Prediction of Airborne Pesticide Distributional Parameters by Physiochemical Properties

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1 Issue

- Exposure models are increasingly used in assessing risk from exposure to pesticides.
- Both stochastic and deterministic models often rely on distributional parameters observed in field studies.
- The mix of current use pesticides is continually changing, but field studies rarely measure emerging pesticides.
- The environmental behavior of a chemical is governed by its intrinsic physicochemical properties.
- In the absence of sufficient field measurement data, is it possible to estimate important distributional parameters based on physiocochemical properties?

2 Approach

- Indoor airborne concentrations of representative organochlorine, organophosphate, and pyrethroid pesticides were obtained from the North Carolina Children's Total Exposure to Persistent Pesticides and Other Persistent Organic Pollutants (CTEPP) study.
- Vapor pressure (VP) values were obtained from the Extension Toxicology Network (EXTOXNET).
- The observed geometric mean concentration (ng/m³) of each compound was regressed on its logged vapor pressure ($\log_{10}$mPa).
- The relationship will be compared to that found with airborne concentrations measured in the EPA Indoor Air Quality Research House following crack-and-crevice type applications.

3 Methods

- CTEPP: Indoor air concentrations of multiple pesticides were available from 129 homes and 13 daycare in North Carolina (Table 1). Samples were collected over 48 hr with quartz fiber filters/XAD-2 cartridges (10 µm inlet) and analyzed by GC/MS.
- Vapor Pressure: Estimates (Table 1) were from Pesticide Information Profiles (PIP) on the Extension Toxicity Network website maintained by Oregon State University (extoxnet.orst.edu).
- Statistical Analysis: Linear regression analysis and plotting was performed using Microsoft Excel.
- Research House: Crack-and-crevice type applications of four pesticides with vapor pressures spanning a wide range (Table 2) were performed to investigate residential translocation.

Class	Compound	VP (mPa)	$\log_{10}$VP	Location	GM (ng/m³)	GSD
organophosphate	chlorpyrifos	2.5	0.40	home	7.0	3.9
				daycare	3.9	3.6
	diazinon	0.097	-1.0	home	2.4	6.1
				daycare	2.5	6.9
pyrethroid	cyfluthrin	0.002	-2.7	home	0.6	1.7
				daycare	0.6	1.4
	cis-permethrin	0.045	-1.3	home	0.46	5.8
				daycare	0.21	4.1
organochlorine	α-chlordane	1.3	0.11	home	1.2	4.7
				daycare	0.79	4.5
	heptachlor	53	1.7	home	7.3	6.6
				daycare	8.9	4.3

VP, vapor pressure; GM, geometric mean; GSD, geometric standard deviation

Table 1. Vapor pressures of selected pesticides and indoor air concentrations measured in CTEPP.

Class	Compound	VP (mPa)	$\log_{10}$VP
phenyl pyrazole	fipronil	0.00037	-3.4
pyrethroid	cypermethrin	0.00041	-3.4
pyrethroid	permethrin	0.045	-1.3
carbamate	propoxur	1.29	0.11

VP, vapor pressure

Table 2. Vapor pressures of pesticides applied in the Indoor Air Quality Research House.

4 Results

- A strong association between geometric mean concentration and logged vapor pressure was observed in both residential (r^2 = 0.65) and daycare (r^2 = 0.66) environments (Figure 1).
- A crude estimate of expected indoor air concentration can be obtained using: $1.7 \cdot \log_{10}(VP) + 3.8$, with VP in mPa.
- Because of the large geometric standard deviations associated with the indoor air concentrations (Table 1), the estimates based on vapor pressure are expected to be imprecise.
- Results of airborne concentrations measurements of pesticides applied in the EPA Indoor Air Quality Research House in support of the model (Table 2) were not yet available.

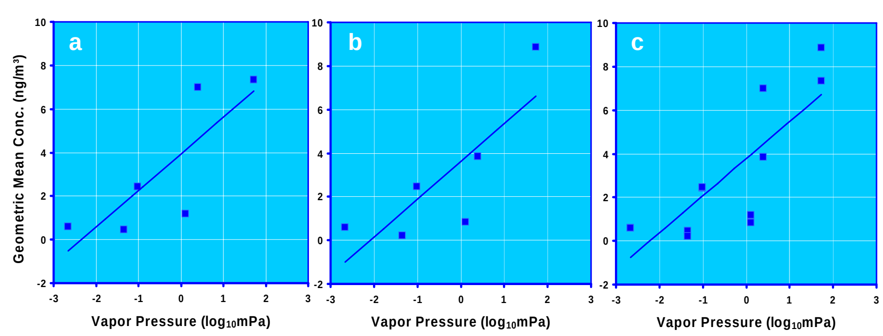
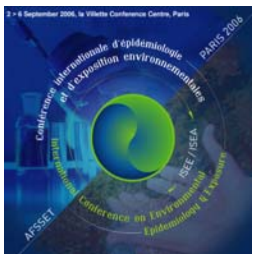


Figure 1. Pesticide concentrations in indoor air as a function of vapor pressure in (a) homes ($y = 1.7x + 3.9$, $r^2 = 0.65$), (b) daycares ($y = 1.7x + 3.6$, $r^2 = 0.66$), and (c) homes and daycares together ($y = 1.7x + 3.8$, $r^2 = 0.65$).

5 Discussion

- These results demonstrate that in the absence of a recent application, a crude estimate of pesticide concentration in indoor air can be made from at least one of the physiochemical properties, namely the vapor pressure.
- Results from applications in the Indoor Air Quality Research House will be available shortly. Those results will be used to assess the how well the relationship between vapor pressure and concentration is maintained following an application.
- Future work should investigate whether including other physiocochemical properties (*e.g.*, molecular weight, melting point, boiling point, water solubility, octanol/water partition coefficient) improves the model.



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