Use of a Simple Two-Media Degradation Model to Evelauate the Environmental Fate of a Semivolatile Transformation Product of Ibuprofen

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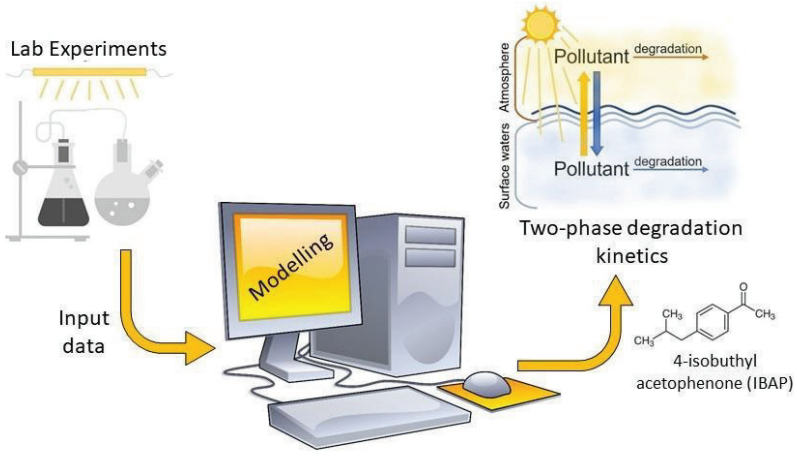
The partitioning of semivolatile contaminants between surface waters and the atmosphere is an important process that influences their fate and transport (Atkinson, 2000). In this work, we used a simple methodology that combines experimental data and modeling to investigate the degradation of 4-Isobutylacetophenone (IBAP) in a two-phase system (surface water and atmosphere). IBAP is a semivolatile toxic pollutant that was chosen as model contaminant. IBAP is a transformation product of the widely use non-steroidal, anti-inflammatory drug ibuprofen (IBP), and it may occur in expired IBP formulations or photochemically formed in sunlit surface waters, mostly upon IBP direct photolysis, and reaction with the triplet states of chromophoric dissolved organic matter (^{3}CDOM*) (Vione et al., 2018).
The atmospheric behavior of IBAP would mainly be characterized by its degradation with OH radicals, while degradation initiated by NO_3 radicals or direct photolysis would be negligible. Furthermore, the gas-phase reactivity of IBAP with OH is faster compared to the likely kinetics of volatilization from aqueous systems. Therefore, it would be extremely difficult to detect gas-phase IBAP. Nevertheless, up to 60% of IBAP occurring in a deep and DOC-rich water body might be degraded via volatilization, and subsequent reaction with gas-phase OH. In conclusion, the present study suggests that the gas-phase chemistry of the semivolatile organic compounds initially occurring in surface waters (like IBAP) is potentially very important in some environmental conditions.



Graphical description of the experimenatl and modelling approach used to evaluate the environmental fate of IBAP

References

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