvents or co-solutes such as surfactants, and (g) removing any data obtained in systems at temperatures greater than 30C or less than 10C (Spurlock, 2008). In approximately 10% of cases, other data sources were used to augment the available data. The three primary alternate sources were the European pesticide properties database ("FOOTPRINT" <http://www.herts.ac.uk/aeru/footprint/>, the U.S. Department of Agriculture-Agricultural Research Service pesticide properties database at: <http://www.ars.usda.gov/Services/docs.htm?docid=14147> and the pyrethroid environmental fate data compilation of Laskowski (2002). The data in Laskowski (2002) were included because that review is the most reliable and comprehensive source for pyrethroid data in the literature. In a few cases KOW values were estimated using Meylan and Howard's (1995) procedure based on group contribution structure-activity relationships (as opposed to a linear free energy relationships with solubility or octanol-water partition coefficients). Finally, for a few legacy pesticides in the model development data described below, property data were obtained from earlier work (Johnson, 1988, 1989, 1992).

Although Spurlock's compilation (2008) included data for hydrolysis half-life (HYDROL), soil photolysis half-life (SPHOT), and aqueous photolysis half-life (AQPHOT), those data are not available for many pesticides. Consequently HYDROL, SPHOT, and AQPHOT were not used as explanatory variables here. The models that were developed used various properties listed in Table 1. Those data are highly collinear, and represent three general underlying chemical

characteristics (Spurlock, 2008): hydrophobicity (SOL, KOW, KOC), persistence (FD, AERO, ANAERO) and volatility (VP, KH). Across a range of pesticides, values for essentially all of these properties span several orders of magnitude, and all are, or are close to, log-normally distributed (Spurlock, 2008). Consequently $\log_{10}$-transformed fate variables were used as explanatory variables.

Model Development Contaminant/Noncontaminant Data
Wilkerson and Kim (1986), and later Johnson (1989, 1992) reviewed numerous ground water monitoring studies from across the nation to determine a list of pesticides classified as known ground water contaminants and noncontaminants. In compiling their data, pesticides were only classified into a contaminant or noncontaminant group if use had been confirmed in the area where wells were sampled. Johnson (1988, 1989, 1992) used these data to calculate DPR's SNVs. These efforts produced a list of 52 pesticides, with 26 classified as contaminants and 26 classified as noncontaminants (Appendix 1). This list of contaminants and noncontaminants was used as the "model development" data set here. However, propylene dichloride (1,2-dichloropropane, "contaminant"), silvex (2-(2,4,5 trichlorophenoxy) propionic acid, "noncontaminant"), and toxaphene ("noncontaminant") were excluded because data for one or more of their eight environmental fate properties were lacking.

Model Validation Data
A second list of 55 pesticides was compiled for validation. This list included many pesticides in the model development data set as well as pesticides not found in that data set. The validation data met the following criteria (Appendix 2):

1. the pesticides had been monitored for in California
2. sampling was conducted by DPR
3. the monitoring had been "targeted" monitoring, with sampling for a pesticide targeted to wells in areas where use had occurred and the detection was determined to be a result of legal agricultural use

All pesticides from targeted monitoring studies were either taken from past GWPL studies or in the study of Johnson et al. (1992). The term "validation" is used loosely in this study. Ideally, model validation is performed using data that are independent of those data used for model development. Because of the limited number of monitoring data meeting criteria 1-3 above, particularly for contaminants, there is overlap between the development and validation data sets. For example, 46% of validation set pesticides were also in the model development data set (26 of 56), including 72% of the validation set known contaminants (8 of 11). Consequently, estimates of model classification error based on the validation data may be low-biased.

Aldoxycarb (aldicarb sulfone) was included in the validation data set as a contaminant even though there have been no aldoxycarb products registered in California. Aldoxycarb has been used as a pesticide outside of California, and is a degradate of aldicarb and has been detected in California ground water. Aldicarb breaks down rapidly, and aldoxycarb's presence in California ground water is due to aldicarb use (Schuette et al., 2005).

RESULTS

Logistic Regression Models

Twenty seven two- and three-parameter models (Table 2) were fitted to the model development data set (Appendix 1) using SAS's maximum likelihood LOGISTIC procedure (Appendix 3). Different persistence and hydrophobicity variables were included in every model, while a volatility variable was not required for every model. The generalized R^2 statistic and Somers' D are measures of predictive power (Allison, 1999). The generalized R^2 is rescaled from it's calculated value such that $0 \leq R^2 \leq 1$ (SAS, 2007). Somers' D is a measure of rank correlation between model predictions and response variable; higher values indicate better concordance between predicted probabilities and the observed data. These two statistics were used to identify the top performing models for further comparisons (Table 3). The third statistic listed in Table 3 is the Hosmer-Lemeshow (H-L) goodness of fit chi-square statistic (SAS, 2007). This statistic is popular and often reported with logistic regression results. That is the primary reason it is included here. Significant H-L *p*-values indicate a lack of model fit, although some researchers now question the usefulness of the H-L statistic for identifying poor models (Allison, 1999). None of the 27 models here yielded significant H-L statistics, meaning that none of the models could be judged incorrect based on fits to the model development data.

Three models yielded both a generalized $R^2 \geq 0.40$ and a Somers' $D > 0.65$ (Table 3). On this basis these models were selected as the top three models. The three models were further compared based on analysis of their (a) cross-validated probabilities for the model development set and (b) predicted contaminant probabilities for the validation data set. Seventeen of 18 models that contained the volatility variables VP or KH yielded coefficients that were not significantly different than zero. Those models were discarded. The one remaining model, case 26 (Table 3) yielded a low generalized R^2 (0.38) and was not retained for further analysis. Model fit information for the top three models is provided in Table 3, and predicted development data set probabilities are shown in Figure 1.

Under the (arbitrary) rule that a pesticide is classified as a contaminant if the cross-validated probability $p_i \geq 0.50$, all models yielded a significant Fisher Exact test of association between cross-validated and actual contaminant status (Table 5, Figure 2). The choice of 0.50 as cutoff for classification as a contaminant/noncontaminant was arbitrarily chosen. While a different cutoff value could have been used the intention was to use a standard basis for comparing the different models and 0.50 fulfilled that objective. The Models 1 and 2 yielded identical

contaminant misclassification rates of 24% based on the cross-validated results, both performing somewhat better than model 3 with a rate of 28% for the actual contaminants (Table 5).

Validation Results
The overall misclassification percentages for the validation data set followed a similar trend as the cross-validated development data in that Models 1 and 2 had lower misclassification rates than model 3 (Table 6, Figure 3). However, all three models correctly classified every actual contaminant.

Noncontaminants are those that have not been detected in targeted California monitoring studies. They may not have been detected because they are not disposed to move to ground water based on their physical-chemical properties. However, they may not have been detected for various other reasons, including low use intensity in the monitoring area, less vulnerable soils in the monitoring area, inadequate time between use and monitoring or use practices that are low risk for ground water contamination. Consequently the overall misclassification rate may be biased by incorrect contaminant/noncontaminant membership. For a protective program such as DPR's, the overall misclassification rate is less important than the ability of the models to accurately classify actual contaminants. From this standpoint all three models performed well, particularly on the validation data set with an error rate of zero for actual contaminants (Table 6). Finally, Appendix 4 presents predicted contaminant probabilities of current GWPL pesticides based on their physical chemical data and Models 1-3.

