

Predicting Pesticide Emissions and Downwind Concentrations Using Correlations with Estimated Vapor Pressures

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Pesticide emissions to air have been shown to correlate with compound vapor pressure values taken from the published literature. In the present study, emissions correlations based on vapor pressures derived from chemical property estimation methods are formulated and compared with correlations based on the literature data. Comparison was made by using the two types of correlations to estimate emission rates for five herbicides, a fungicide, and an insecticide, for which field-measured emission rates from treated soil, foliage, and water were available. In addition, downwind concentrations were estimated for two herbicides, three fungicides, four insecticides, and two fumigants, for which concentration measurements had been made near treated sources. The comparison results demonstrated that correlations based on vapor pressures derived from chemical property estimation methods were essentially equivalent to correlations based on literature data. The estimation approach for vapor pressures is a viable alternative to the inherently more subjective process of selecting literature values.

Keywords: Pesticides; emissions; vapor pressure; chemical property estimation

INTRODUCTION

Correlation techniques have been developed for estimating pesticide emission rates from treated soil, foliage, and water (*1*). These correlations of measured emission rate versus pesticide physicochemical properties were derived from emissions measured within the first 24 h after application because losses are typically the greatest during this time period. These correlations were intended as a simpler and less costly and time-consuming alternative to measuring emissions. They were also an alternative to measuring air concentrations as modeled emissions could be used in atmospheric dispersion models to estimate concentrations in air for assessment of exposure.

The pesticide physicochemical properties—vapor pressure, water solubility, and soil organic carbon adsorption—were used to formulate the three correlations for pesticides applied to soil, foliage, and water. Vapor pressure, a critically important pesticide property common to all three of these correlations, can be regarded as the underlying driving force leading to emissions of deposited residues. Other properties, such as soil adsorption and water solubility, act as operators on vapor pressure, resulting in a modified, or effective, pressure under a particular set of conditions. For example, for soil, vapor pressure (VP) is attenuated by soil adsorption (K_{oc}) and water solubility (S_w) acting together [VP/($K_{oc}S_w$)]; for foliage, vapor pressure is assumed to act alone for a brief period after application so that pesticide residues volatilize from an essentially non-interactive surface (*1*); and for water, interaction of the chemical

aqueous solubility and vapor pressure is commonly expressed as the Henry's law ratio (VP/ S_w).

A common source for chemical vapor pressure data is the published literature. However, published vapor pressure data are notoriously variable for individual compounds, and in the process of selecting data there is a chance for subjective bias, even when one exercises professional judgment. The use of a computer-based, chemical property estimation program was explored as a more objective way of obtaining chemical vapor pressure values for use in the correlations discussed in this paper. Below, we describe the program and its use in generating a new set of emissions correlations. These new correlations are compared with the earlier ones presented in ref *1* and are evaluated by comparing calculations of environmental interest with measured data. The results presented in this paper are best understood as an extension of our earlier work (*1*), and it is recommended that the two papers be read together.

METHODS

The computer-based program for determining chemical vapor pressure, known as the Estimation Programs Interface (EPI), was developed by the Syracuse Research Corp. (*2*). It is a combination of programs that uses chemical structure to estimate the following: (1) melting point using an adapted Joback method (*3*) and the Gold and Ogle method (*4*); (2) boiling point using an adapted Stein and Brown method (*5*); and (3) vapor pressure using the Antoine relationship (*6–8*) and the modified Grain (*4*, *8*) and Mackay methods (*4*). These three vapor pressure estimation methods are all derived from the Clausius–Clapeyron equation, which correlates compound vapor pressure with temperature:

$$\ln(P_2/P_1) = -(\Delta H_v/R)[(T_1 - T_2)/T_1 T_2]$$

This simple expression has been modified by setting $P_1 = P_b$ (vapor pressure at the boiling point) and $T_1 = T_b$ (boiling point)

