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How do we protect the environment for the future: the rising population creating an ever-growing need

Surfactants are chemicals that increase solubility and dispersion of hydrocarbons and oils and they are widely used in detergents and other cleaning products. These include well-known brands such as Dettol, Persil and Fairy Liquid. They are necessary to remove stubborn stains like dirt that otherwise would require substantial amounts of water. After use, they are discharged into sewage systems (domestic or industrial), ending up dispersed in the environment polluting the water, the soil and other sediments.

The toxic effects of surfactants on various aquatic organisms are published in a variety of well-known medical journals, such as PubMed. The discharge of wastewater polluted with massive quantities of surfactants could have serious effects on the ecosystem. Currently most surfactants are greatly reduced by secondary wastewater treatment. However, the global surfactant market is predicted to be worth $40 bn by 2021, in response to population growth. A new production methodology for non-toxic and more biodegradable surfactants is required to decrease their final impact on future global water resources.

There has already much research into the design of environmentally-friendly surfactants through computational modelling and experimental validation by both synthesis and toxicity analysis. This involves collaborative work between leading academics from various Universities. The key steps involved in their work rotates around using customising computational tools to design and evaluate surfactants of different structures. This permits the creation of virtual chemicals and by simulating performance conditions, allows the evaluation ‘in silico’ (in the computer).

An average computer simulation requires no physical maintenance throughout, the user simply submits the file to the organisations ‘high performance computing computer’. This usually consists of multiple computers working in series. The most promising simulated surfactants can be synthesised in the lab, and critical toxic concentration and biodegradability can be evaluated at various conditions. This can include temperature, surfactant concentration and pressure. This avoids the issues generated with having to test literally thousands of possible surfactant chemicals.

Current research efforts must aim to capitalise on a recent proposal for the design methodology, created by Herdes et al, which incorporates experimental and computational elements. In particular experimental evaluation from one research department can feed back to a team working on the novel molecular simulation methodology for the design of surfactants. The main result of this work should be a database relating surfactant chemical building blocks, structure and toxicity. The main challenge of this project would be linking the computational and experimental components. This is because a computer simulation code assumes various environmental factors that can be found in some laboratories are

negligible. Indeed, any discrepancy between the two is usually due to shortcomings in the simulation code.

Support can be obtained through various routes; the UK research council (RCUK) offers studentships, which cover tuition fees and provide a living allowance to PhD researchers. It is possible that companies interested in this research can partner with Universities as industrial collaborators. In this case companies like Unilever or P&G may be interested. Many University departments have access to High Performance Computers which can provide the CPU needed to carry out detailed simulations. It is not necessary for researchers to have prior experience in computational modelling, as they can be mentored by knowledgeable University professors. What is really required for the researchers is to have an enthusiastic attitude to new scientific matters, as well as being able to explain information in a clear, concise manner.

In conclusion, whilst the current wastewater infrastructure for many countries can treat the waste surfactants, there are still those that cannot. In any case, the future will bring with it a higher human impact on our natural environment. It is the responsibility of scientists across the UK to investigate and characterise new chemicals with which we can make the products we use everyday to live in dignity. There is a clear benefit for both parties involved; the methodology listed above is the most productive to filter out the chemicals that are unsuitable. The use of computational simulation means that less time is spent requesting lab sessions in busy research facilities. Most people can be taught the basic coding language in a matter of weeks, and will learn transferrable skills that are highly valuable in both industry and academia.