While the misclassification percentages of Models 1 and 2 were comparable, Model 2 does have the potential advantage that the model includes log KOW as an explanatory variable instead of log KOC as in Model 1. Both variables are a measure of hydrophobicity, but KOW data are intrinsically much less variable than KOC. In a recent analysis of pesticide environmental fate data (Spurlock, 2008), the median coefficient of variation for repeated determinations of KOW on the same pesticide was 0.11 (n = 109 pesticides) as compared to 0.51 for KOC (n = 1229 pesticides). Consequently the KOW-based model might be preferable when few KOC data are available.

These logistic models yield probabilities that a pesticide is a ground water contaminant based solely on pesticide physical-chemical properties. The models do not consider the myriad of other factors that influence pesticide movement to ground water (e.g. use intensity, application practices, crop management practices, irrigation, timing of application, etc.) and so are necessarily limited. Moreover, there are some inconsistencies between the development and validation data sets. For instance, cyanazine, metolachlor, and alachlor are all listed as contaminants in the development set, but they are classified as noncontaminants in the validation set because they haven't been detected in targeted California monitoring. Other validation set noncontaminants have been reported as "detects" in the U.S. Geological Survey National Water Quality Assessment monitoring (Kolpin et al., 1998), although most had relatively low detection

frequencies. For all of these reasons, the regression models should be considered as only one of a suite of tools or methods to identify potential ground water contaminants.

In addition to prioritizing pesticides for GWPL monitoring, logistic models might also be a useful tool for screening new pesticide active ingredients as to their potential to contaminate ground water. In this capacity, these models might provide additional support to Environmental Monitoring's current probabilistic modeling procedure used to evaluate new active ingredients (Troiano and Clayton, 2004).

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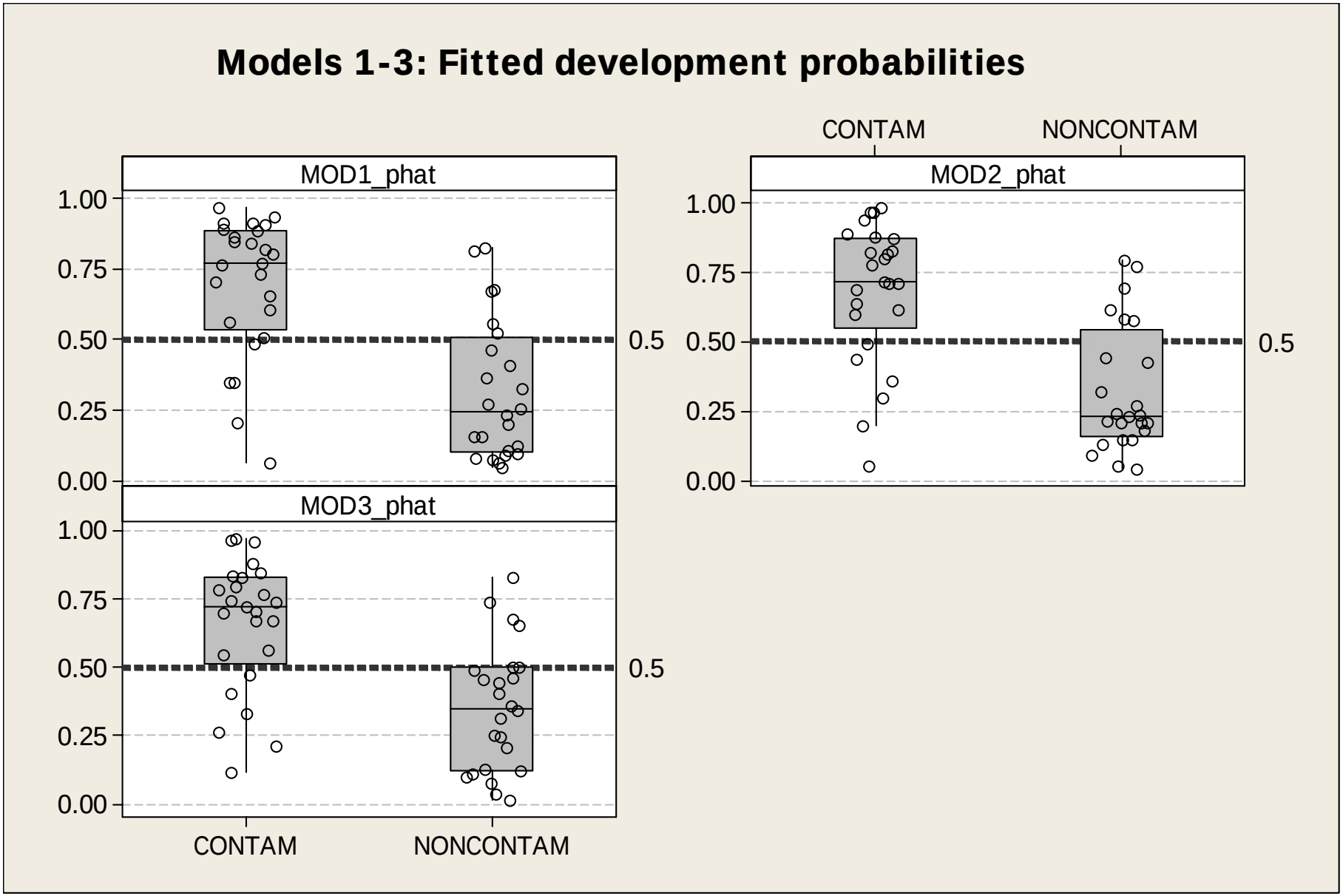

Figure 1. Box plots of fitted development data contaminant probabilities for models 1-3. The box borders are the 25th and 75th percentiles, the center line is the median and the whiskers extend to the 5th and 95th percentiles. The term "phat" refers to predicted probability.