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Table 1. Soil Adsorption (K_{oc}), Water Solubility (S_w), and Measured and Estimated Vapor Pressure (VP) for Correlation with Emission Rates (ER) for Pesticides Applied to Soil at 25–30 °C

compound	K_{oc} (mL/g)	S_w (mg/L)	vapor pressure (Pa)		Ln [VP/($K_{oc}S_w$)]		Ln ER ^a
			measured	estimated	measured VP	estimated VP	
Beacon oil	1000	100	200	248	-6.215	-5.999	17.786
Chevron oil	1000	100	47	63	-7.663	-7.370	16.274
Eptam	240	375	4.53	3.87	-9.897	-10.054	12.578
PCNB	5000	0.44	1.47E-02	3.44E-03	-11.916	-13.368	8.292
trifluralin	8000	0.3	1.47E-02	3.79E-03	-12.003	-13.360	8.700
fonofos	870	13	4.53E-02	7.33E-02	-12.428	-11.946	8.987
lindane	1100	7	8.60E-03	10.2E-03	-13.705	-13.532	6.916
dieldrin	9817	0.2	1.33E-03	1.69E-03	-14.205	-13.964	5.660
chlorpyrifos	6070	0.982	2.49E-03	2.71E-03	-14.688	-14.605	4.525
diazinon	1000	48.6	6.40E-03	7.24E-03	-15.843	-15.720	3.292
atrazine	100	33	9.00E-04	3.07E-03	-15.115	-13.889	4.426
dacthal	3200	0.5	3.33E-04	4.61E-04	-15.385	-15.059	2.996/3.144
<i>p,p'</i> -DDT	139959	0.00335	9.60E-05	11.9E-05	-15.401	-15.184	3.825
prometon	150	720	1.10E-02	2.81E-02	-16.100	-15.161	2.526

^a ER = $\mu\text{g}/\text{m}^2\cdot\text{h}$.

and expanded by adding terms that fit the expression to measured data. For example, a common form for the Antoine relationship is

$$\text{Ln}(P/P_b) = \Delta H_b(T_b - C)^2/RT_b^2[1/(T - C) - 1/(T_b - C)]$$

For the Grain method, expressions for liquids and solids take the respective forms

$$\text{Ln}(P/P_b) = \Delta H_b/RT_b[1 - (3 - 2T_\rho)^m/T_\rho - 2m(3 - 2T_\rho)^{m-1} \text{Ln } T_\rho]$$

$$\text{Ln}(P_s/P_l) = 0.61 \text{Ln}(RT_m) [1 - (3 - 2T_{\rho m})^m/T_{\rho m} - 2m(3 - 2T_{\rho m})^{m-1} \text{Ln } T_{\rho m}]$$

where $T_\rho = T/T_b$, $T_{\rho m} = T/T_m$, T_m = melting point, and m is a constant determined by T/T_b (liquid) and T/T_m (solid). Finally, for both liquids and solids, the Mackay method takes the form

$$\text{Ln } P = -(4.4 + \text{Ln } T_b)[1.803(T_b/T - 1) - 0.803 \text{Ln}(T_b/T)] - 6.8(T_m/T - 1)$$

The last term is dropped for liquids (i.e., $T_m < T$) (4, 8).

The EPI program uses all three of the methods to estimate vapor pressure, but the program outputs a "suggested" value. For solids, the EPI program uses the modified Grain method exclusively to calculate the vapor pressure. For liquids and gases, the program calculates an average vapor pressure from the Antoine and modified Grain methods. The Mackay method is restricted in use to the chemical classes for which it was derived (hydrocarbons and halocarbons).

