

# Supplementary Information: Modelling the Sources and Fate of Perfluorooctane Sulfonate (PFOS) in the River Rhine

Alexander G. Paul<sup>1</sup>, Martin Scheringer<sup>2</sup>, Konrad Hungerbühler<sup>2</sup>, Robert Loos<sup>3</sup>,  
Kevin C. Jones<sup>1</sup> and Andrew J. Sweetman<sup>1\*</sup>

<sup>1</sup>Centre for Chemicals Management, Lancaster Environment Centre, Lancaster University,  
Lancaster, LA1 4YQ, UK

<sup>2</sup>Institute for Chemical and Bioengineering, ETH Zürich, CH-8093 Zürich, Switzerland

<sup>3</sup>European Commission, Joint Research Centre, Institute for Environment and Sustainability,  
21020 Ispra, Italy

\*Corresponding Author: a.sweetman@lancaster.ac.uk

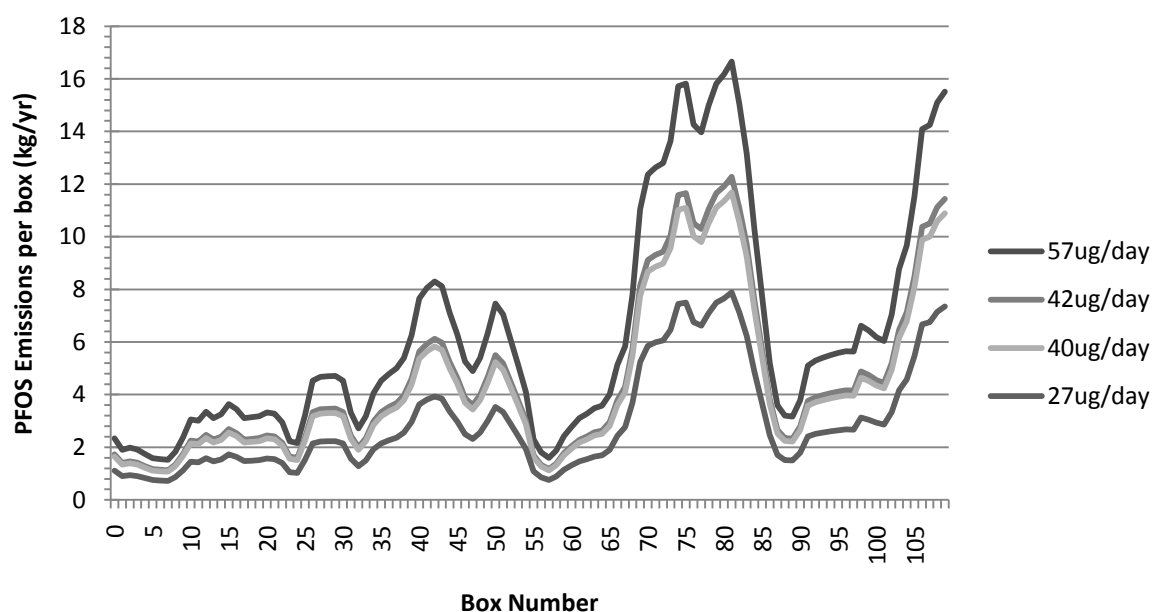


Figure S11: Estimated per capita PFOS emissions into each River Rhine box, calculated using ArcGIS using a 50km buffer zone.

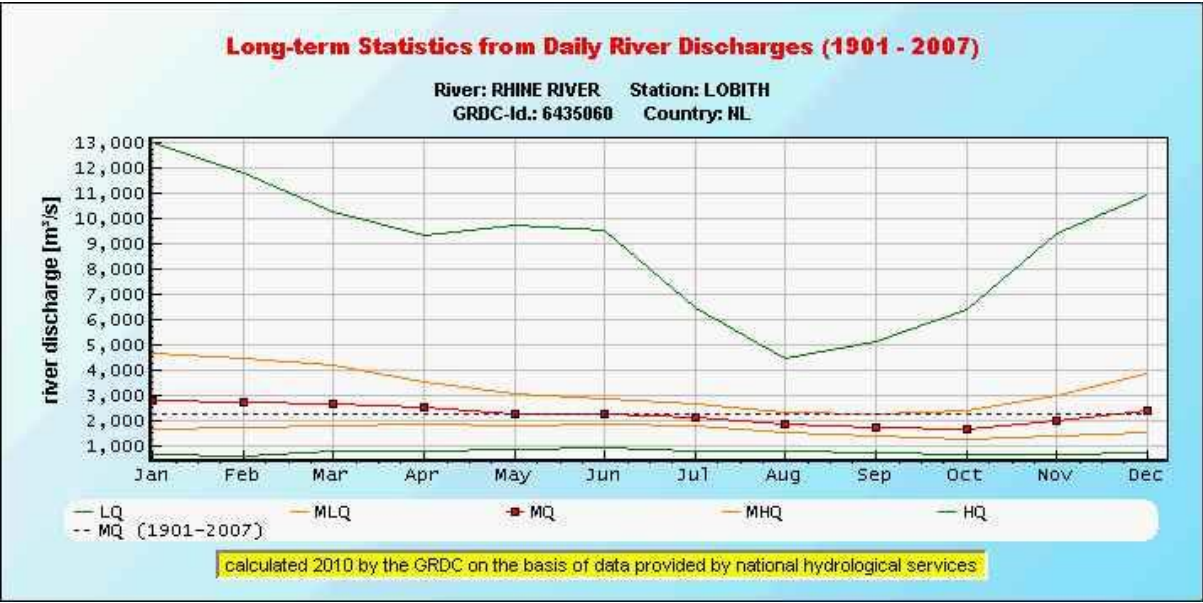


Figure SI2: Long-term statistics from Lobith (The Netherlands) gauging station. Data provided by the FRIEND project.

| Rhine Statistics        |          |
|-------------------------|----------|
| Mean                    | 2228.9   |
| Standard Error          | 45.1     |
| Median                  | 2224.5   |
| ±%                      | 0.21     |
| Standard Deviation      | 466.5    |
| Sample Variance         | 217582.8 |
| Kurtosis                | -0.59    |
| Skewness                | -0.12    |
| Range                   | 2042.2   |
| Minimum                 | 1098.9   |
| Maximum                 | 3141.1   |
| Sum                     | 238486.2 |
| Count                   | 107      |
| Confidence Level(95.0%) | 89.4     |

Table SI1: Flow variation calculations at Lobith (The Netherlands) gauging station over 107 years.

