Environmental Fate Prediction via Atom-Based Computer Simulations

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Project Introduction

The objective of this project was to calculate physical properties of 1-perfluorooctanol (PFO), a synthetic fluorinated surfactant, to determine the toxicity of the compound.

State of Knowledge

PFO is a surfactant that is used in the production semiconductors, as adhesives, repellants and in aqueous film forming foams [1]. This surfactant, along with other fluorinated compounds, has a high strength carbon-fluorine bond that gives it unique physical properties. Unfortunately, PFO and like fluorinated compounds are known to be carcinogenic and unable to biodegrade in the environment [2]. With little experimental data, computer simulations are used to calculate thermodynamic properties which will determine the behavior of these surfactants. Understanding these properties will hopefully lead to the development of abatement technologies and replacement materials that will be more sustainable.

Relation Sustainable Mg.

Fluorinated surfactants are used in semiconductor manufacturing during III-V processing, and in aqueous film forming foams for fire fighting purposes. This research will assist in the environmental analysis of the manufacturing of semiconductors, and hopefully predict the fate of these harmful chemicals.

Table 1 Comparison of hydration free energy and air-water partitioning coefficients in 1-perfluorooctanol and 1-octanol

	ΔG (kcal/mol)	K
PFO	-0.4397	2.1031
1-Octanol	3.7933	0.0016

Approach

Molecular dynamics simulations were used to calculate the free energy of hydration (ΔG), air-water partitioning coefficient (K), and radial distribution function (g(r)), for PFO and 1-octanol in solutions with varying concentrations of water. These calculations provide insight into the role fluorination plays in the environmental fate of fluorinated surfactants.

Results

PFO exhibits a low partition coefficient compared to 1-octanol, shown in Table 1. Plots in Figure 1 show a comparison between the radial distribution of oxygen atoms within the solutions of varying concentrations between PFO and 1-octanol. Figure 2 gives a visual insight on the behavior of the compounds.

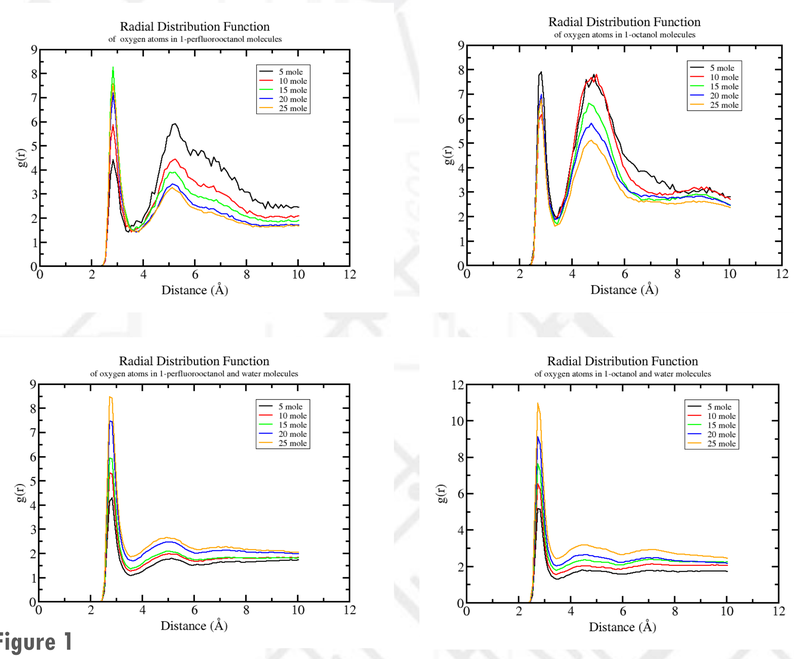

Figure 1
Structural analysis and comparison of radial distribution function between oxygen atoms in PFO (left-top) and 1-octanol (right-top) and oxygen atoms found in PFO and water (left-bottom) and 1-octanol and water (right-bottom).

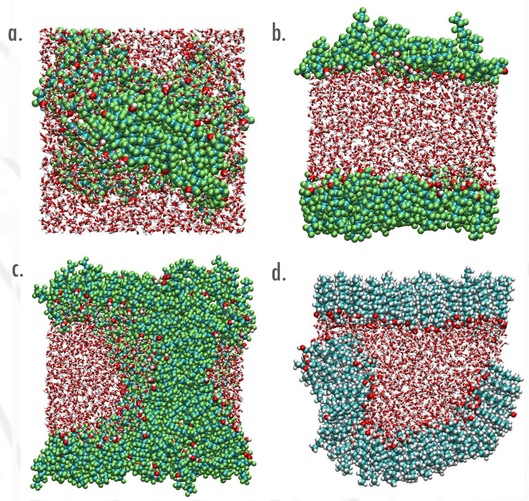

Figure 2
a. PFO at 5 mole percent in water with micelle behavior after equilibration.
b. PFO at 5 mole percent in water with layers forming in air-water simulation.
c. PFO at 15 mole percent in water with formation of reverse micelles.
d. 1-Octanol at 15 mole percent in water exhibiting formation of bi-layers.

Conclusions

In regards to the physical properties observed in PFO, we see that this surfactant will accumulate in aqueous regions, hence the low K value and distribution amongst the oxygen atoms. Future work will include the analysis of the effects PFO has on surface tension.

Acknowledgements

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About Me

Thalia Quinn is a fourth year student studying chemical engineering at the New Mexico Institute of Mining and Technology. Most of her research includes molecular dynamics such as this project. She plans to graduate in May 2017, and is still contemplating graduate school for a PhD in chemical engineering.

References

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