Vapor pressure is estimated from the melting (solids) and boiling points, but the EPI program does not always give consistently reliable data for the latter properties, especially the melting point. The melting point, however, is important only if it is above the temperature for which the vapor pressure is to be estimated; otherwise, the melting point is not needed. The best results occur when measured boiling and melting point data are used, which lead to fairly reliable calculated vapor pressures. Unfortunately, boiling point data, especially for semivolatiles, are not always available. Melting point data are often available, and melting point is usually more reliable than boiling point, especially if the chemical is unstable at higher temperatures. For the most part, the EPI program is able to calculate reasonable vapor pressures with the melting point as the only input and with the program-calculated boiling point. The EPI program estimates boiling points by using an adaptation of the Stein and Brown method (5), which is based on the method of Joback and Reid (9). These methods are quantitative structure-activity relationships that calculate the boiling point (T_b) of a compound through a

Table 2. Measured and Estimated Vapor Pressure (VP) and Emission Rates (ER) for Pesticides on Non-interactive (Plant, Glass, and Plastic) Surfaces at 20–30 °C

compound	surface	Ln VP (Pa)		Ln ER ^a
		measured	estimated	
Beacon oil	glass	5.298	5.513	17.155
Chevron oil	glass	3.850	4.139	14.845
dodecane	plastic	2.507	3.060	13.805
<i>n</i> -octanol	glass	2.851	3.009	14.116
tridiphane	giant foxtail	-3.530	-2.957	8.872
trifluralin	weedy turf	-4.220	-5.631	7.371
pendimethalin	turfgrass	-5.521	-7.118	6.947
2,4-D (isooctyl)	wheat	-5.926	-5.903	6.507
diazinon	dormant peach orchard	-6.509	-6.722	6.812
toxaphene	cotton	-7.537	-6.982	5.293
dieldrin	weedy turf	-7.325	-7.098	5.147
<i>p,p'</i> -DDT	cotton	-10.031	-9.034	3.824

^a ER = $\mu\text{g}/\text{m}^2\cdot\text{h}$.

summation of group increment values (7)

$$T_b = 198.2 + \sum n_i \delta_i$$

where n_i is the number of i groups in the molecule and δ_i is the Joback contribution of group i to the boiling point.

In the discussion of the emissions correlations below, the EPI program yielded unsatisfactory vapor pressure values for a few of the compounds because of poor boiling point estimates. In these cases, we went back to the method of Joback and Reid (9), as discussed in ref 7, and hand-entered the group values. The boiling points estimated in this way were used as input to the EPI program, along with measured melting point, resulting in some improvement in the quality of the calculated vapor pressure for these few compounds. Overall, the error inherent in the estimation of vapor pressure using the EPI program (with input melting and boiling points) is comparable to measurement error, even for vapor pressures of $< \sim 1$ Pa, for which measurement is relatively difficult (8).

RESULTS AND DISCUSSION

Tables 1–3 summarize the data used to establish the pesticide emissions correlations for pesticides applied to soil, foliage, and water. Literature data were from ref 1, with a few minor changes. The measured vapor pressure value for diazinon applied to soil was changed from 1.6×10^{-2} Pa to 6.4×10^{-3} Pa, which was more in line with the field temperature during the measurement of the emission rate for this compound (Table 1). Total vapor pressures (P_i) for the hydrocarbon weed oil

Table 3. Henry's Law Ratio (VP/S_w), Derived from Measured and Estimated Vapor Pressure (VP), and Emission Rates (ER) for Pesticides Applied to Water

compound	S _w (mg/L) ^a	VP (Pa)		Ln (VP/S _w)		Ln [ER/(mg/L)] ^b
		measured	estimated	measured VP	estimated VP	
deltamethrin	0.002	2.00E-06	1.17E-06	-6.908	-7.444	8.230
diazinon	48.6	6.40E-03	4.07E-03	-8.935	-9.388	5.870
eptam	375	4.53	3.869	-4.416	-4.574	9.390
ethyl parathion	15	6.93E-04	2.48E-03	-9.982	-8.708	5.150
methyl parathion	25	8.40E-04	1.71E-03	-10.301	-9.590	4.350
mevinphos	6E05	0.293	0.291	-14.532	-14.539	0.830
molinate	688	0.746	0.973	-6.827	-6.561	7.420
molinate	688	0.746	0.973	-6.827	-6.561	7.690
molinate	800	0.413	0.595	-7.569	-7.204	6.440
thiobencarb	30	2.00E-03	4.65E-03	-9.616	-8.772	5.640
thiobencarb	30	2.00E-03	4.65E-03	-9.616	-8.772	5.470

