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Modelling emissions of perfluorinated chemicals to the Danube River Basin

The emissions of two perfluoroalkyl acids (PFAAs) into the Danube River Basin have been estimated in a test of four different hypotheses regarding the factors affecting those emissions. The results were used to simulate water concentrations for comparison with measured data. The researchers found that incorporating wastewater treatment information and wealth distribution alongside population data can improve the accuracy of emissions estimates.

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Source: Lindim, C., Cousins, I. & vanGils, J. (2015). Estimating emissions of PFOS and PFOA to the Danube River catchment and evaluating them using a catchment-scale chemical transport and fate model. *Environmental Pollution*, 207: 97-106. DOI: 10.1016/j.envpol.2015.08.050

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Perfluoroalkyl acids (PFAA) are highly persistent synthetic chemicals that have been identified in natural environments worldwide[1]. Perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA) are of greatest concern, as they are the most environmentally abundant and have been associated with wildlife and human health effects.

Due to their ability to reduce the surface tension of a liquid, increasing its spreading and wetting properties, PFOS and PFOA have been used in a wide range of industrial applications and consumer products, from semiconductors and fire-fighting foams to waterproof textiles, adhesives and paint.

The EU places restrictions on the use and import of PFOS, which is identified as a priority hazardous substance under the Environmental Quality Standard Directive[2] (daughter of the Water Framework Directive (WFD[3]) and listed by the Stockholm Convention on Persistent Organic Pollutants due to its persistence, bioaccumulative potential and toxicity. Similar restrictions on the production and use of PFOA are currently under discussion under REACH[4,5].

Despite efforts to limit use and production, these substances continue to contaminate surface waters in Europe. A 2008 study measured contaminant concentrations in 100 European rivers and found the prevalence of PFOS to be 94% and PFOA 97%. High concentrations were found in a number of large European rivers and concentrations of PFOS frequently exceeded the WFD environmental quality standard for inland surface waters (0.65 ng/l)[6]. No Europe-wide regulatory limit yet exists for PFOA in surface waters.

Emission estimates are important for developing new regulations, but previous attempts at estimating the emissions of PFAA have been hampered by the many different sources, and scarce data regarding the production, use and transformation of PFAA. Most have also focused solely on population as an emissions predictor.

In this study, which is part of the European Commission project SOLUTIONS[7], the authors set out to improve emissions estimates for PFOA and PFOS. They explored new approaches using the Danube River catchment — the second longest river in Europe — as a case study.

The researchers assessed the relevance of three parameters to the estimation of emissions: population, wastewater treatment, and wealth (based on gross domestic product (GDP) data). They obtained different emissions estimates using each of the three parameters individually and in combination, and then applied the STREAM-EU (Spatially and Temporally Resolved Exposure Assessment Model for European basins[8]) model to simulate concentrations of PFOA and PFOS in the Danube.

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Finally, to determine which of the emissions estimates was most accurate, the model predictions were compared to measured values obtained during the Joint Danube Survey 3, which was conducted in 2013 and sampled 68 locations along the Danube River for PFOS and PFOA.

The emissions estimates that resulted in simulated concentrations most different from the measured values were those made using population data alone, which suggests this approach is too simplistic. When population data were combined with other factors that influence emissions, such as wastewater treatment or GDP information, the accuracy of the emission predictions improved. The GDP information improved results markedly, which suggests that economic wealth has an effect on the consumption, use and disposal of products containing PFOS and PFOA. The most accurate estimates were obtained by considering the combined contributions of human population, wealth and wastewater treatment.

This study shows that human population alone cannot reliably explain the levels of PFOS and PFOA found in the Danube catchment waters. The multifaceted approach employed in the study is likely to be useful for estimating emissions from other pollutants.

Footnotes:

1. Lau, C., Anitole, K., Hodes, C., Lai, D., Pfahles-Hutchens, A. & Seed, J. (2007). Perfluoroalkyl Acids: A Review of Monitoring and Toxicological Findings. *Toxicological Sciences*, 99(2), pp.366-394.

2. Directives 2008/105/EC and 2013/39/EU: http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2008:348:0084:0097:en:PDF; http://eur-lex.europa.eu/LexUriServ/LexUriServ.do?uri=OJ:L:2013:226:0001:0017:EN:PDF

3. Water Framework Directive (2000/60/EC): http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32000L0060

4. http://www.hse.gov.uk/reach/

5. Regulation (EC) No 1907/2006: http://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:02006R1907-20150601

6. Germany and Norway propose a restriction on PFOA, its salts and PFOA related substances. http://echa.europa.eu/documents/10162/3b6926a2-64cb-4849-b9be-c226b56ae7fe

7. SOLUTIONS is supported by the European Commission under the Seventh Framework Programme. See: http://www.solutions-project.eu/

8. Lindim, C., J. van Gils, & I. T. Cousins (2016). A large-scale model for simulating the fate & transport of organic contaminants in river basins. *Chemosphere* 144: 803-810.