

Assignment

Thursday, 19 November 2020 16:29

$$1a) \Delta F_{mix} = k_B T \left[\chi \phi (1-\phi) + \frac{\phi}{N_x} \ln \phi + \frac{(1-\phi)}{N_y} \ln (1-\phi) \right]$$

$$\chi = A + \frac{B}{T} \quad \phi = \text{volume fraction of particle } x$$

From data sheet:

$$N_x = 200$$

$$N_y = 150$$

$$A = 0.003$$

$$B = 2.8$$

$$T = 280$$

$$\phi_c = \frac{\sqrt{N_y}}{\sqrt{N_x} + \sqrt{N_y}} = \frac{\sqrt{200}}{\sqrt{150} + \sqrt{200}} = 0.5358983849 = 0.536$$

$$\begin{aligned} \chi_c &= \frac{1}{2} \left[\frac{1}{N_x \phi_c} + \frac{1}{N_y (1-\phi_c)} \right] \\ &= \frac{1}{2} \left[\frac{1}{200 \cdot 0.535...} + \frac{1}{150 (1-0.535...)} \right] \\ &= 0.01184739864 \\ &= 0.0118 \end{aligned}$$

$$\text{using } \chi = A + \frac{B}{T}$$

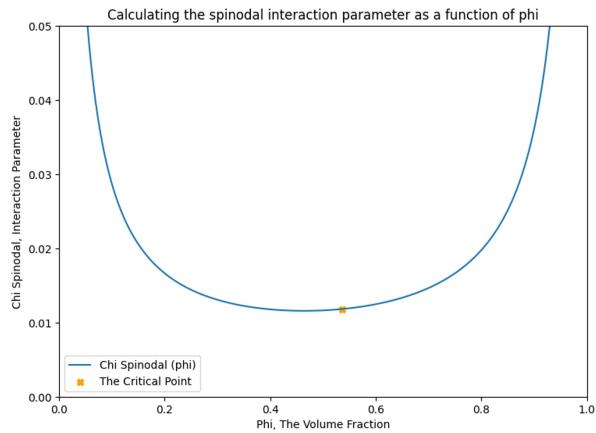
$$\therefore \frac{B}{x-a} = T$$

$$\Rightarrow T_c = \frac{2.8}{0.0118... - 0.003} = 316.4772059 \text{ K} = 316.48 \text{ K}$$

$$B) \chi = f(\phi)$$

$$\begin{aligned} \chi_{\text{spinodal}} &= \frac{1}{2} \left[\frac{1}{N_x \phi} + \frac{1}{N_y (1-\phi)} \right] \\ &= \frac{1}{2} \left[\frac{1}{200\phi} + \frac{1}{150(1-\phi)} \right] \end{aligned}$$

χ_{spinodal} for ϕ between 0 and 1:



C) Plotting free energy curve as a function of ϕ

$$\Delta F_{\text{mix}} = k_B T \left[\frac{\phi \ln \phi}{N_x} + \frac{1-\phi \ln(1-\phi)}{N_y} + \chi \phi (1-\phi) \right]$$