^a S_w = water solubility. ^b ER = μg/m²·h.

mixtures Beacon oil and Chevron oil were calculated from the hydrocarbon component mole fraction (X_i) (10) and component saturation vapor pressure (P_i°) using Raoult's law

$$P_i = \gamma_i X_i P_i^\circ$$

and

$$P_t = \sum P_i$$

where P_i is component partial pressure and γ_i is component activity coefficient, assumed to be unity for a mixture of normal alkanes. Component vapor pressure, P_i° , was calculated using the Harlacher equation, which is valid for temperatures up to critical conditions (11):

$$\ln P_i^\circ = A + (B/T) + C \ln T + (D P_i^\circ)/T^2$$

The terms A , B , C , and D were taken from Appendix A in ref 11. This process led to no change in the "measured" vapor pressure value for Beacon oil but a slight increase in the value for Chevron oil compared to our earlier results (Tables 1 and 2). The Harlacher equation was also used to more accurately calculate the saturation vapor pressure for dodecane under emission measurement conditions (12), leading to the value of 12.27 Pa (Ln VP = 2.507), as compared to our earlier value of 18.69 Pa (Ln VP = 2.928) (Table 2).

The estimated vapor pressures listed in Tables 1–3 were derived from the EPI computer program using measured melting point data along with measured boiling point data, when available. Measured weed oil component boiling points were used to derive component vapor pressures, from which component partial pressures and total vapor pressures for the hydrocarbon mixtures were calculated using Raoult's law. To achieve a better data fit for some of the semivolatile pesticides, the method of Joback and Reid (7, 9) was used to estimate boiling points for dacthal and p,p' -DDT (Table 1), p,p' -DDT (Table 2), and eptam and molinate (Table 3). This approach was taken with these compounds because measured boiling points were not available and results from the EPI program were not as reliable as the hand-calculated results using the method of Joback and Reid. For example, boiling points calculated using the EPI program for the above compounds were 343.2, 368.0, 287.6, and 298.7 °C for dacthal, p,p' -DDT, eptam, and molinate, respectively. The respective hand-calculated values using the Joback and Reid method were 360.2, 406.1, 257.2, and 274.3 °C. These latter estimated

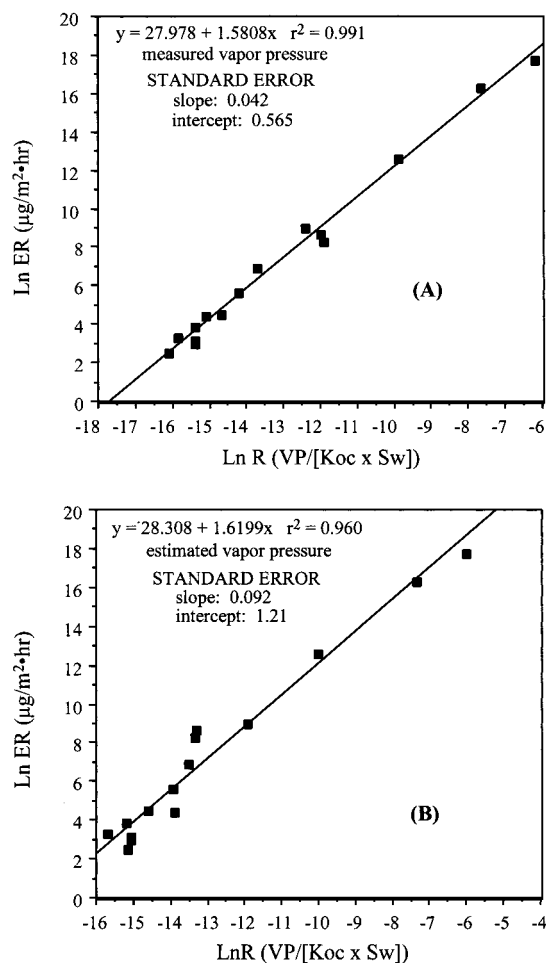


Figure 1. Correlation of pesticide emission rates from soil with chemical properties: (A) literature vapor pressure; (B) estimated vapor pressure.