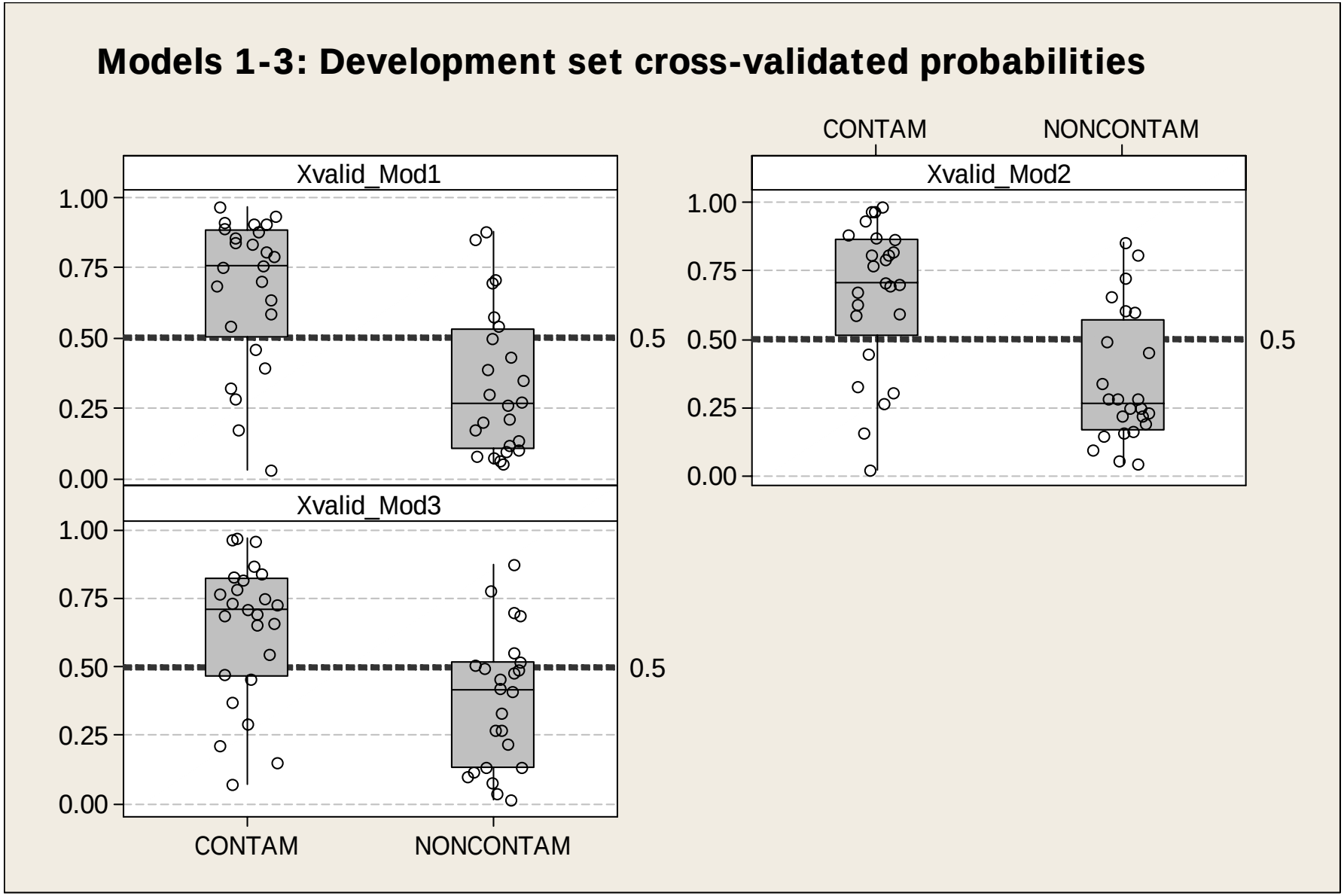

Figure 2. Box plots of estimated cross-validated contaminant probabilities based on the "leave one out approach" for models 1-3. The box borders are the 25th and 75th percentiles, the center line is the median and the whiskers extend to the 5th and 95th percentiles. The term "phat" refers to predicted probability.

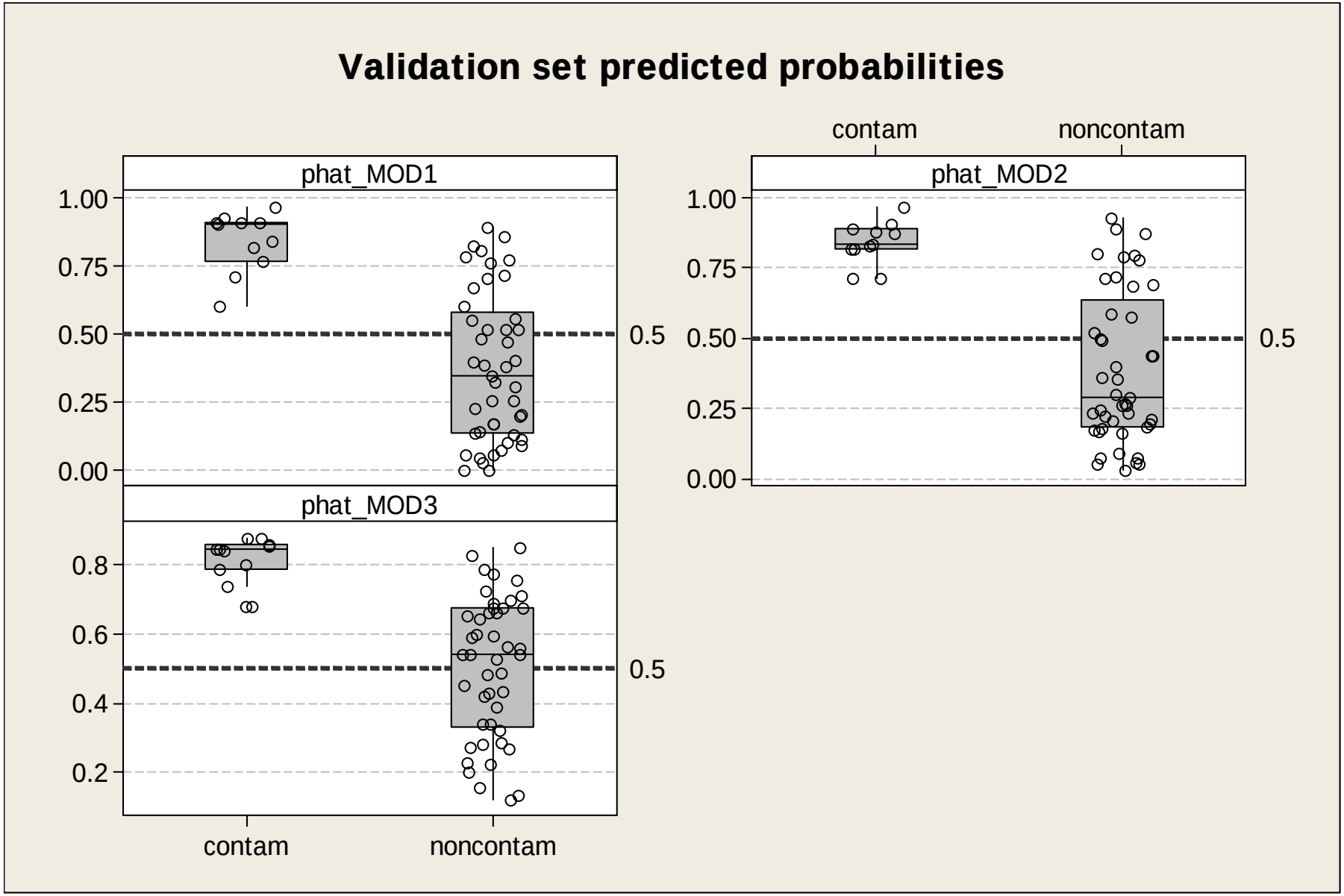

Figure 3. Box plots of estimated validation contaminant probabilities for models 1-3. The box borders are the 25th and 75th percentiles, the center line is the median and the whiskers extend to the 5th and 95th percentiles. The term "phat" refers to predicted probability.

