Week 9 Workshop Solution Proposal

The first method is using a **graphical approach** and the second method uses a **numerical approach.**

Graphical Methodology

The **cumulative number density** of particles is given by the relationship.

$$\lim_{\Delta L \to 0} \frac{\Delta N(L)}{\Delta L} = \frac{dN(L)}{dL} = n(L)$$

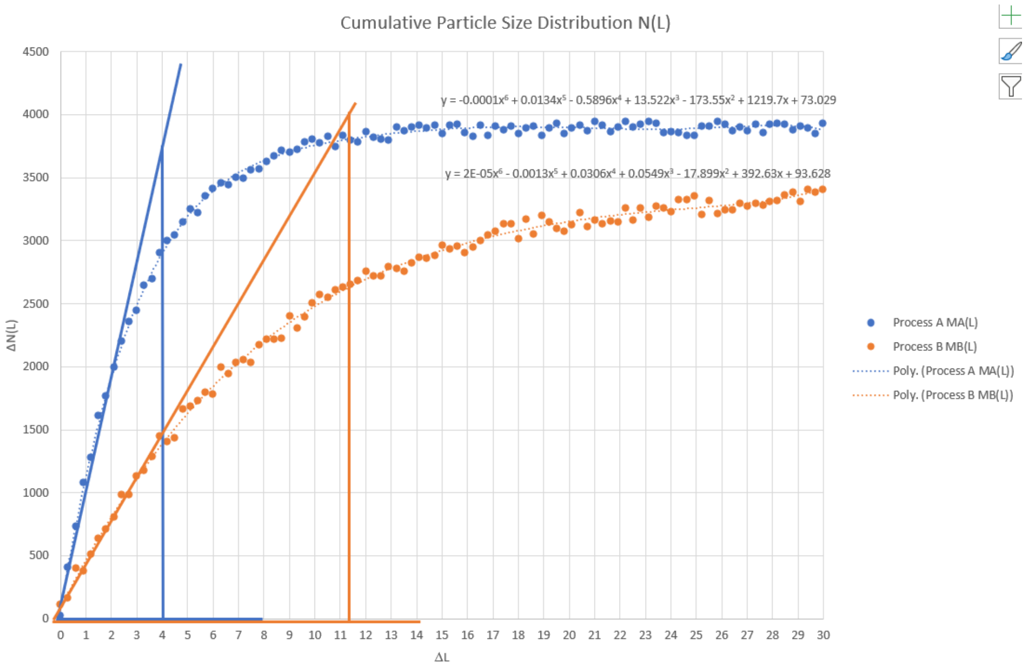
Where the **number population density** is given by.

$$n(L) = n_0 e^{\left(-\frac{L}{G\tau}\right)}$$

Whereby $n_o = \frac{J}{G}$ and $\tau = \frac{V}{\dot{Q}}$

Considering an initial crystal length at the **MSMPR** input of $n(L = 0\mu m)$, we obtain the **number population density** at the point $L = 0\mu m$, by finding the gradient of the **tangent** at that point, this allows us to obtain the **integration constant.** We assume the crystals have a constant nucleation and growth rate.

$$\lim_{\Delta L \to 0} \frac{\Delta N(L)}{\Delta L} = n(L = 0\mu m) = n_o e^0 = n_o$$



Thus, for crystal populations A and B, we obtain an **integration constant** of

$$n_{o,A} = \frac{J_A}{G_A} = \frac{\Delta N_A(L)}{\Delta L} = \frac{3700}{4} = 925$$

$$n_{o,B} = \frac{J_B}{G_B} = \frac{\Delta N_B(L)}{\Delta L} = \frac{4000}{11.3} = 353.9822 = 353$$

We can identify the **total number of crystals** using the equation.

$$N_T = \int_{0\mu m}^{30\mu m} n(L)dL$$

$$N_T = n_o G\tau$$

For the **Graphical methodology,** we assume that the **total number of crystals** within the MSMPR crystalliser is given by the number of crystals of length $30\mu m$ on the chart, giving.

$$N_{T,A} = 3938.5$$

$$N_{T,B} = 3411.2$$

Although this is a rough approximation for polymorph B, as we can identify from the increasing gradient at $L = 30\mu m$, that the crystal population has not yet achieved its final total population.