boiling point values, along with measured melting points, were used as input to the EPI program to estimate vapor pressure for these particular compounds.

Figures 1–3 show the emissions correlations expressed as Ln–Ln regressions, along with standard errors for slope and intercept. Percent relative standard deviations (%RSD) for slope and intercept were, respectively, for soil, 2.6 and 2.0% (literature vapor pressure) and 5.7 and 4.3% (estimated vapor pressure); for plants, 3.2 and 1.4% (literature vapor pressure) and 4.3 and 1.8% (estimated vapor pressure); and for water, 5.3 and 3.0% (literature vapor pressure) and 9.2 and 5.2% (estimated vapor pressure). Although the standard error

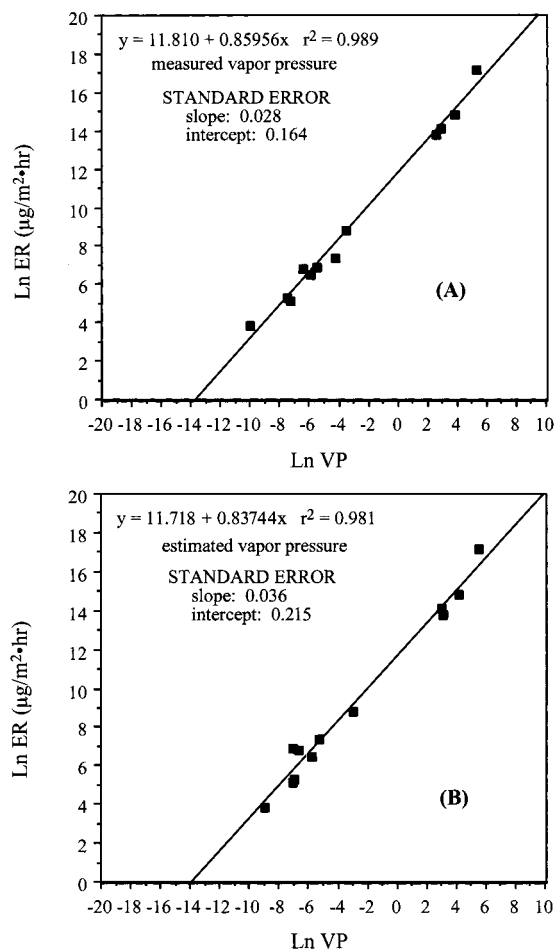


Figure 2. Correlation of pesticide emission rates from inert surfaces (plant, glass, and plastic) with vapor pressure: (A) literature vapor pressure; (B) estimated vapor pressure.

statistics reflected a greater scatter of the data points about the regression lines for all of the correlations derived from estimated vapor pressure, the resulting regression lines compared reasonably well—in slope and intercept—with the regressions derived from literature vapor pressure data. Furthermore, a comparison of the confidence intervals (CI) for the two types of regressions showed that the estimated regression lines were not significantly different from the regression lines derived from the literature data at the 95% CI.

