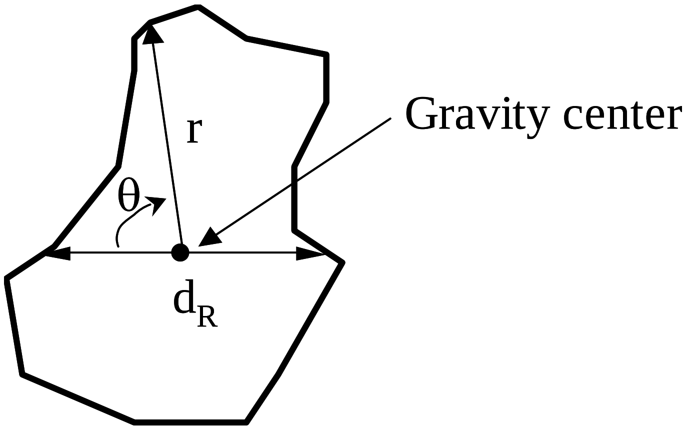
# 7. Number balance and size distribution modeling

***- Particle size***

Statistical size ( $\overline{d_R}$ )




$$\overline{d_R} = \frac{1}{\pi}\int_0^{2\pi} r\,d\theta$$

cf) Definition of Diameter

volume diameter, surface diameter, projected diameter, Feret diameter, Martin's diameter, Stoke's diameter, etc.

Method of Analysis

Microscopy, sieve, settling, gas adsorption, Coulter counter, Inertial separation, light scattering etc.

***- Mean particle size***

1) Number-length mean diameter

$$d_{NL} = \frac{\sum N_i d_i}{\sum N_i}$$

2) Geometrical mean diameter by number

$$d_{GN} = \log_{10} \frac{\sum N_i \log_{10} d_i}{\sum N_i}$$

3) Number-surface mean diameter

$$d_{NS} = \left(\frac{\sum N_i d_i^{\,2}}{\sum N_i}\right)^{1/2}$$

4) Number-volume mean diameter

$$d_{NV} = \left(\frac{\sum N_i d_i^{\,3}}{\sum N_i}\right)^{1/3}$$

5) Length-surface mean diameter

$$d_{SL} = \frac{\sum N_i d_i^{\,2}}{\sum N_i d_i}$$

6) Length-volume mean diameter

$$d_{VL} = \left(\frac{\sum N_i d_i^{\,3}}{\sum N_i d_i}\right)^{1/2}$$

7) Surface-volume mean diameter

$$d_{VS} = \frac{\sum N_i d_i^{\,3}}{\sum N_i d_i^{\,2}}$$

8) Volume-moment mean diameter

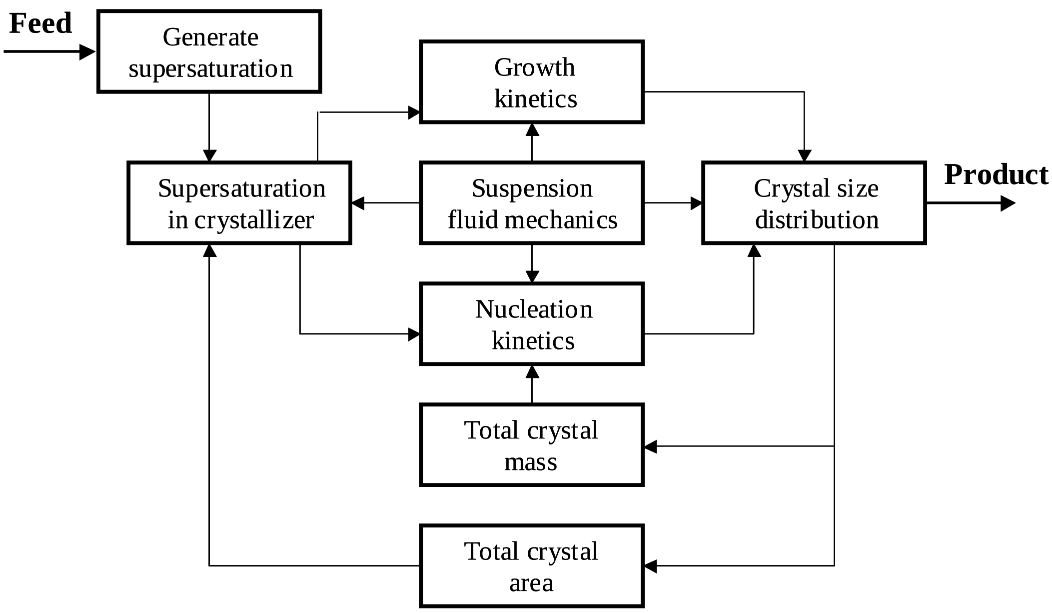
$$d_{VM} = \frac{\sum N_i d_i^{\,4}}{\sum N_i d_i^{\,3}}$$