Table 1. Explanatory variables (log_{10} transformation used in models)

Variable	Abbreviated Name
water solubility mg L^{-1}	**SOL**
octanol-water partition coefficient	**KOW**
organic carbon normalized sorption coefficient [ml (gm organic carbon)$^{-1}$]	**KOC**
vapor pressure (torr)	**VP**
Henry's law constant (Pa m^3 mol^{-1})	**KH**
aerobic soil metabolism half-life (day^{-1})	**AERO**
anaerobic soil metabolism half-life (day^{-1})	**ANAER**
field dissipation half-life (day^{-1})	**FD**

Table 2. Top three models based on R^2 and Somers' D. [A]

explanatory variables:	Model 1 logKOC logFD	Model 2 logKOW logFD	Model 3 logKOW logANAERO
generalized R^2 [B]	0.46	0.44	0.40
Somers'D	0.71	0.70	0.65
Hosmer Lemeshow goodness of fit	$p = 0.74$	$p = 0.73$	$p = 0.67$

[A] All other model fits had $R^2 < 0.40$ and Somers' D < 0.65.

[B] Called the "max-rescaled R^2" in SAS.

Table 3. Models tested for ability to predict ground water contaminant probabilities. Hydrophobicity and persistence variables were included in all models. There were no volatility variables in models 1-9.

case	hydrophobicity	persistence	volatility	Model Number	generalized R^2	Somers D
1	KOC	aero	---	**---**	0.38	0.64
2	KOC	FD	---	**1**	0.46	0.71
3	KOC	anaero	---	**---**	0.39	0.63
4	KOW	aero	---	**---**	*	*
5	KOW	FD	---	**2**	0.44	0.70
6	KOW	anaero	---	**3**	0.40	0.65
7	SOL	aero	---	**---**	*	*
8	SOL	FD	---	**---**	0.29	0.54
9	SOL	anaero	---	**---**	*	*
10	KOC	aero	VP	**---**	*	*
11	KOC	FD	VP	**---**	*	*
12	KOC	anaero	VP	**---**	*	*
13	KOW	aero	VP	**---**	*	*
14	KOW	FD	VP	**---**	*	*
15	KOW	anaero	VP	**---**	*	*
16	SOL	aero	VP	**---**	*	*
17	SOL	FD	VP	**---**	*	*
18	SOL	anaero	VP	**---**	*	*
19	KOC	aero	KH	**---**	*	*
20	KOC	FD	KH	**---**	*	*
21	KOC	anaero	KH	**---**	*	*
22	KOW	aero	KH	**---**	*	*
23	KOW	FD	KH	**---**	*	*
24	KOW	anaero	KH	**---**	*	*
25	SOL	aero	KH	**---**	*	*
26	SOL	FD	KH	**---**	0.38	0.64
27	SOL	anaero	KH	**---**	*	*

* = p-value for one or more coefficients >0.05; model rejected

Table 4. Summary of parameter estimates

MODEL		parameter estimate	Standard Error	*p*-value	odds ratio point estimate
Model 1	intercept	1.8521	1.1275	-----	-----
	logKOC	-1.8318	0.5125	<0.001	0.160
	logFD	1.7451	0.6933	0.012	5.727
Model 2	intercept	0.7085	0.9647	-----	-----
	logKOW	-1.0796	0.3178	<0.001	0.633
	logFD	1.5887	0.6425	0.013	17.253
Model 3	intercept	0.9289	0.9620	-----	-----
	logKOW	-0.8570	0.2799	0.002	0.735
	logANAERO	0.9434	0.4640	0.042	6.378

Table 5. Misclassification percentages of development data based on estimated cross-validated probabilities

	percent incorrectly classified			
	actual contaminants	actual noncontaminants	all data	two-sided probability Fisher Exact test for association
Model 1	24	25	24	5.4×10^{-4}
Model 2	24	25	24	5.4×10^{-4}
Model 3	28	29	29	4.2×10^{-3}

Table 6. Misclassification percentages of validation data based on model estimated contaminant probabilities

	percent incorrectly classified			
	actual contaminants	actual noncontaminants	all data	two-sided probability Fisher Exact test for association
Model 1	0	36	29	8.8×10^{-5}
Model 2	0	33	27	5.2×10^{-5}
Model 3	0	56	45	4.8×10^{-3}

chem	mg/L SOL	- KOW	ml /(g OC) KOC	torr VP	atm m^3/mol KH	day FD	day AERO	day ANAERO	Classification
24-D	9.00E+02	1.48E-01	3.84E+01	1.52E-07	1.80E-15	5.93E+01	8.00E+00	6.00E+01	contam
ALACHLOR	2.40E+02	1.22E+03	1.28E+02	1.40E-05	2.48E-08	1.32E+01	1.50E+01	5.40E+00	contam
ALDICARB	5.87E+03	1.41E+01	4.98E+01	2.90E-05	1.23E-09	1.67E+01	1.78E+00	1.84E+00	contam
ATRAZINE	3.25E+01	4.50E+02	8.65E+01	2.34E-07	1.96E-09	8.59E+01	1.46E+02	1.59E+02	contam
BENTAZON	5.70E+02	3.47E-01	3.50E+01	3.45E-06	2.20E-09	2.70E+01	6.50E+01	3.65E+02	contam
BROMACIL	7.00E+02	7.59E+01	1.41E+01	3.10E-07	1.53E-10	1.46E+02	3.44E+02	7.25E+01	contam
CARBOFURAN	3.51E+02	4.60E+01	2.57E+01	2.36E-07	5.10E-09	3.04E+01	2.21E+01	1.97E+01	contam
CHLORAMBEN	7.00E+02	7.94E+01	2.10E+01	6.98E-03	3.90E-11	1.40E+01	5.00E+01	5.90E+01	contam
CHLOROTHALONIL	1.20E+00	7.62E+02	1.11E+03	2.00E-06	1.40E-07	6.00E+01	2.41E+01	7.60E+00	contam
CHLORTHAL-DIMETHYL	5.00E-01	2.00E+05	5.60E+03	2.50E-06	2.20E-06	2.14E+01	2.58E+01	4.80E+01	contam
CYANAZINE	1.55E+02	1.27E+02	2.37E+02	1.60E-09	6.60E-11	3.75E+01	1.54E+01	1.08E+02	contam
dbcp	1.00E+03	4.27E+02	8.00E+01	9.03E+02	2.80E-04	2.03E+02	1.80E+02	7.40E+02	contam
DICAMBA	1.85E+04	1.62E+02	1.30E+01	3.70E-03	1.20E-07	4.90E+00	2.00E+01	8.81E+01	contam
dieldrin	1.20E-01	2.00E+05	7.10E+03	1.82E-07	6.50E-07	1.00E+03	1.00E+03	2.70E+02	contam
dinoseb	7.50E+01	1.95E+02	1.17E+02	7.40E-05	4.60E-07	3.00E+01	3.00E+01	2.30E+01	contam
DIURON	3.64E+01	6.98E+02	5.40E+02	6.90E-08	5.10E-10	1.15E+02	3.72E+02	9.95E+02	contam
EDB	4.30E+03	5.80E+01	4.40E+01	1.10E+01	4.66E-04	1.00E+02	3.50E+01	2.32E+02	contam
FONOFOS	1.69E+01	8.70E+03	1.05E+03	2.73E-04	6.50E-06	2.24E+01	6.28E+01	1.50E+02	contam
METOLACHLOR	4.93E+02	8.50E+02	2.11E+02	3.14E-05	2.40E-08	1.13E+02	2.60E+01	3.70E+01	contam
METRIBUZIN	1.03E+03	5.38E+01	5.00E+01	3.20E-07	3.51E-11	8.88E+01	1.40E+02	2.76E+02	contam
OXAMYL	2.80E+05	3.60E-01	3.16E+01	2.30E-04	2.40E-10	3.18E+01	1.07E+01	5.63E+00	contam
PICLORAM	4.30E+02	1.20E+01	2.90E+01	6.20E-07	4.70E-10	1.08E+02	3.83E+02	5.09E+03	contam
PROMETON	3.94E+02	4.92E+02	1.00E+02	7.70E-06	3.20E-09	2.47E+02	4.59E+02	5.57E+02	contam
PROPACHLOR	6.55E+02	4.10E+01	9.21E+01	2.30E-04	9.56E-10	4.40E+00	5.00E+00	1.46E+02	contam
SIMAZINE	6.15E+00	1.22E+02	1.52E+02	2.21E-08	5.40E-10	8.35E+01	1.10E+02	6.42E+01	contam
1,3-DICHLOROPROPENE	2.25E+03	1.06E+02	6.60E+01	2.51E+01	1.62E-03	5.16E+01	3.27E+01	4.65E+00	noncontam
ALDRIN	2.70E-02	4.60E+05	1.26E+04	2.30E-05	1.33E-03	3.65E+02	1.80E+03	1.18E+02	noncontam
AMETRYNE	1.12E+02	4.23E+02	2.36E+02	2.74E-06	2.49E-09	7.30E+01	3.70E+01	3.22E+02	noncontam
CARBARYL	1.13E+02	2.29E+02	1.39E+02	1.17E-06	2.74E-09	9.49E+00	5.50E+00	8.66E+01	noncontam
chlordane	1.90E+00	1.45E+06	3.36E+04	9.88E-06	9.51E-05	3.65E+02	5.40E+01	8.20E+03	noncontam
CHLORPYRIFOS	1.39E+00	5.01E+04	9.37E+03	2.44E-05	6.60E-06	4.60E+01	8.25E+01	1.36E+02	noncontam
DDT	3.00E-03	8.13E+06	1.60E+05	1.90E-07	8.30E-06	2.74E+03	3.80E+03	5.30E+01	noncontam
DIAZINON	6.00E+01	1.98E+03	1.86E+03	1.10E-04	8.70E-07	9.07E+00	3.97E+01	1.56E+01	noncontam
DIMETHOATE	3.98E+04	5.06E+00	1.00E+01	1.85E-06	1.40E-11	7.80E+00	2.38E+00	2.20E+01	noncontam
DISULFOTON	2.50E+01	9.71E+03	4.90E+02	6.00E-05	2.10E-06	2.86E+00	8.65E+00	2.40E+00	noncontam