The similarity of the two types of regressions for soil, plants, and water is further illustrated in Table 4, which compares measured emission rate data for a series of pesticides applied to soil, foliage, and water with emission rates estimated from the two types of correlations. The ranges of values listed for the measured emission rates were due partly to application to different kinds of soil [varying K_{oc} values—fenpropimorph (13)] and partly to different experimental conditions [wind tunnel vs field—diflufenican and terbuthylazine (14, 15)]. The two measured emission values each for trifluralin and triallate were obtained using two different field methods for measuring the emission rate from treated soil—relaxed eddy accumulation and aerodynamic gradient (16). The two measured and estimated emission values for molinate were for two different concentrations in rice field water—1.80 and 3.43 mg/L (17, 18). The estimated emission rates for soil were calculated by using the listed values for vapor pressure (VP), soil adsorption (K_{oc}), and water solubility (S_w) in the regression equa-

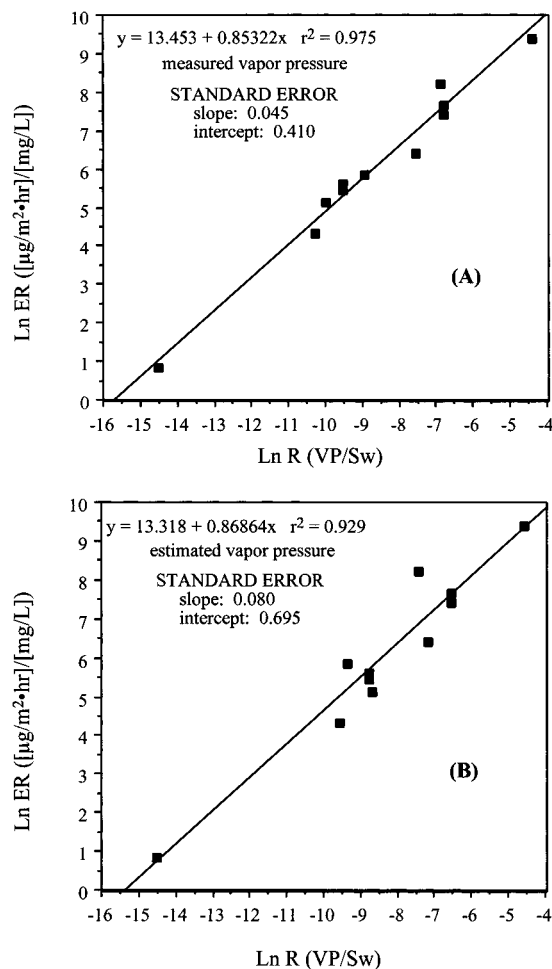


Figure 3. Correlation of water concentration normalized pesticide emission rates from water with chemical properties: (A) literature vapor pressure; (B) estimated vapor pressure.

tions in Figure 1. The estimated emission rate for parathion-methyl on foliage was calculated by using vapor pressure only in the regression equations in Figure 2, and the estimated emission rate for molinate in rice water was calculated by using vapor pressure and water solubility in the regression equations in Figure 3. These property values were obtained from the investigators who measured emission rates for the compounds listed in Table 4.

The percent differences between the estimated emission values in Table 4 and the measured values were 3–60% (average = 20%; median = 13%) for the correlation derived from literature vapor pressure and 5–64% (average = 24%; median = 24%) for the correlation derived from estimated vapor pressure. For soil treated with fenpropimorph, diflufenican, and terbuthylazine, comparison was made with the midrange points of the measured values—60.8, 0.052, and 8.66, respectively. Finally, the percent differences between the estimated values themselves were 8–44%, with an average of 23% and a median of 24%.

Table 5 continues the comparisons by summarizing measured and estimated pesticide concentrations downwind of treated fields. This may be the most valuable type of comparison because concentrations in air are often used to assess exposure to pesticides. The estimated concentrations were obtained from a numerical atmospheric dispersion model (19), which is derived from the U.S. EPA's screening procedures (20, 21). As

Table 4. Comparison of Measured Emission Rates (ER) with Those Derived from Emissions Correlations