$$k_B = 1.38 \times 10^{-23}$$

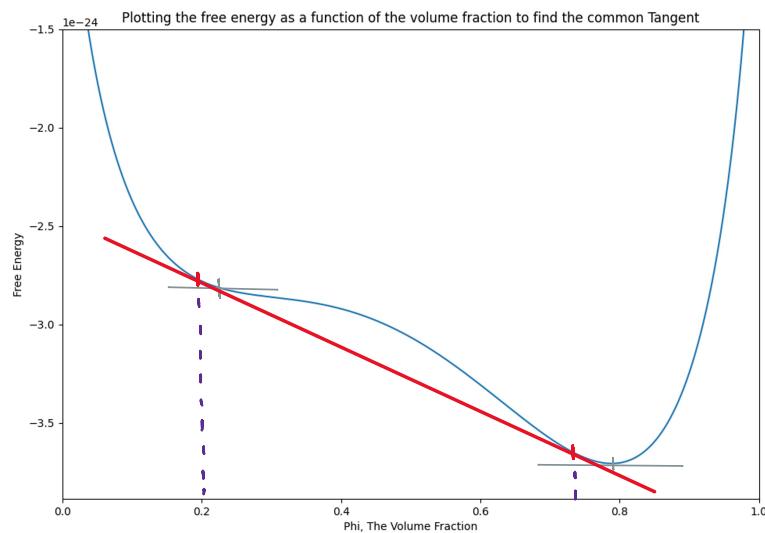
$$T = 280$$

$$N_x = 200$$

$$N_y = 150$$

$$\chi = A + \frac{B}{T} = 0.003 + \frac{2.8}{280} = 0.013$$

$$\Rightarrow \Delta F_{\text{mix}}(\phi) = 1.38 \times 10^{-23} \cdot 280 \left[\frac{\phi \ln \phi}{200} + \frac{1-\phi \ln(1-\phi)}{150} + 0.013 \phi (1-\phi) \right]$$



Marking points where gradient = 0

Finding common tangent

This gives us our two equilibrium points at $\phi = 0.2$ and $\phi = 0.75$

D) Spinodal line: $\chi_s = \frac{1}{2} \left[\frac{1}{N_x \phi} + \frac{1}{N_y (1-\phi)} \right]$ crit point $\frac{\partial \chi}{\partial \phi} = 0$

Binodal line: $\chi_B = \frac{1}{2\phi-1} \left[\frac{\ln \phi}{N_x} - \frac{\ln(1-\phi)}{N_y} \right] = \frac{\ln(\phi/(1-\phi))}{(2\phi-1)N}$

$$\chi = A + \frac{B}{T} \Rightarrow \frac{B}{\chi - A} = T$$

$$T_B = \frac{B}{\chi_{B-A}} = \frac{2.8}{\left(\frac{\ln(\phi/(1-\phi))}{(2\phi-1)N} - 0.003 \right)}$$

$$T_S = \frac{B}{\chi_{S-A}} = \frac{2.8}{\left(\frac{1}{2} \left[\frac{1}{200\phi} + \frac{1}{150(1-\phi)} \right] \right) - 0.003}$$

$$\Delta F_{\text{mixing}} = kT \left[\frac{\chi\phi(1-\phi)}{N_x} + \frac{\phi \ln \phi}{N_x} + \frac{(1-\phi) \ln(1-\phi)}{N_y} \right]$$

Co-existence / binodal curve, $\frac{dF}{d\phi} = 0$

$$\frac{dF}{d\phi} = kT \left[\chi(1-2\phi) + \frac{1+\ln\phi}{N_x} + \frac{1}{(1-\phi)N_y} (\phi-1) - \frac{\ln(1-\phi)}{N_y} \right] = 0$$

$$= kT \left[\chi(1-2\phi) + \frac{1+\ln\phi}{N_x} + \frac{1}{N_y} \left(\frac{\phi}{1-\phi} - \frac{1}{1-\phi} - \ln(1-\phi) \right) \right] = 0$$

$$= \chi(1-2\phi) + \frac{1+\ln\phi}{N_x} + \frac{1}{N_y} \left[\frac{\phi-1}{1-\phi} - \ln(1-\phi) \right] = 0$$

$$\Rightarrow \chi_{\text{Bin}} = - \frac{1}{1-2\phi} \left[\frac{1+\ln\phi}{N_x} + \frac{1}{N_y} \left(\frac{\phi-1}{1-\phi} - \ln(1-\phi) \right) \right]$$

$$T_{\text{Binodal}} = \frac{2.8}{\left(- \frac{1}{1-2\phi} \left[\frac{1+\ln\phi}{N_x} + \frac{1}{N_y} \left(\frac{\phi-1}{1-\phi} - \ln(1-\phi) \right) \right] \right) - 0.003}$$

$$N_x = 200, N_y = 150$$

$$\Rightarrow T_{\text{Binodal}} = \frac{2.8}{\left(- \frac{1}{1-2\phi} \left[\frac{1+\ln\phi}{200} + \frac{1}{150} \left(\frac{\phi-1}{1-\phi} - \ln(1-\phi) \right) \right] \right) - 0.003}$$

2a) Enzyme is usually a protein and thus has a diffusion constant, $D \sim 10^{-12} \text{ m}^2/\text{s}$