EUROFRIEND Project 3. Global Runoff Data Centre (GRDC), Federal Institute of Hydrology, Koblenz, Germany. <http://ne-friend.bafg.de/servlet/is/7413/>

**Table SI2: PFOS Partition Coefficient Comparison**

| Matrix            | Kd (L/kg) | Koc  | Log Koc | Notes / Reference                                |
|-------------------|-----------|------|---------|--------------------------------------------------|
| Clay              | 18.3      | 704  | 2.8     | Beech et al. <sup>1</sup>                        |
| Clay Loam         | 9.72      | 374  | 2.6     | Beech et al. <sup>1</sup>                        |
| Sandy Loam        | 35.3      | 1260 | 3.1     | Beech et al. <sup>1</sup>                        |
| River Sediment    | 7.42      | 571  | 2.8     | Beech et al. <sup>1</sup>                        |
| Domestic Sludge   | 120       | n/a  | n/a     | Beech et al. <sup>1</sup>                        |
| Sediments         |           |      | 2.68    | Higgins & Luthy, Regression Log Koc <sup>2</sup> |
| Sediments         |           |      | 2.57    | Higgins & Luthy, Log normal average <sup>2</sup> |
| Rhine Sed Field   | 4.3       |      |         | PERFORCE <sup>3</sup>                            |
| Rhine Sed Field   | 11        |      |         | PERFORCE <sup>3</sup>                            |
| Rhine Sed Lab     | 3         |      |         | PERFORCE <sup>3</sup>                            |
| Rhine Sed Lab     | 10        |      |         | PERFORCE <sup>3</sup>                            |
| Scheldt Sed Field | 5.2       |      |         | PERFORCE <sup>3</sup>                            |
| Scheldt Sed Lab   | 8         |      |         | PERFORCE <sup>3</sup>                            |
| Scheldt Sed Lab   | 97        |      |         | PERFORCE <sup>3</sup>                            |
| North Sea Sed.    | 2.1       |      |         | PERFORCE <sup>3</sup>                            |

**Table SI3: Fraction of Organic Carbon in Sediments (f<sub>oc</sub>%)**

| Minimum | Maximum | Region / River               | Reference                  |
|---------|---------|------------------------------|----------------------------|
| 0.02    | 4.15    | Rhine, Scheldt and North Sea | PERFORCE <sup>3</sup>      |
| 0.08    | 0.8     | Roter Main river, Germany    | Becker et al. <sup>4</sup> |
| 0.56    | 9.66    | United States                | Higgins & Luthy            |
| 1.6     | 4.8     | River Rhine                  | Möller et al. <sup>5</sup> |

**Table SI4: Sensitivity analysis of the model.**

| Parameter            | Explanation                                   | Unit                | Original Value | Range ( $\pm 10\%$ ) | Change in Concentration L1 (%) |
|----------------------|-----------------------------------------------|---------------------|----------------|----------------------|--------------------------------|
| $U$                  | Water flow velocity                           | m/s                 | 1              | 0.9 - 1.1            | $+10 - -10$                    |
| SPM                  | Concentration of suspended particulate matter | kg/m <sup>3</sup>   | 0.01           | 0.009 - 0.011        | 0                              |
| $\rho_{\text{sed}}$  | Sediment density                              | kg/m <sup>3</sup>   | 2500           | 2250 - 2750          | 0                              |
| $\phi$               | Porosity of sediment                          | -                   | 0.9            | 0.81 - 0.99          | 0                              |
| $u_{\text{sed}}$     | Settling velocity of SPM                      | m/s                 | 5.79E-06       | 5.21E-06 - 6.37E-06  | 0                              |
| $\mu_{\text{resup}}$ | Resuspension rate                             | kg/m <sup>2</sup> d | 1.00E-04       | 9.00E-05 - 1.10E-04  | 0                              |

Note: Concentration of PFOS in the moving water layer (L1) shows limited sensitivity to changes in the model parameters. The majority of the model parameters relate to sedimentation factors and have little or no influence on the moving water layer.

## References:

1. S. Beach, J. Newsted, K. Coady and J. Giesy, *Rev. Environ. Contam. Toxicol.*, 2006, 133-174.
2. C. P. Higgins and R. G. Luthy, *Environ. Sci. Technol.*, 2006, **40**, 7251-7256.
3. P. de Voogt, U. Berger, W. de Coen, W. de Wolf, E. Heimstad, M. S. McLachlan, S. P. J. van Leeuwen and A. van Roon, *Perfluorinated Organic Compounds in the European Environment*, Institute for Biodiversity and Ecosystem Dynamics, University of Amsterdam, 2006.
4. A. M. Becker, S. Gerstmann and H. Frank, *Environ. Poll.*, 2008, **156**, 818-820.
5. A. Möller, L. Ahrens, R. Surm, J. Westerveld, F. van der Wielen, R. Ebinghaus and P. de Voogt, *Environmental Pollution*, **158**, 3243-3250.