chem	mg/L SOL	- KOW	ml /(g OC) KOC	torr VP	atm m^3/mol KH	day FD	day AERO	day ANAERO	Classification
ENDOSULFAN	3.20E-01	5.84E+04	1.20E+04	1.30E-05	3.70E-05	8.98E+01	3.16E+01	1.48E+02	noncontam
ETHOPROP	8.43E+02	3.89E+03	1.83E+02	3.80E-04	1.44E-09	2.33E+01	3.41E+01	1.30E+02	noncontam
FENAMIPHOS	3.29E+02	1.64E+03	2.24E+02	2.44E-05	3.36E-08	9.95E+00	2.42E+01	8.79E+01	noncontam
heptachlor	6.00E-02	6.31E+05	1.60E+04	4.03E-04	3.53E-03	2.50E+02	2.00E+03	3.90E+01	noncontam
LINDANE	7.00E+00	3.14E+03	1.64E+03	3.30E-05	1.80E-06	1.72E+02	9.80E+02	3.70E-03	noncontam
LINURON	7.72E+01	1.02E+03	4.17E+02	1.40E-06	5.80E-09	6.59E+01	4.89E+01	2.20E+01	noncontam
MALATHION	1.25E+02	5.62E+02	1.65E+02	1.32E-05	1.19E-08	9.00E+00	2.50E+00	3.00E+01	noncontam
METHIOCARB	2.70E+01	2.20E+03	6.17E+02	3.53E-07	2.70E-09	1.20E+01	6.44E+01	6.44E+01	noncontam
METHYL BROMIDE	1.75E+04	5.15E+01	1.26E+02	1.77E+03	1.60E-02	3.80E+00	9.63E+00	3.82E+00	noncontam
NALED	2.00E+02	9.20E+01	2.21E+02	2.63E-07	5.01E-08	1.53E+00	3.00E+00	1.53E+00	noncontam
PENDIMETHALIN	2.75E-01	1.52E+05	1.50E+04	9.40E-06	1.27E-08	4.20E+01	1.32E+03	2.14E+01	noncontam
PHORATE	2.90E+01	8.39E+03	5.38E+02	6.44E-04	7.63E-03	1.76E+00	3.00E+00	1.44E+01	noncontam
PROMETRYN	3.29E+01	1.24E+03	2.40E+02	1.05E-06	7.11E-09	7.11E+01	2.61E+02	3.16E+02	noncontam
TRIFLURALIN	3.00E-01	1.18E+05	3.53E+03	1.03E-04	6.11E-04	1.15E+02	1.89E+02	3.50E+01	noncontam

