

## A SIMPLE TWO-MEDIA DEGRADATION MODEL TO EVALUATE THE ENVIRONMENTAL FATE OF 4-ISOBUTYLACETOPHENONE, 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<sup>1</sup>. We proposed a simple methodology that combines experimental data and modelling to investigate the degradation of 4-Isobutylacetophenone (IBAP) in a two-phase system (surface water and atmosphere). IBAP is a semivolatile and toxic transformation product of the widely used drug ibuprofen (IBP), photochemically formed in sunlit surface waters.<sup>2</sup> The atmospheric behaviour of IBAP would mainly be characterized by its degradation with OH radicals (degradation by NO<sub>3</sub> 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.

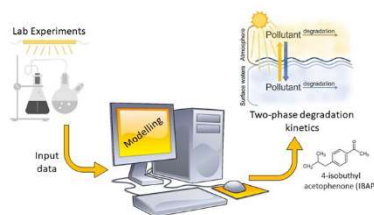


Figure 1: Description of the experimental/modelling approach used to evaluate the IBAP environmental fate

### References:

1. Atkinson, R., *Atmospheric Environment* 34 (2000) 2063-2101.
2. Vione, D. ... & Calza, P. *Chemosphere* 198 (2018) 473-481.

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