Comment on "Visualising the equilibrium distribution and mobility of organic contaminants in soil using the chemical partitioning space [Wong and Wania, J. Environ. Monit., 2011, 13, 1569-1578]"

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In their article, Wong and Wania [1] employ the "chemical partitioning space, defined by the air-water partition coefficient (K_{AW}) and the soil organic carbon-water partition coefficient (K_{OC}) ... to visualize the equilibrium distribution of organic contaminants between the air-filled pores, the pore water and the solid phases of the bulk soil and the relative importance of the three transport processes [for] removing contaminants from soil (evaporation, leaching and particle erosion)." Wong and Wania [1] state that "[t]he partitioning properties of twenty neutral organic chemicals (i.e. herbicides, pharmaceuticals, polychlorinated biphenyls and volatile chemicals) were estimated using poly-parameter linear free energy relationships and superimposed onto these maps [which] allows instantaneous estimation of the equilibrium phase distribution and mobility of neutral organic chemicals in soil."

Five of the 20 compounds in ref. [1] have ionizable functional groups with the following environmentally relevant pK_a values: zearalenone: 7.62 (acidic) [2]; triclosan: ∼8.0 (acidic) [3]; fluorouracil: 7.93 (acidic) [4]; cyromazine: 5.22 (basic) [5]; and bromacil: 9.3 (acidic) [6]. As such, these five compounds are not "neutral" as Wong and Wania [1] incorrectly claim. Consequently, the K_{AW} and K_{OC} values for these compounds are highly pH dependent, rendering the modeling approach applied in ref. [1] subject to a fatal conceptual and practical flaw.

References

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