Using this information for the **total number of crystals** and the **integration constant** information, we can obtain the value for $G\tau$ for polymorphs A and B.

$$G\tau = \frac{N_T}{n_o}$$

$$G_A\tau_A = \frac{N_{T,A}}{n_{o,A}} = \frac{3938.5}{925} = 4.257837838$$

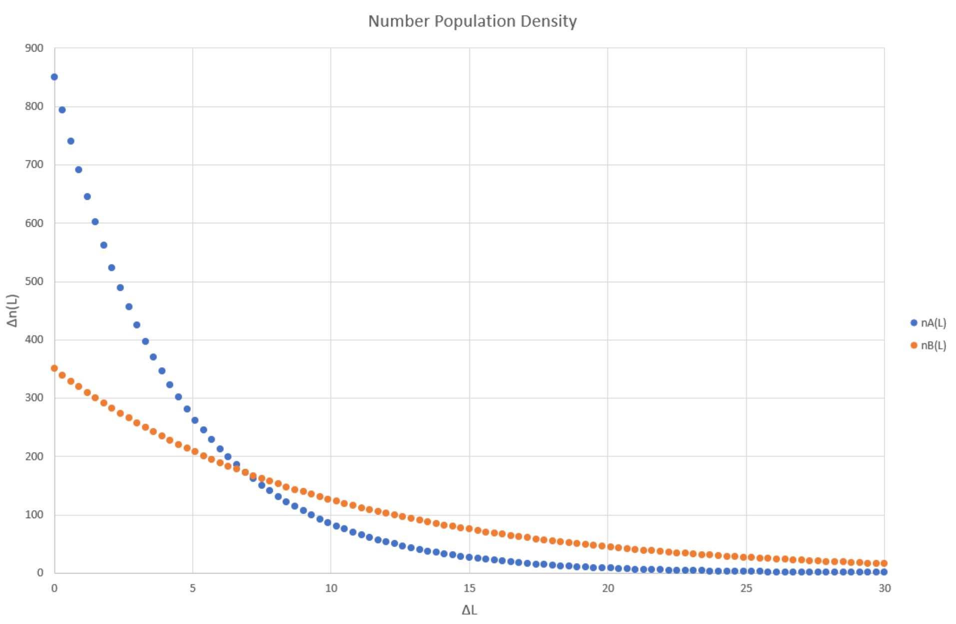
$$G_B\tau_B = \frac{N_{T,B}}{n_{o,B}} = \frac{3411.2}{353} = 9.663456091$$

We can thus use all of this collected information to plot the distribution for the **number population density.**

$$n_A(L) = n_{0,A} e^{\left(-\frac{L}{G_A\tau_A}\right)} = 925 e^{\left(-\frac{L}{4.2578}\right)}$$

$$n_B(L) = n_{0,B} e^{\left(-\frac{L}{G_B\tau_B}\right)} = 353 e^{\left(-\frac{L}{9.663456}\right)}$$

Using **Excel,** this can be plotted.

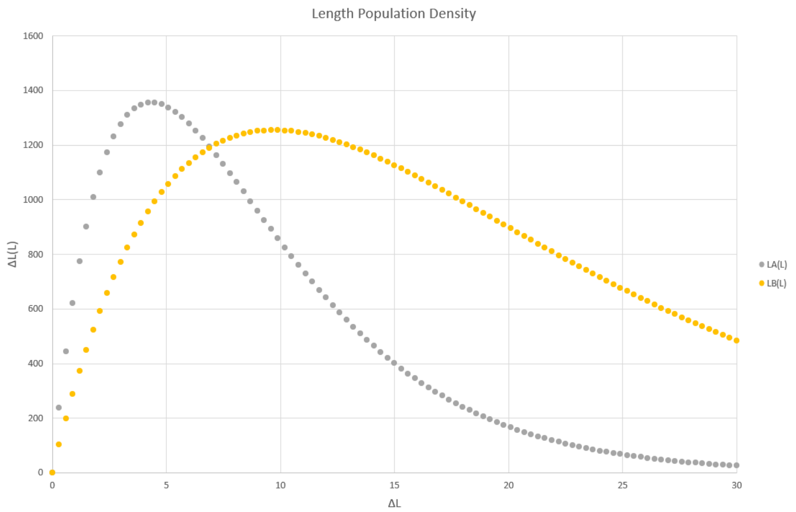


Where the plot for the Length and Area, is given by the moments.

