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Addition/Correction

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Correction to An Improved Screening Tool for Predicting Volatilization of Pesticides Applied to Soils

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Supporting Information

In our article describing a screening tool for predicting pesticide volatilization from soils,[1] we used eq 1 to estimate the air diffusion coefficient (D_{air}) at the specified atmospheric temperature (T).

$$D_{air} = D_{air(ref)}\left(\frac{T}{T_{ref}}\right)^{1.75} \tag{1}$$

where $D_{air(ref)}$ is the reference air diffusion constant (0.0179 m^2 h^{-1}) at the reference temperature (T_{ref}) (293.15 K). According to the original literature source from which this equation was derived,[2] the temperatures must be expressed in Kelvin. However, this was not specified in our article[1] nor in the Pesticide Leaching Model user manual,[3] which we referenced as the source of the equation, and we erroneously used values in degrees Celsius for the calculations reported in our article. The correct use of Kelvin in this equation is important because, for example, if 15 and 20 °C are used for the T and T_{ref} values, respectively, the calculated D_{air} is 0.0108 m^2 h^{-1}. However, if 288.15 K and 293.15 K are used, the calculated D_{air} is 0.0174 m^2 h^{-1}. As our sensitivity analysis showed,[1] 24-h cumulative percentage volatilization (CPV_{24h}) values can be highly dependent on D_{air}, depending on the properties of the pesticide. The CPV_{24h} values for all pesticides (except chloropicrin, dichlorvos, and thiram) were higher when D_{air} was calculated correctly using temperatures in Kelvin than the values reported in our article. The three exceptions occurred because these pesticides were predicted to completely volatilize within 24 h (i.e., CPV_{24h} = 100%) regardless of whether the D_{air} value was derived from temperatures given in degrees Celsius or Kelvin. Among the 224 pesticides for which we listed CPV_{24h} values under standard conditions in the Supporting Information (pages S7−13),[1] the maximum increase in CPV_{24h} occurred by a factor of 1.6 (e.g., the CPV_{24h} of dithianon increased from 1.25×10^{-9}% to 2.01×10^{-9}%). However, for half the listed pesticides, the absolute increase in the reported CPV_{24h} values was less than 0.1%.

There were 57 pesticides (out of 224) that exhibited an absolute increase in CPV_{24h} of greater than 1%. These pesticides were located within the boundaries between high CPV_{24h} (>50%, red) and low CPV_{24h} (<5%, purple) on the chemical space diagrams and were sensitive to the correction because the boundaries shifted outward when the correction was made. Figure 1 shows the position of the 57 pesticides on a chemical space diagram under standard conditions (T 288.15 K, soil organic carbon fraction (f_{OC}) 0.02, relative humidity (RH) 100%). Additionally, in the original manuscript, we stated that 21 pesticides had vapor pressures above the European Union Tier I trigger value and CPV_{24h} less than 0.005%. However, this has changed to 15 pesticides with the correction (Supporting Information Table S7).

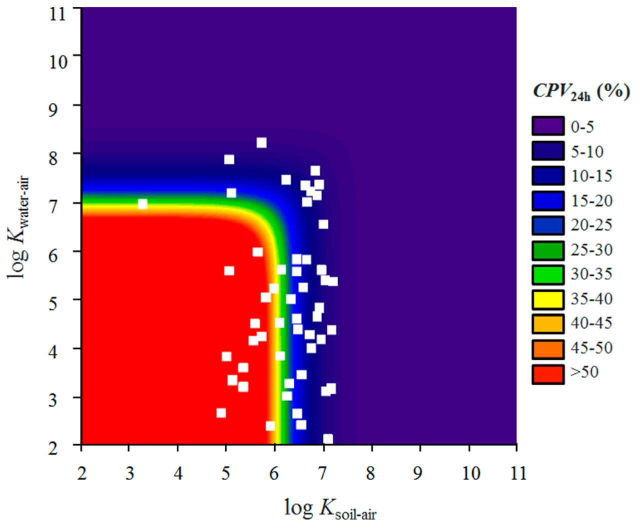

Figure 1. Chemical space diagram showing Flux IV CPV_{24h} values for hypothetical pesticides under standard conditions (T 288.15 K, f_{OC} 0.02, RH 100%). The white squares represent the 57 real pesticides whose CPV_{24h} values increased by greater than 1%, all of which are located along the boundary between high (>50%) and low (<5%) CPV_{24h}.

Although we felt that it was important to report this correction and emphasize the importance of using Kelvin in eq 1, the correction we report here had no impact on the overall volatilization and sensitivity trends reported in the original article nor on any of the conclusions drawn.

We also note here that the default volume of water (V_w) used in the standard agricultural system was listed incorrectly on page S3 of the Supporting Information and should have read 1.39×10^3 L; however, we used the correct value of V_w in all of our calculations.

ASSOCIATED CONTENT

Supporting Information

An updated version containing the corrected CPV_{24h} values is available free of charge via the Internet at http://pubs.acs.org.

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REFERENCES

(1) Davie-Martin, C. L.; Hageman, K. J.; Chin, Y. P. An improved screening tool for predicting volatilization of pesticides applied to soils. *Environ. Sci. Technol.* **2013**, *47* (2), 868−876.

(2) Fuller, E.; Schettler, P.; Giddings, J. A new binary method for prediction of binary gas-phase diffusion coefficients. *Ind. Eng. Chem* **1966**, *58* (5), 19−28.

(3) Klein, M. *PELMO: Pesticide Leaching Model Version 4.0 User Manual*; Fraunhofer Institute for Molecular and Applied Ecology: Aachen, Germany, 2011.