2B) estimate 10^3 viruses/min
droplets last ~ 30 mins

$$\text{size of lounge} \approx 3\text{m} \cdot 3\text{m} \cdot 2.5\text{m} \\ = 22.5\text{m}^3$$

after $\frac{1}{2}$ hour we reach
max virus number at 30 mins
 $\geq 10^3 \cdot 30\text{mins} = 30000$ Viruses
in air

$$30000 / 22.5 = 1333.3 \text{ viruses/m}^3$$

human breathes $\sim 1\text{m}^3$ of
air / hour

\Rightarrow human breathes in ~ 1300 virus droplets
per hour

Action 1: Wear a mask

- According to CDC multi-layer cloth masks can block 50-70% of fine droplets from leaving the source i.e. the infected person and limit forward spread of other droplets
- According to same source multi-layer cloth masks can also filter up to 50% of fine particles for filtration personal protection

<https://www.cdc.gov/coronavirus/2019-ncov/more/masking-science-sars-cov2.html#:~:text=Human%20Studies%20of%20Masking%20and%2050%20%20%20Transmission&text=In%20a%20study%20of%20124,within%20the%20households%20by%2079%25.>

if

- The transmitter wore a face mask
 - up to 70% of viruses would not enter air
 - thus only 9000 in room and only 400 viruses per hour
- non-infected member wore mask

- thus only 4000 in room and only 400 viruses per hour
- non-injected member wore mask
 - up to 50% would not be breathed in
 - $1300 \cdot 0.5 = 650$ viruses/hour
- both wore mask
 - up to 70% don't enter air
 - up to 50% not breathed in
 - in best case scenario up to 85% not breathed in
 - $1300 \cdot 0.15 \sim 200$ viruses/hour

Action 2: ventilation

- according to UK Gov ventilation either through opening a window or through non-recirculated AC can reduce 'risk of infection' by 70%.
- The reasoning for this is that fresh air dilutes the virus particles in the room

<https://www.gov.uk/government/news/new-film-shows-importance-of-ventilation-to-reduce-spread-of-covid-19>

Applying this to our estimate of 30000 particles in room:

$$0.3 \cdot 30000 = 9000 \text{ virus particles in room}$$

$$9000 / 22.5 \text{ m}^3 = 400 \text{ viruses/m}^3$$

~ 400 viruses breathed in hour

$$3a) D_{O_2} \sim 10^{-9} \text{ m}^2/\text{s}$$

$$10^{-10} \text{ m}^2/\text{s} < D_{O_2} < 10^{-8} \text{ m}^2/\text{s}$$

$$d(t) = (D_{O_2} \cdot t)^{1/2} \text{ m}$$

Bi) Dataset d1 is consistent with diffusion

ii)

rearranging our equation for diffusion constant

$$D_{O_2} = \frac{d^2}{t} \text{ m}^2/\text{s}$$

$$\bar{D}_{O_2} = \frac{1}{n} \sum D_{O_2,t} \quad \text{mean}$$

$$\sigma = \sqrt{\frac{\sum (D_{O_2,t} - \bar{D}_{O_2})^2}{n}} \quad \text{Standard deviation}$$

Using the value $D_{O_2} = 1 \times 10^{-9}$ for the following

Dataset 1 gives us:

$$D_{02,1} = 0.9 \times 10^{-9} \pm 0.3$$

Dataset 2 gives us:

$$D_{02,2} = 2 \times 10^{-9} \pm 1$$

This allows us to say through a basic analysis that dataset 1 provides a more accurate prediction of D_{02} , this is because its uncertainty is an order smaller giving us a more precise measurement i.e. it is less noisy.

Next, we calculate the coefficient of determination, R^2 , which provides a measure of how well observed outcomes are replicated by a model

here we compare dispersion at time t to the modeled dispersion as given by the equation in part a

We calculate the mean $\bar{d} = \frac{1}{n} \sum_{t=0}^T d_t$

We calculate the total sum of squares (proportional to variance) $SS_{\text{tot}} = \sum_t (d_t - \bar{d})^2$

calculate the sum of squares of residuals $SS_{\text{res}} = \sum_t (d_t - \hat{d}_t)^2$

Thus we calculate the definition of the coefficient of determination as:

$$R^2 = \frac{SS_{\text{res}}}{SS_{\text{tot}}}$$

for Diffusion constant 1

$$R^2 = 0.86$$

for Diffusion constant 2

$$R^2 = 0.29$$

where the value closest to 1 shows values observed matching modeled values. Thus showing the first dataset matches the model whereas the second dataset is a noisy one not matching the model.

The first dataset matches the model whereas the second dataset is a noisy one not matching the model.

iii)