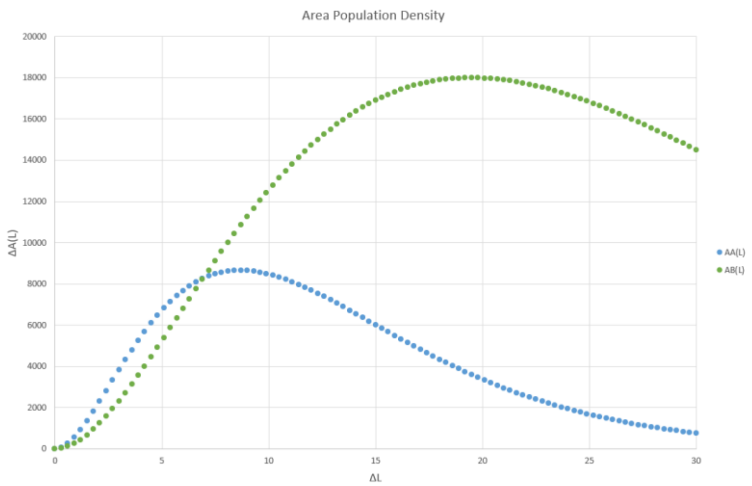
$$L_T = \int_{0\mu m}^{30\mu m} Ln(L)\, dL$$

$$A_T = \int_{0\mu m}^{30\mu m} L^2 n(L)\, dL$$

Where the **length population density distribution,** is given by a plot of $\boldsymbol{Ln(L)}$



The **area population density distribution** is given by a plot of $\boldsymbol{L^2 n(L)}$

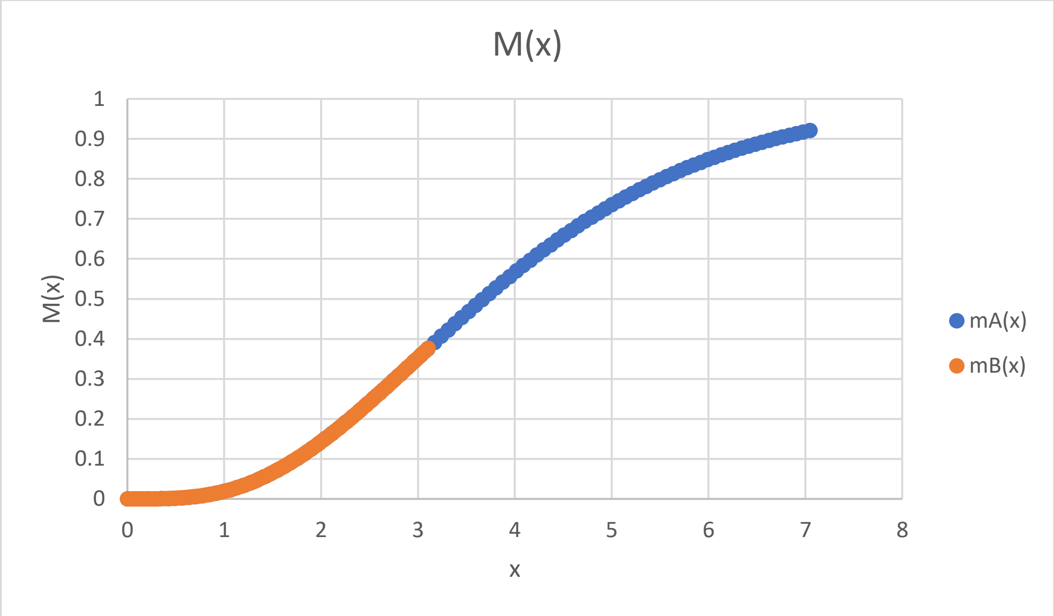


The **cumulative mass distribution** can be obtained using the below equation, where $x = \frac{L}{G\tau}$

$$M(x) = 1 - \left(1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3\right) e^{(-x)}$$

$$x_A = \frac{L}{G_A \tau_A}$$

$$x_B = \frac{L}{G_B \tau_B}$$



Predominant Crystal Length

The **characteristic lengths of the crystals** are given by the relationship.