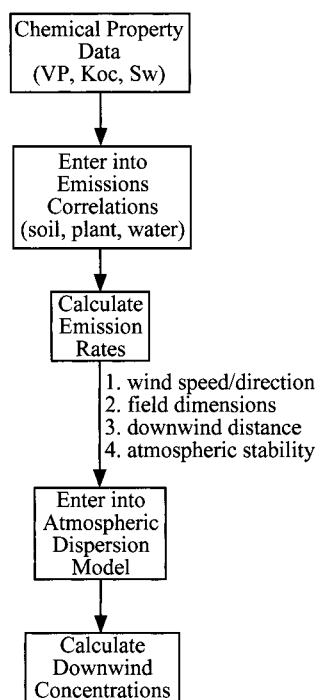
compound ^a	type	VP ^b (Pa)	K _{oc} ^c	S _w ^d	ER (μg/m ² ·h)		
					measured	lit. VP	estimated VP
fenpropimorph ^e	fungicide	2.30E-03	1970	4.3	32.8–88.9	59.0	45.4
diflufenican ^f	herbicide	4.25E-06	38500	<0.05	0.0042–0.1001	0.0293	0.0187
parathion-methyl ^f	insecticide	4.40E-04			154	175	190
terbuthylazine ^g	herbicide	1.50E-04	212	8.5	5.51–11.8	9.10	6.69
trifluralin ^h	herbicide	1.06E-02	8000	0.3	3028/3833 ⁱ	4849	4165
triallate ^h	herbicide	1.52E-02	1164	4	2699/3417 ⁱ	3007	2552
molinate ^j	herbicide	0.746		688	3935/5725 ^k	3700/7050 ^k	2910/5544 ^k

^a Parathion-methyl applied to foliage, molinate applied to water, and all others applied to soil. ^b VP = vapor pressure. ^c Soil organic carbon adsorption coefficient, mL/g. ^d Water solubility, mg/L. ^e Reference 13. ^f Reference 14. ^g Reference 15. ^h Reference 16. ⁱ The first value was obtained using the relaxed eddy accumulation method; the second value was obtained using the aerodynamic gradient method. ^j References 17 and 18. ^k The first value was for the field concentration 1.80 mg/L and the second for the field concentration 3.43 mg/L.

Table 5. Measured and Estimated Downwind Concentrations of Pesticides in Air Resulting from Emissions from Treated Foliage, Water, and Soil

pesticide	type	commodity	downwind concn (μg/m ³) (9–23 m)		
			measured	lit. VP	estimated VP
azinphos-methyl	insecticide	walnuts ^a	<LOQ ^b	0.21–0.30	0.25–0.36
benomyl	fungicide	almonds ^a	<LOQ ^c	9.54E-04	13.9E-04
bromoxynil	herbicide	wheat ^a	2.34	2.28	2.54
captan	fungicide	vineyard ^a	<LOQ ^d	0.014	0.016
carbofuran	insecticide	alfalfa ^a	0.53	0.30–0.61	0.33–0.67
chlorothalonil	fungicide	celery ^a	0.06–0.12	0.05–0.24	0.06–0.28
methidathion	insecticide	oranges ^a	1.40–3.16	1.39–4.20	1.55–4.71
parathion-methyl	insecticide	rice ^e	0.20–0.32	0.14–0.39	0.11–0.30
molinate	herbicide	rice ^e	11.3–22.6	8.21–22.5	6.48–17.8
MITC	fumigant	– ^f	0.030–0.900 ^g	0.036–0.770 ^{g,h}	0.044–1.008 ^{g,i}
methyl bromide	fumigant	– ^j	10.7–242 ^k	9.72–194 ^{k,h}	10.1–202 ^{k,i}

^a Emission from plant surface. ^b LOQ (limit of quantitation) = 0.28 μg/m³. ^c LOQ = 0.22 μg/m³. ^d LOQ = 0.15 μg/m³. ^e Emission from water. ^f Metam sodium applied by drip irrigation at a soil depth of ~10 cm. MITC (methyl isothiocyanate) emission from soil. ^g Downwind distance = 1.6–4.8 km. ^h Emission correlation: Ln ER (μg/m²·s) = 3.7406 + 0.92177 Ln R, where R = (VP × AR)/(K_{oc}S_wd) (AR = application rate and d = depth of injection). ⁱ r² = 0.991. ^j Emission correlation: Ln ER (μg/m²·s) = 3.8235 + 0.84632 Ln R, where R = (VP × AR)/(K_{oc}S_wd) (AR = application rate and d = depth of injection). ^k r² = 0.994. ^j Injected into soil at a depth of 30 cm as a mixture of 67:33 methyl bromide/chloropicrin. ^k Downwind distance = 5–615 m.

