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Modelling the fate of per- and polyfluoroalkyl substances in the North- and Baltic Sea

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Per- and polyfluoroalkyl substances (PFASs) present themselves as a large self-imposed risk to human health and the environment as a whole. This risk is amplified by the high persistence and long-range transport in oceans. Therefore, this study considers the marine transport of the most widely used PFAS: Perfluorooctanoic acid (PFOA) in the North- and Baltic-Sea, to determine and quantify the relationship between the physico-chemical properties and the potential for long range transport, temporary storage and permanent degradation respectively.

For this purpose, an extensive model chain was established. It contains a newly developed emission model for PFOA approximating global emissions centred around the year 2001 by combining specific point sources (e.g., PTFE production sites) and diffuse emissions by population, from which total PFOA- loads of European rivers are obtained by a hydrological-discharge-model (HDM). This discharge as well as approximations of the air sea exchange based on observed atmospheric concentrations form the input for the Hamburg Shelf Ocean Model (HAMSOM) which is combined with the ecosystem-model ECOSMO. These models are complemented by several newly implemented, locally resolved mechanisms, including photolytic and bio-chemical degradation, adhesion to dissolved and particulate organic matter as well as sedimentation.

To relate the properties of PFOA to its environmental fate, this novel system has been used to consider the PFOA budgets of the major input and output pathways and the exchange between the North and Baltic Sea. In multiple simulations these uncertain physico-chemical properties, as well as boundary conditions for input and output were varied and the simulation was run over multiple years until a quasi-equilibria state was reached.

The simulated budgets show that degradation plays in general a minor role for the North- and Baltic-Sea while the ratio of PFOA stored in sediments compared to the amount lost to the Arctic- and Atlantic Ocean strongly depends on the chosen partitioning coefficients. Furthermore, the comparison of simulated concentrations to actual marine measurements allowed to narrow the plausible range of these uncertain physico-chemical properties, based on marine conditions in contrast to lab measurements.

Understanding the sensitivity of the transport and long-term fate of PFOA depending on its

properties may point to simpler approaches to assess the fate of other PFASs where, due to their limited use, less data is available.