chem	mg/L SOL	- KOW	ml /(g OC) KOC	torr VP	atm m^3/mol KH	day FD	day AERO	day ANAERO	Classification
ALDOXYCARB	1.00E+04	6.76E-01	1.00E+01	1.20E-04	2.70E-09	2.00E+01	2.10E+01	7.80E+01	contam
ATRAZINE	3.25E+01	4.50E+02	8.65E+01	2.34E-07	1.96E-09	8.59E+01	1.46E+02	1.59E+02	contam
BROMACIL	7.00E+02	7.59E+01	1.41E+01	3.10E-07	1.53E-10	1.46E+02	3.44E+02	7.25E+01	contam
dbcp	1.00E+03	4.27E+02	8.00E+01	9.03E+02	2.80E-04	2.03E+02	1.80E+02	7.40E+02	contam
DIURON	3.64E+01	6.98E+02	5.40E+02	6.90E-08	5.10E-10	1.15E+02	3.72E+02	9.95E+02	contam
EDB	4.30E+03	5.80E+01	4.40E+01	1.10E+01	4.66E-04	1.00E+02	3.50E+01	2.32E+02	contam
HEXAZINONE	3.30E+04	1.50E+01	4.52E+01	1.45E-07	1.10E-12	1.39E+02	2.26E+02	2.32E+02	contam
NORFLURAZON	3.37E+01	2.80E+02	4.60E+02	2.90E-08	3.44E-10	1.80E+02	1.30E+02	3.48E+02	contam
PROMETON	3.94E+02	4.92E+02	1.00E+02	7.70E-06	3.20E-09	2.47E+02	4.59E+02	5.57E+02	contam
SIMAZINE	6.15E+00	1.22E+02	1.52E+02	2.21E-08	5.40E-10	8.35E+01	1.10E+02	6.42E+01	contam
ACETOCHLOR	2.23E+02	1.07E+03	2.03E+02	4.00E-03	3.80E-06	1.40E+01	3.40E+01	1.93E+01	noncontam
ALACHLOR	2.40E+02	1.22E+03	1.28E+02	1.40E-05	2.48E-08	1.32E+01	1.50E+01	5.40E+00	noncontam
ALDICARB	5.87E+03	1.41E+01	4.98E+01	2.90E-05	1.23E-09	1.67E+01	1.78E+00	1.84E+00	noncontam
AZINPHOS METHYL	2.80E+01	3.60E+02	7.77E+02	1.60E-06	2.55E-08	8.12E+00	4.40E+01	6.80E+01	noncontam
BENOMYL	2.00E+00	1.32E+02	1.21E+03	9.88E-08	4.90E-09	8.20E+01	7.92E-01	1.00E+00	noncontam
BROMOXYNIL OCTANOATE	8.00E-02	1.15E+05	1.90E+02	1.39E-06	9.21E-06	4.31E+00	2.82E+00	4.15E+00	noncontam
BUTYLATE	4.40E+01	1.40E+04	4.22E+02	1.37E-02	4.40E-05	1.23E+01	5.37E+01	6.36E+01	noncontam
CARBOFURAN	3.51E+02	4.57E+01	5.01E+01	2.36E-07	5.10E-09	3.04E+01	2.21E+01	1.97E+01	noncontam
CYANAZINE	1.55E+02	1.27E+02	2.37E+02	1.60E-09	6.60E-11	3.75E+01	1.54E+01	1.08E+02	noncontam
CYCLOATE	9.50E+01	1.27E+04	2.72E+02	1.60E-03	4.76E-06	1.07E+01	4.31E+01	1.07E+02	noncontam
CYPERMETHRIN	4.00E-03	3.98E+06	3.10E+05	1.30E-09	1.90E-07	2.70E+01	2.30E+01	7.67E+01	noncontam
DIAZINON	6.00E+01	1.98E+03	1.86E+03	1.10E-04	8.70E-07	9.07E+00	3.97E+01	1.56E+01	noncontam
DICOFOL	8.30E-01	1.91E+04	6.99E+03	3.95E-07	2.35E-07	6.56E+01	6.64E+01	1.59E+01	noncontam
DIETHATYL-ETHYL	1.20E+02	3.61E+03	2.02E+02	1.82E-05	6.70E-08	2.00E+01	9.00E+00	6.00E+00	noncontam
DIMETHENAMID	1.20E+03	1.58E+02	1.08E+02	3.70E-06	8.60E-08	1.30E+01	3.80E+01	1.40E+01	noncontam
DIMETHOATE	3.98E+04	5.06E+00	1.00E+01	1.85E-06	1.40E-11	7.80E+00	2.38E+00	2.20E+01	noncontam
DISULFOTON	2.50E+01	9.71E+03	4.90E+02	6.00E-05	2.10E-06	2.86E+00	8.65E+00	2.40E+00	noncontam
EPTC	3.45E+02	2.20E+04	1.45E+02	2.65E-02	1.73E-05	2.07E+00	3.85E+01	7.63E+01	noncontam
ESFENVALERATE	1.31E-03	4.17E+05	4.37E+05	1.50E-09	6.30E-07	3.11E+01	1.05E+02	1.43E+02	noncontam
ETHOPROP	8.43E+02	3.89E+03	1.83E+02	3.80E-04	1.44E-09	2.33E+01	3.41E+01	1.30E+02	noncontam
FENAMIPHOS	3.29E+02	1.64E+03	2.24E+02	2.44E-05	3.36E-08	9.95E+00	2.42E+01	8.79E+01	noncontam
FLUOMETURON	1.11E+02	2.42E+02	8.72E+01	9.38E-07	1.59E-09	1.03E+02	1.09E+01	2.86E+01	noncontam
FONOFOS	1.69E+01	8.70E+03	1.05E+03	2.73E-04	6.50E-06	2.24E+01	6.28E+01	1.50E+02	noncontam
IMIDACLOPRID	5.14E+02	3.70E+00	2.89E+02	1.52E-09	2.00E-15	5.89E+01	9.97E+02	2.71E+01	noncontam
LINURON	7.72E+01	1.02E+03	4.17E+02	1.40E-06	5.80E-09	6.59E+01	4.89E+01	2.20E+01	noncontam

chem	mg/L SOL	- KOW	ml /(g OC) KOC	torr VP	atm m^3/mol KH	day FD	day AERO	day ANAERO	Classification
METALAXYL	7.10E+03	3.30E+01	1.67E+02	5.63E-06	1.49E-10	6.53E+01	6.24E+01	6.84E+01	noncontam
METHIOCARB	2.70E+01	2.20E+03	6.17E+02	3.53E-07	2.70E-09	1.20E+01	6.44E+01	6.44E+01	noncontam
METOLACHLOR	4.93E+02	8.50E+02	2.11E+02	3.14E-05	2.40E-08	1.13E+02	2.60E+01	3.70E+01	noncontam
METRIBUZIN	1.03E+03	5.38E+01	5.00E+01	3.20E-07	3.51E-11	8.88E+01	1.40E+02	2.76E+02	noncontam
MOLINATE	9.70E+02	7.56E+02	2.17E+02	5.00E-03	1.30E-06	1.45E+01	5.10E+01	1.29E+02	noncontam
NALED	2.00E+02	9.20E+01	2.21E+02	2.63E-07	5.01E-08	1.53E+00	3.00E+00	1.53E+00	noncontam
NAPROPAMIDE	7.40E+01	2.10E+03	6.68E+02	1.70E-07	8.10E-10	1.00E+01	4.55E+02	5.06E+01	noncontam
ORYZALIN	2.60E+00	5.37E+03	8.87E+02	1.00E-08	1.70E-09	1.21E+02	6.33E+01	1.00E+01	noncontam
OXADIAZON	1.00E+00	8.13E+04	2.31E+03	7.76E-07	3.50E-07	1.30E+02	5.25E+02	5.74E+03	noncontam
OXYDEMETON METHYL	1.20E+06	1.80E-01	1.00E+01	3.30E-05	4.00E-12	5.00E+00	6.05E+00	3.60E+00	noncontam
PARATHION	1.25E+01	6.76E+03	1.42E+03	9.40E-06	2.40E-07	1.73E+01	6.40E+01	3.50E+00	noncontam
PENDIMETHALIN	2.75E-01	1.52E+05	1.50E+04	9.40E-06	1.27E-08	4.20E+01	1.32E+03	2.14E+01	noncontam
PHOSMET	2.50E+01	9.00E+02	6.29E+03	4.90E-07	1.01E-08	8.24E+00	7.20E+00	2.67E+01	noncontam
PROMETRYN	3.29E+01	1.24E+03	2.40E+02	1.05E-06	7.11E-09	7.11E+01	2.61E+02	3.16E+02	noncontam
PROPANIL	1.52E+02	1.93E+02	4.68E+02	7.77E-07	1.47E-09	1.38E+00	2.20E+00	2.77E+00	noncontam
PROPARGITE	1.93E+00	5.31E+03	7.28E+03	4.19E-08	1.02E-08	8.70E+01	4.69E+01	2.90E+02	noncontam
PROPAZINE	8.60E+00	8.91E+03	1.61E+02	1.70E-07	1.30E-08	1.23E+02	1.05E+02	5.60E+01	noncontam
PROPYZAMIDE	1.29E+01	1.57E+03	8.25E+02	4.35E-07	9.80E-09	5.35E+01	3.92E+02	7.62E+02	noncontam
S,S,S-TRIBUTYL PHOSPHO	2.30E+00	3.31E+05	9.47E+03	4.10E-06	3.10E-07	3.15E+01	7.45E+02	2.22E+02	noncontam
TRIFLURALIN	3.00E-01	1.18E+05	3.53E+03	1.03E-04	6.11E-04	1.15E+02	1.89E+02	3.50E+01	noncontam
TRIFLURALIN	3.00E-01	3.53E+03	1.18E+05	1.03E-04	6.11E-04	1.15E+02	1.89E+02	3.50E+01	noncontam