**Figure 4.** Diagram illustrating the procedure for starting with chemical properties and ending with environmental data.

outlined in Figure 4, calculated pesticide emission rates—derived from chemical property data and the emissions correlations discussed above—were used as input to the dispersion model, along with field dimen-

sions, downwind distance, wind speed/direction, and atmospheric stability that existed during the field measurements. The field-measured values and environmental/application conditions were taken from a series of reports by the California Department of Pesticide Regulation and the California Air Resources Board. Most of the examples in the table involve pesticide application to foliage (correlations in Figure 2). For treated orchards (walnuts, almonds, and oranges), however, it was necessary to adjust the calculated emission rates for foliage to take into consideration orchard tree density and leaf surface area (orchards are essentially cubic emitters, in contrast to the approximate two-dimensional, planar characteristics of cultivated fields). The technique for doing this is explained in ref 1. There are also two examples of pesticide applications to flooded rice fields (no rice foliage; correlations in Figure 3) and of two fumigants applied to bare soil. Unlike the surface-applied pesticides, emissions correlations for soil fumigants also include the influence of injection depth and application rate, both of which will affect diffusion to the surface. The fumigant correlations that appear in Table 5 were derived from physicochemical property and application data for methyl bromide (MeBr), chloropicrin, 1,3-D (Telone), and methyl isothiocyanate (MITC). Although these fumigant correlations are preliminary and will be discussed in full in a later report, they and their estimated downwind concentrations for MeBr and MITC were included to show the versatility of the correlation approach in its applicability to very volatile chemicals.

In Table 5, ranges of concentration values reflect differing environmental conditions and application scenarios. However, in all cases, measured and estimated concentrations compared reasonably well. Even for the field values that were less than the limit of quantitation (LOQ), the estimated values were near or less than the LOQ. Percent differences between the measured concentration values and the estimated values fell in the ranges of <1–100% (average = 23%; median = 18%) and 0–133% (average = 29%; median = 18%) for the literature vapor pressure and estimated vapor pressure correlations (Figures 1–3), respectively. The large differences (100 and 133%) were for chlorothalonil, which had a measured range of concentrations of 0.06–0.12 $\mu\text{g}/\text{m}^3$. Whereas percent differences between measured and estimated low-end values were small (0 and 17% difference), the estimated high-end values were 2–2.3 times the measured value. Even so, a factor of ~ 2 agreement between modeled and measured concentrations in air is still reasonable. Percent differences between the estimated concentrations themselves fell in the range of 4–37%, with an average of 17% and a median of 17%.

Vapor pressure is a critically important pesticide property in emissions models because vapor pressure is the primary driving force for moving pesticides from a consolidated state to the vapor. Therefore, it becomes important to select the “best” vapor pressure values from the literature or to estimate them in a consistent and reliable manner. To avoid the possibility of bias, inherent in the process of selecting published vapor pressure data, vapor pressure values, in the range of ~ 250 kPa to as low as 10^{-6} Pa, were derived from the computer-based EPI chemical property estimation method. Emission rate correlations derived from estimated vapor pressure compared well with the correlations derived from literature values when these correlations were used to estimate emission rates and downwind concentrations for different pesticide/application scenarios. Overall, the results of this study clearly show that vapor pressure estimation, coupled with the emissions correlations and atmospheric dispersion models, is a practical and reliable way to obtain dissipation and exposure data for pesticides under normal use conditions.

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