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To Reggie Cheatham/DC/USEPA/US@EPA
cc
Subject EPA data quality

Dear Dr. Cheatham,

a small article in the July issue of ES&T made me aware of the current dispute between the EPA and the US Chamber of Commerce.

Here are a number of thoughts that may be helpful when you are thinking of revising your data bases.

1) There are probably more wrong physico-chemical data published than one might expect. One reason for this is that most scientists are not able to check their experimental data for plausibility and consistence. We have shown how such a data check can work and not work in

Goss, K.-U.; Wania, F.; McLachlan, M.S.; Mackay, D.; Schwarzenbach, R.P.,
Comments on 'Re-Evaluation of Air-Water Exchange Fluxes of PCBs in Green Bay and Southern Lake Michigan'.
Environ. Sci Technol., 2004. 38: p. 1626-1628.

Fenner, K.; Roth, C.; Goss, K.-U.; Schwarzenbach, R.P.,
Comment on "High-Resolution Gas Chromatography Retention Data as Basis of the Estimation of Kow Values using PCB Congeners as Secondary Standards".
Environ. Sci Technol., 2004. 38: p. 2286-2287.

Goss, K.-U.,
Comment on 'Influence of Soot Carbon on the Soil-Air Partitioning of Polycyclic Aromatic Hydrocarbon'.
Environ. Sci Technol., 2004. 38: p. 1622-1623.

Goss, K.-U.; Schwarzenbach, R.P.,
Gas/Solid and Gas/Liquid Partitioning of Organic Compounds: Critical Evaluation of the Interpretation of Equilibrium Constants.
Environ. Sci. Technol., 1998. 32: p. 2025-2032.

In a similar way we are going to show that the published physico-chemical data on fluorinated telomer alcohols are wrong (although some of them have been reproduced with two completely different experimental methods).

2) Another, more severe problem, however, goes far beyond the quality of the physical-chemical data in your and other data bases. The parameters that are used to predict the environmental partitioning of organic compounds like water solubility, vapor pressure, octanol/water and octanol/air partitioning are not adequate. We have shown this in a theoretical analysis including some examples in

Goss, K.-U.; Schwarzenbach, R.P.,
Linear Free Energy Relationships Used to Evaluate Equilibrium Partitioning of Organic Compounds.
Environ. Sci. Technol., 2001. 35: p. 1-9.

Meanwhile we have been collecting thousands of data that support this (see attached pdf file). The best available cure to this problem lies in the use of so called LSER equations (proposed by MH Abraham and coworkers). These equations allow a reliable prediction of all kinds or partitioning data for all kinds of non-ionic organic compounds based on 5 compound descriptors (four of which must be determined experimentally from various kinds of partition data). In the attachment you will see a comparison between the LSER approach and the traditional predictions based on Kow or vapor pressure based on hundred's of experimental data.
The advantages of this LSER method can be summarized as follows:
- partitioning can be predicted much more precisely with the LSER method than with traditional methods for a large variety of organic compounds and phases. (because separate descriptors are used for the van der Waals and H-bond interactions of both the compounds and the phases).
- the compound descriptors that are required can be determined from a variety of partition experiments. This allows to leave out experiments that are technically demanding. For example: data on Henry's Law constant and Kow can be used among others to derive these descriptors. If, however, one finds that Henry's Law constant or Kow cannot be determined reliably for a given compound
then one can switch to other partition data (e.g. HPLC retention data) to determine the required descriptors. Furthermore, the consistency of the descriptors can be easily checked if more than the minimum number of partition data are available.

Obviously, an email does not give enough room for a comprehensive discussion of all this. If you are interested in further information please feel free to contact me.

Sincerely

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