Molecular Characteristics of the Surfactants Considered

Ionic surfactants are described using the following molecular characteristics:

Ionic Surfactant	n_t	a_h [Å ^{2}]	l_h [Å]	d_z [Å]	z_A	z_C	r_C [Å]
C_iTAB	$i-1$	32.0	5.76	2.5	+1	-1	2.10
$NaC_{10}S$	9	25.0	6.27	3.7	-1	+1	2.18

where n_t is the number of carbon atoms in the hydrophobic portion of the tail, a_h is the cross-sectional area of the head, l_h is the length of the ionic surfactant head, d_z is the distance from the tail (as measured from the first hydrophobic carbon atom) to the location of the charge in the head, z_A is the valence of the head, z_C is the valence of the counterion, and r_C is the hydrated radius of the counterion.

Two molecular characteristics are required to describe nonionic surfactants, n_t and a_h. For C_iE_j surfactants, n_t is $(i-1)$ and a_h is estimated using the following temperature-dependent equation:

$$a_h(j,T) = a_{h0}\left[1 - H\left(T - T_0\right)\right]\left(\frac{j}{6}\right)^z \tag{1}$$

where j denotes the number of ethylene oxide units, T is the temperature in K, T_0 is 273 K, $a_{h0} = 49.4$ Å^2 denotes the cross-sectional area of a hexa(ethylene oxide) head ($j = 6$) at T_0, $H = 0.0057$ K^{-1} models the temperature dependence of the head area due to hydration effects, and $z = 0.8$ models the scaling of the head cross-sectional area with j.