The LOGISTIC Procedure

Model 1: explanatory variables = logKOC, logFD

Data Set	WORK.PROPS	
Response Variable	leach	leach
Number of Response Levels	2	
Model	binary logit	
Optimization Technique	Fisher's scoring	

Number of Observations Read	49
Number of Observations Used	49

Response Profile

Ordered Value	leach	Total Frequency
1	l	25
2	nl	24

Probability modeled is leach='l'.

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

Criterion	Intercept Only	Intercept and Covariates
AIC	69.908	52.920
SC	71.800	58.595
-2 Log L	67.908	46.920

R-Square 0.3484 Max-rescaled R-Square 0.4646

Testing Global Null Hypothesis: BETA=0

Test	Chi-Square	DF	Pr > ChiSq
Likelihood Ratio	20.9881	2	<.0001
Score	18.0853	2	0.0001
Wald	12.9614	2	0.0015

The LOGISTIC Procedure

Analysis of Maximum Likelihood Estimates

Parameter	DF	Estimate	Standard Error	Wald Chi-Square	Pr > ChiSq
Intercept	1	1.8521	1.1275	2.6982	0.1005
logKOC	1	-1.8318	0.5125	12.7733	0.0004
logFD	1	1.7451	0.6933	6.3364	0.0118

Odds Ratio Estimates

Effect	Point Estimate	95% Wald Confidence Limits	
logKOC	0.160	0.059	0.437
logFD	5.727	1.472	22.285

Association of Predicted Probabilities and Observed Responses

Percent Concordant	85.3	Somers' D	0.707
Percent Discordant	14.7	Gamma	0.707
Percent Tied	0.0	Tau-a	0.361
Pairs	600	c	0.853

Profile Likelihood Confidence Interval for Parameters

Parameter	Estimate	95% Confidence Limits	
Intercept	1.8521	-0.2431	4.2755
logKOC	-1.8318	-2.9901	-0.9393
logFD	1.7451	0.5135	3.2859

Wald Confidence Interval for Parameters

Parameter	Estimate	95% Confidence Limits	
Intercept	1.8521	-0.3578	4.0621
logKOC	-1.8318	-2.8364	-0.8273
logFD	1.7451	0.3863	3.1039

The LOGISTIC Procedure

Partition for the Hosmer and Lemeshow Test

		leach = l		leach = nl	
Group	Total	Observed	Expected	Observed	Expected
1	5	1	0.33	4	4.67
2	5	0	0.58	5	4.42
3	5	1	1.06	4	3.94
4	5	2	1.67	3	3.33
5	5	2	2.39	3	2.61
6	5	3	3.05	2	1.95
7	5	4	3.66	1	1.34
8	5	3	4.12	2	0.88
9	5	5	4.41	0	0.59
10	4	4	3.74	0	0.26

Hosmer and Lemeshow Goodness-of-Fit Test

Chi-Square	DF	Pr > ChiSq
5.1629	8	0.7400

The LOGISTIC Procedure

Model 2: explanatory variables = logKOW, logFD

Data Set	WORK.PROPS	
Response Variable	leach	leach
Number of Response Levels	2	
Model	binary logit	
Optimization Technique	Fisher's scoring	

Number of Observations Read	49
Number of Observations Used	49

Response Profile

Ordered Value	leach	Total Frequency
1	l	25
2	nl	24

Probability modeled is leach='l'.

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

Criterion	Intercept Only	Intercept and Covariates
AIC	69.908	54.312
SC	71.800	59.987
-2 Log L	67.908	48.312

R-Square 0.3296 Max-rescaled R-Square 0.4396

Testing Global Null Hypothesis: BETA=0

Test	Chi-Square	DF	Pr > ChiSq
Likelihood Ratio	19.5965	2	<.0001
Score	16.2856	2	0.0003
Wald	11.8621	2	0.0027

The LOGISTIC Procedure

Analysis of Maximum Likelihood Estimates

Parameter	DF	Estimate	Standard Error	Wald Chi-Square	Pr > ChiSq
Intercept	1	0.7085	0.9647	0.5394	0.4627
logKOW	1	-1.0796	0.3178	11.5400	0.0007
logFD	1	1.5887	0.6425	6.1139	0.0134

Odds Ratio Estimates

Effect	Point Estimate	95% Wald Confidence Limits	
logKOW	0.340	0.182	0.633
logFD	4.897	1.390	17.253

Association of Predicted Probabilities and Observed Responses

Percent Concordant	84.8	Somers' D	0.698
Percent Discordant	15.0	Gamma	0.699
Percent Tied	0.2	Tau-a	0.356
Pairs	600	c	0.849

Profile Likelihood Confidence Interval for Parameters

Parameter	Estimate	95% Confidence Limits	
Intercept	0.7085	-1.1703	2.7010
logKOW	-1.0796	-1.7938	-0.5289
logFD	1.5887	0.4205	2.9766

Wald Confidence Interval for Parameters

Parameter	Estimate	95% Confidence Limits	
Intercept	0.7085	-1.1823	2.5994
logKOW	-1.0796	-1.7025	-0.4567
logFD	1.5887	0.3294	2.8480

The LOGISTIC Procedure

Partition for the Hosmer and Lemeshow Test

		leach = l		leach = nl	
Group	Total	Observed	Expected	Observed	Expected
1	5	1	0.37	4	4.63
2	5	1	0.89	4	4.11
3	5	0	1.10	5	3.90
4	5	2	1.50	3	3.50
5	5	2	2.39	3	2.61
6	5	3	3.07	2	1.93
7	5	4	3.53	1	1.47
8	5	3	3.98	2	1.02
9	5	5	4.30	0	0.70
10	4	4	3.87	0	0.13

Hosmer and Lemeshow Goodness-of-Fit Test

Chi-Square	DF	Pr > ChiSq
5.2732	8	0.7280

The LOGISTIC Procedure

Model 3: explanatory variables = logKOW, logANAERO

Data Set	WORK.PROPS	
Response Variable	leach	leach
Number of Response Levels	2	
Model	binary logit	
Optimization Technique	Fisher's scoring	

Number of Observations Read	49
Number of Observations Used	49

Response Profile

Ordered Value	leach	Total Frequency
1	l	25
2	nl	24

Probability modeled is leach='l'.

