INTERFACIAL CHEMISTRY CH-341

Week 1 - Solutions

1.1 The total interaction energy of two molecules (or atoms) is described by the Lennard-Jones potential:

$$V(r) = \frac{C_1}{r^{12}} - \frac{C_2}{r^6} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

- What is the relation between parameters C_1, C_2 and parameters ε, σ ?
  Calculate the minimum potential energy between two molecules (or atoms) and the distance that corresponds to this minimum.
- For argon the parameters are as following: $\sigma = 3.4 \cdot 10^{-10}$ m and $\varepsilon = 1.65 \cdot 10^{-21}$ J. Calculate the value of the potential energy at the minimum and the corresponding distance between argon atoms.

Solution:

The relation between parameters is $C_1 = 4\varepsilon\sigma^{12}$ and $C_2 = 4\varepsilon\sigma^6$

In the minimum of the potential energy, the derivative of the potential is equal to

$$\frac{dV}{dr} = 0 = -12\frac{C_1}{r^{13}} + 6\frac{C_2}{r^7}$$

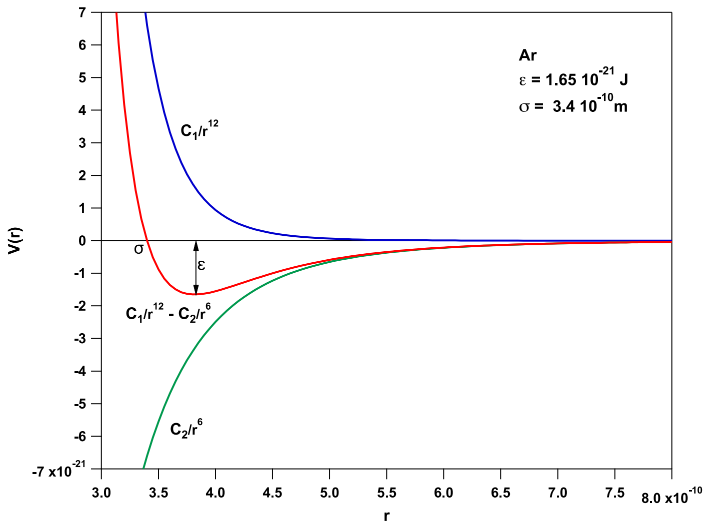
$$r_{min}^6 = 2\frac{C_1}{C_2} \implies r_{min} = 2^{1/6}\sigma$$

$$V = -\frac{C_2^2}{4C_1} = -\varepsilon$$

For argon, the corresponding distance and potential energy are:

$$r_{min} = 3.82 \cdot 10^{-10}\ \mathrm{m}$$

$$V_{min} = -1.65 \cdot 10^{-21}\ \mathrm{J}.$$



1.2 Calculate the surface tension work done when spherical droplets with an average radius of 1.0×10^{-3} mm agglomerate to form a sphere of 1 litre of water at 20°C. The surface tension of water is 72.8×10^{-3} J/m^2 at 20°C.

Solution:

Volume of the sphere: $V_s = \frac{4}{3}\pi r^3$

Total volume of the liquid: V

Number of the spheres: $N = \frac{V}{V_s} = \frac{3V}{4\pi r^3}$

Surface of the sphere: $S_s = 4\pi r^2$

Total surface of N spheres: $S_{tot} = S_s \cdot N = \frac{3V}{4\pi r^3} 4\pi r^2 = \frac{3V}{r}$

Total surface energy before the aggregation is:

$$E_{initial} = \gamma S_{tot} = \frac{3V}{r}\gamma = \frac{3 \cdot 10^{-3}\ m^3}{1 \cdot 10^{-6}\ m} 72.8 \cdot 10^{-3} J \cdot m^{-2} = 218.4\ \mathrm{J}$$

After the aggregation, one sphere with a radius R is formed:

$$V_s = \frac{4}{3}\pi R^3 \Longrightarrow R = \left(\frac{3V_s}{4\pi}\right)^{\frac{1}{3}} \qquad S_s = 4\pi R^2 = (4\pi)^{1/3}(3V)^{2/3}$$

The final surface energy is then:

$$E_{final} = \gamma S_s = \gamma(4\pi)^{1/3}(3V)^{2/3} = 3.5 \cdot 10^{-3}\ \mathrm{J}$$

Therefore, the surface work is $E_{surface} = E_{final} - E_{initial} = -218.4\ \mathrm{J}$

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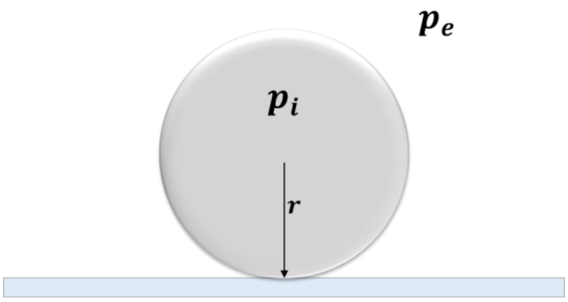
1.3 Droplets of mercury are deposited on a glass plate. What is the pressure difference between the inner and the outer part of a droplet (supposed to be spherical) if its diameter is 1mm or 0.1 mm? ($\gamma_{Hg} = 484\ \mathrm{mNm^{-1}}$ at $T = 20°\mathrm{C}$). What fraction of an atmosphere does this difference in pressure represent?

Solution :

The difference between inner and outer pressure of the droplet is given by Young equation:

$$\Delta p = \frac{2\gamma}{r}$$



The pressure difference:

$\Delta p = p_i - p_e$

Surface work needed for one droplet:

$dw = \gamma ds = \gamma d(4\pi r^2) = 8\pi\gamma r dr$

Force exerted by the presssure difference:

$dw' = -\Delta p dV = -\Delta p 4\pi r^2 dr$

The equilibrium condition between the force induced by pressure and the surface work:

$$dw + dw' = 0$$

By combining this condition and the equations above, we can derive Young equation:

$$\Delta p = \frac{2\gamma}{r}$$

Calculate the difference between inner and outer pressure:

$r_1 = 0.5mm$, $r_2 = 0.05mm$, $\gamma_{Hg} = 0.484\frac{N}{m}$ $a\ T = 20°C$, $1atm = 1.01325 \cdot 10^5 Pa$

$$\Delta p_1 = \frac{2\gamma}{r_1} = \frac{2 * 0.484\ \frac{N}{m}}{5 \cdot 10^{-4}\ m} = 1936 \left[\frac{N}{m^2} = Pa\right]$$

$$\Delta p_2 = \frac{2\gamma}{r_2} = \frac{2 * 0.484\frac{N}{m}}{5 \cdot 10^{-5}\ m} = 19360 \left[\frac{N}{m^2} = Pa\right]$$

We can compare these pressures with the atmospheric pressure:

$$F_1 = \frac{\Delta p_1}{1atm} = \frac{1936\ Pa}{1.01325 \cdot 10^5 Pa} = 1.91\ \%$$

$$F_2 = \frac{\Delta p_2}{1atm} = \frac{19360 Pa}{1.01325 \cdot 10^5 Pa} = 19.1\%$$

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