J. Pharm. Pharmacol. 1998, 50 (Supplement): 57

SURFISS—an interactive program for surfactant interfacial structure simulation

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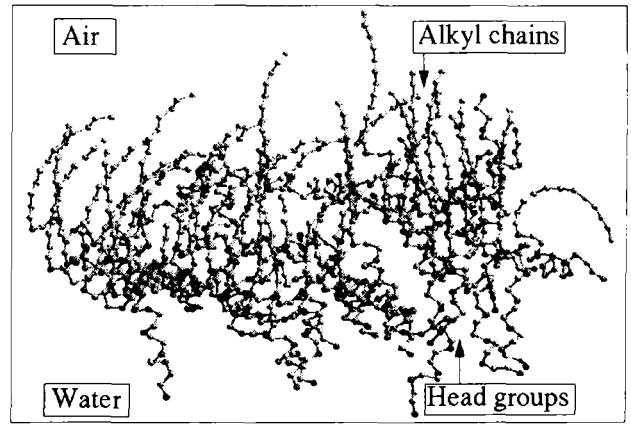
In the rational design and exploitation of surfactant-based drug delivery systems, crude indicators like the critical packing parameter and surfactant HLB value have limited utility (Lawrence 1994). Our relatively poor understanding of the relationship between surfactant covalent structure and aggregate structure therefore demands further fundamental and systematic investigations of the behaviour of surfactants at interfaces. Over recent years such information has been most elegantly furnished by neutron reflectivity experiments (Thomas & Penfold 1996), yielding highly detailed information on the molecular architecture of surfactant layers, able to distinguish, for example, the widths and relative separations of the interfacial distributions of the surfactant hydrophobe, head group and associated solvent. Sadly, the volume fraction profiles produced at the culmination of such studies give no clear picture of the arrangements of the surfactant molecules nor their conformation. It would thus be advantageous to have the means to produce molecular models consistent with these volume fraction profiles so that the neutron data can be extended to give information at an atomistic level.

A Fortran 90 program, SURFISS, has been developed for this purpose. The user supplies details of the surfactant(s) of interest, and the reflectivity-derived surfactant interfacial surface area, number densities (n_i), Gaussian distribution widths (σ_i) and distribution separations (δ_{ij}) for the surfactant components (i, j). The program then generates atomic coordinates for the molecule(s) of interest and produces a molecular model in which copies of the molecule (typically 100) are arranged on a square lattice. The experimentally-derived volume fraction profiles are then produced using the input values of σ_i, n_i, and δ_{ij} and these are compared with the corresponding profiles calculated from the molecular model. The conformations and positions of the molecules in the model are subsequently modified in an iterative manner until the calculated and observed profiles are matched.

Simulations have been carried out for the monolayers formed at the air/water interface by monododecyl hexaethylene glycol ($C_{12}E_6$) using neutron reflectivity data taken from Lu et al (1993). Fig 1 shows the molecular model obtained when the calculated and observed volume fraction profiles are identical. Inspection of the model reveals that the alkyl chains are tilted away from the surface normal with the head groups very disordered, and the C_{12} and E_6 chains markedly intermixed. The model is consistent with findings from more detailed reflectivity experiments of Lu et al (1993), and it is concluded that the SURFISS program will provide a valuable and robust utility to help further our knowledge of surfactant interfacial behaviour.

Figure 1. SURFISS-generated molecular model of a $C_{12}E_6$ monolayer.



Lawrence, M. J. (1994) Eur. J. Metabolism and Pharmacokin. 3: 257-269

Lu, J, R. , Li, Z. X., Thomas, R. K., Staples, E. J., Tucker, I., Penfold, J. (1993) J. Phys. Chem. 97: 8012-8020

Thomas, R. K., Penfold, J. (1996) Current Opinion in Colloid Interf. Sci. 1: 23-33