Model Convergence Status

Convergence criterion (GCONV=1E-8) satisfied.

Model Fit Statistics

Criterion	Intercept Only	Intercept and Covariates
AIC	69.908	56.423
SC	71.800	62.098
-2 Log L	67.908	50.423

R-Square 0.3001 Max-rescaled R-Square 0.4002

Testing Global Null Hypothesis: BETA=0

Test	Chi-Square	DF	Pr > ChiSq
Likelihood Ratio	17.4854	2	0.0002
Score	14.4371	2	0.0007
Wald	10.2640	2	0.0059

The LOGISTIC Procedure

Analysis of Maximum Likelihood Estimates

Parameter	DF	Estimate	Standard Error	Wald Chi-Square	Pr > ChiSq
Intercept	1	0.9289	0.9620	0.9322	0.3343
logKOW	1	-0.8570	0.2799	9.3731	0.0022
logANAERO	1	0.9434	0.4640	4.1332	0.0420

Odds Ratio Estimates

Effect	Point Estimate	95% Wald Confidence Limits	
logKOW	0.424	0.245	0.735
logANAERO	2.569	1.034	6.378

Association of Predicted Probabilities and Observed Responses

Percent Concordant	82.2	Somers' D	0.648
Percent Discordant	17.3	Gamma	0.652
Percent Tied	0.5	Tau-a	0.331
Pairs	600	c	0.824

Profile Likelihood Confidence Interval for Parameters

Parameter	Estimate	95% Confidence Limits	
Intercept	0.9289	-0.9297	2.9361
logKOW	-0.8570	-1.4905	-0.3735
logANAERO	0.9434	0.1242	1.9416

Wald Confidence Interval for Parameters

Parameter	Estimate	95% Confidence Limits	
Intercept	0.9289	-0.9567	2.8144
logKOW	-0.8570	-1.4056	-0.3083
logANAERO	0.9434	0.0339	1.8529

The LOGISTIC Procedure

Partition for the Hosmer and Lemeshow Test

		leach = l		leach = nl	
Group	Total	Observed	Expected	Observed	Expected
1	5	0	0.32	5	4.68
2	5	2	0.78	3	4.22
3	5	2	1.41	3	3.59
4	5	1	1.95	4	3.05
5	5	1	2.39	4	2.61
6	5	3	2.94	2	2.06
7	5	4	3.48	1	1.52
8	5	4	3.78	1	1.22
9	5	4	4.15	1	0.85
10	4	4	3.80	0	0.20

Hosmer and Lemeshow Goodness-of-Fit Test

Chi-Square	DF	Pr > ChiSq
5.8023	8	0.6694

code	Chem	KOC_FD model 1	KOW_FD model 2	KOW_ANAERO model 3
83	BROMACIL	0.971	0.893	0.745
1810	TEBUTHIURON	0.965	0.964	0.916
379	METALDEHYDE	0.952	0.985	0.954
1871	HEXAZINONE	0.928	0.945	0.896
499	PROMETON	0.914	0.832	0.771
2340	IMAZETHAPYR	0.898	0.912	0.890
1692	METRIBUZIN	0.895	0.874	0.852
636	24-D	0.885	0.988	0.965
166	FLUOMETURON	0.859	0.791	0.565
1685	ACEPHATE	0.845	0.885	0.918
45	ATRAZINE	0.843	0.714	0.675
216	DIMETHOATE	0.829	0.797	0.831
1900	ETHOFUMESATE	0.822	0.754	0.793
1944	BENTAZON	0.821	0.970	0.977
383	METHOMYL	0.816	0.950	0.873
2143	CHLORSULFURON	0.796	0.980	0.973
106	CARBOFURAN	0.790	0.781	0.674
2129	VINCLOZOLIN	0.782	0.738	0.368
509	PYRAZON	0.776	0.912	0.920
382	OXYDEMETON METHYL	0.776	0.932	0.890
531	SIMAZINE	0.770	0.819	0.700
1996	METOLACHLOR	0.765	0.692	0.474
2132	METALAXYL	0.720	0.876	0.796
2019	NORFLURAZON	0.713	0.839	0.774
575	ALDICARB	0.706	0.804	0.548
112	DICHLOBENIL	0.690	0.626	0.805
502	PROMETRYN	0.673	0.577	0.654
2289	ISOXABEN	0.631	0.372	*
2081	IPRODIONE	0.622	0.603	0.425
231	DIURON	0.608	0.713	0.789
3849	IMIDACLOPRID	0.607	0.948	0.857
2149	SULFOMETURON METHYL	0.576	0.956	0.960
1640	CYANAZINE	0.562	0.719	0.740
3835	RIMSULFURON	0.559	0.976	0.967
361	LINURON	0.556	0.587	0.405
404	ETHOPROP	0.523	0.270	0.462
1868	ORYZALIN	0.522	0.498	0.210
81	DICHLORAN	0.507	0.813	0.498
678	ALACHLOR	0.487	0.300	0.264

Appendix 4 - modeled contaminant probabilities for section 6800(b) pesticides
(sorted by model 1 predicted probabilities descending)

code	Chem	KOC_FD model 1	KOW_FD model 2	KOW_ANAERO model 3
1987	VERNOLATE	0.486	0.130	*
1995	DIETHATYL ETHYL	0.475	0.256	0.200
439	NITRAPYRIN	0.459	0.379	0.433
136	CHLOROPICRIN	0.452	0.312	*
105	CARBARYL	0.409	0.429	0.676
3	ACROLEIN	0.409	0.870	0.819
449	MOLINATE	0.402	0.365	0.611
694	PROPYZAMIDE	0.384	0.501	0.713
677	CHLOROTHALONIL	0.349	0.604	0.330
1857	FENAMIPHOS	0.329	0.236	0.502
49	TRIALLATE	0.320	0.109	*
516	CYCLOATE	0.308	0.110	0.338
565	BUTYLATE	0.258	0.115	0.284
254	FONOFOS	0.209	0.198	0.402
375	METHIOCARB	0.202	0.234	0.443
264	EPTC	0.175	0.030	0.266
1728	NAPROPAMIDE	0.171	0.216	0.423
590	PEBULATE	0.148	0.087	0.448
459	PARATHION	0.146	0.188	0.137
314	AZINPHOS METHYL	0.135	0.353	0.615
2260	TRIFLUMIZOLE	0.123	0.061	0.251
437	NAPTALAM, SODIUM SALT	0.095	0.950	*
230	DISULFOTON	0.093	0.054	0.106
198	DIAZINON	0.078	0.209	0.316
70	BENSULIDE	0.065	0.123	0.606
478	PHORATE	0.062	0.042	0.207
233	DAZOMET	0.021	0.245	0.813
392	METHYL ISOTHIOCYANATE	0.000	0.591	*

*** = no model prediction - anaerobic half-life data unavailable**
diquat dibromide and fosetyl-Al omitted - sorption is not soil OC mediated, so KOC not a valid concept for this pesticide