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Prediction of PFAS interfacial partitioning under a wide range of environmentally relevant conditions

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Per- and polyfluoroalkyl substances (PFAS) are emerging contaminants that have been used extensively as firefighting agents and in a wide range of commercial applications around the world. As such PFAS are pervasive in the environment (i.e., groundwater, surface water, sediment, soils and atmospheric dust), even in very remote locations with no local PFAS source (e.g., The Arctic). As PFAS are surfactants, they readily partition to interfaces - a process that governs their environmental fate. For example, some PFAS readily sorb to soil and sediment, partition to the air/water interface in the vadose zone or partition to atmospheric dust. In order to predict their environmental fate the development of predictive PFAS interfacial partitioning models is essential. This study will present a predictive model, developed from first principles, to predict a wide range of PFAS interfacial partitioning under a range of environmental relevant geochemical conditions (i.e., as a function of ionic strength and salt valency). The impact of PFAS mixtures will be discussed as will prediction of interfacial partitioning of novel PFAS, in which no data exist. Finally, the practical utility of the model for a range of scenarios will be discussed.