$$L_{pd} = 3G\tau$$

$$L_{pd,A} = 3G_A\tau_A = 3(4.257837838) = 12.77\mu m$$

$$L_{pd,B} = 3G_B\tau_B = 3(9.663456091) = 28.99\mu m$$

Residence Time

The **residence** time can be analysed by **assuming** that the **growth rate** is independent from both temperature and composition and that it is constant ($G = const$).

$$G_A\tau_A = 4.257837838$$

$$G_B\tau_B = 9.663456091$$

Thus,

$$G_A = G_B$$

Giving us,

$$\frac{4.257837838}{\tau_A} = \frac{9.663456091}{\tau_B}$$

$$\tau_A = 0.4406123\tau_B$$

Hence, the residence time of $\tau_A \ll \tau_B$.

Highest Temperature

The process operating at the highest temperature can be determined from the Arrhenius relationship.

$$J = Ae^{\left(-\frac{B}{T}\right)}$$

Where we assume that the constants have values of $A = 1$ and $B = 1$.

Using once again the fact that $G_A = G_B$

Contemplating that

$$n_{o,A} = \frac{J_A}{G_A} = 925$$

$$n_{o,B} = \frac{J_B}{G_B} = 353$$

$$J_B = 0.381622 J_A$$

Contemplating $J_A = 10$ and $J_B = 3.81622$

Where the temperature is given by rearranging the **Arrhenius** type equation.

$$J = e^{\left(-\frac{1}{T}\right)}$$

$$T = \frac{1}{\ln\left(\frac{1}{J}\right)}$$

We thus obtain a $T_A = -0.43429K$ and $T_B = -0.74668078K$

Although this answer is not physically possible, as we go below absolute zero, considering all of the above assumptions, we can conclude that T_A would present the highest operating temperatures. Ideally, we should have calculated the temperature using the constants, and the actual **nucleation rate,** however, due to the absence of data this is not possible, and error propagation and the assumptions made had a significant impact on the final results.

Numerical Methodology (Only the first Part)

Alternatively, a **trendline** can be plot using **excel** (shown on the graph above), and approximated using a **polynomial line** of **6th degree,** or by using a **Vandermonde Matrices** for polynomial equations.

$$N_A(L) = (-0.0001)L^6 + (0.0134)L^5 + (-0.5896)L^4 + (13.522)L^3 + (-173.55)L^2 + (1219.7)L + (73.029)$$

$$\frac{dN_A(L)}{dL} = n_A(L) = n_{o,A} e^{\left(-\frac{L}{G\tau}\right)} = 6(-0.0001)L^5 + 5(0.0134)L^4 + 4(-0.5896)L^3 + 3(13.522)L^2 + 2(-173.55)L + 1219.7$$

$$\frac{dN_B(L)}{dL} = n_B(L) = n_{o,B} e^{\left(-\frac{L}{G\tau}\right)} = 6(0.00002)L^5 + 5(-0.0013)L^4 + 4(0.0306)L^3 + 3(0.0549)L^2 + 2(-17.899)L + 392.63$$

At $L = 0\mu m$, we can solve for the **integration constants.**

$$n_{o,A} = 1219.7$$

$$n_{o,B} = 392.63$$

This is different from the values obtained using the previous method.

$$N_T = \int_{0\mu m}^{30\mu m} n(L)dL$$

$$N_{T,A} = \int_{0\mu m}^{30\mu m} 6(-0.0001)L^5 + 5(0.0134)L^4 + 4(-0.5896)L^3 + 3(13.522)L^2 + 2(-173.55)L + 1219.7\ dL = 20613$$

$$N_{T,B} = 6(0.00002)L^5 + 5(-0.0013)L^4 + 4(0.0306)L^3 + 3(0.0549)L^2 + 2(-17.899)L + 392.63\ dL = 4928.1$$

Whereby, the total population for Process B is significantly closer to the value obtained using the graphical approach. The population for Process A however, is far greater, this may be a consequence of the over-fitting of the data using the numerical method and a 6th order polynomial.

The remaining calculations are conducted as shown above.