***- Particle morphology***

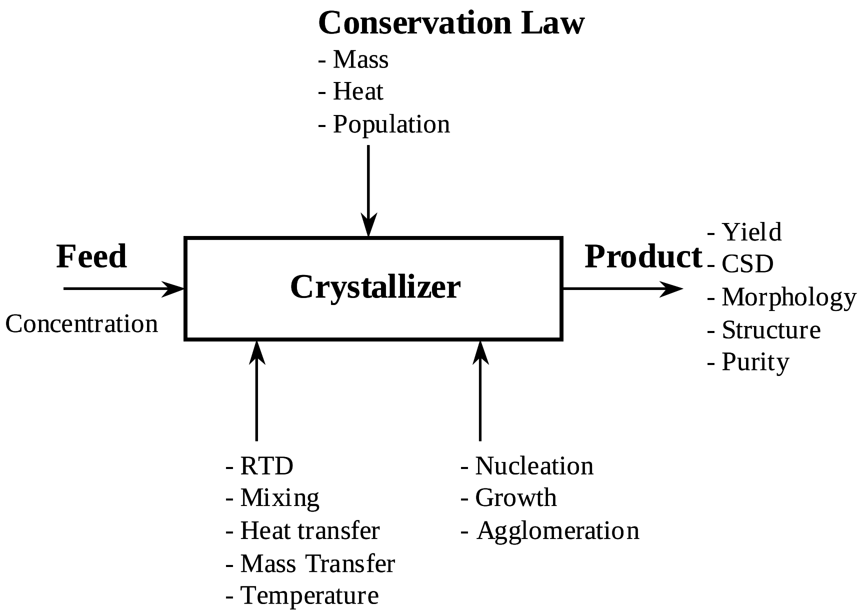
| | | |
|---|---|---|
| Sphere | one dimension | diameter |
| Cylinder | two dimension | diameter and length |
| Cube | one dimension | length |
| Irregular | many dimensions | |

## 7.1 The importance of crystal size distribution

***- Inter-relationship of crystal size distribution with crystallization kintics.***



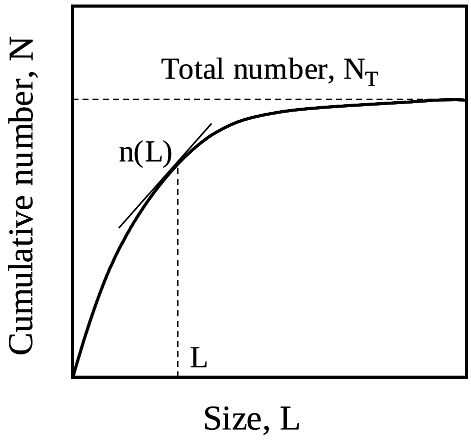

***- Conservation laws for modeling the crystallizer***



## 7.2 Characterization of size distribution

***- Number of crystals, N(L)***

*N(L)* is the number of crystals that are smaller than size L in unit volume of suspension.




***- Population density, n(L)***

$$n(L) = \frac{dN(L)}{dL}$$

- number of crystals in size range $dL$; $dN = n\,dL$

- number of crystals in size range $L_1$ to $L_2$; $N_{1,2} = \int_{L_1}^{L_2} ndL$

- total number of crystals in distribution; $N_T = \int_0^{\infty} ndL$

***- Family of mean size;*** $\overline{L}_{j,0}$ ***and*** $\overline{L}_{j,j-1}$

$$\overline{L}_{j,0} = \left[ \frac{\int_0^{\infty} L^j ndL}{\int_0^{\infty} ndL} \right]^{1/j} = \left[ \frac{\mu_j}{\mu_0} \right]^{1/j}$$

$$\overline{L}_{j,j-1} = \left[ \frac{\int_0^\infty L^j n dL}{\int_0^\infty L^{j-1} n dL} \right] = \frac{\mu_j}{\mu_{j-1}}$$

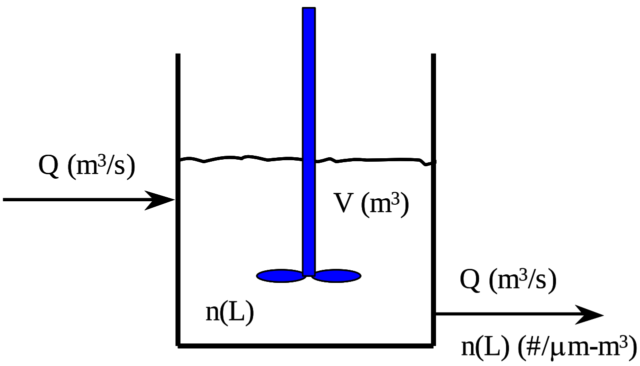
where *j*th moment of distribution is defined as,

$$\mu_j = \int_0^\infty L^j n dL$$

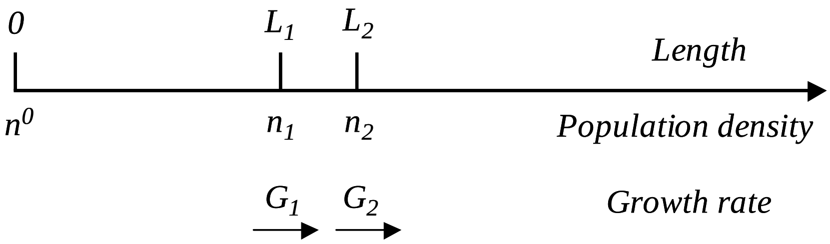
## 7.3 The continuous mixed suspension mixed product removal (MSMPR) reactor

***- Basic assumptions***

1) Continuous operation
2) Steady state
3) Perfect mixing of liquid and suspension
4) No classification of suspension in outlet streams
5) No crystals in inlet streams
6) No breakage and agglomeration
7) Same shape of crystals in whole range of size
8) Size-independent growth rate (McCabe's ΔL Law)



***- Population balance in control scale and volume of $\Delta L$ (=$L_2$-$L_1$) and V***




*Input rate* - *output rate* + *generation rate* = *Accumulation rate*

Input rate of population : $n_1 V G_1 \Delta T$

Output rate of population : $n_2 V G_2 \Delta T \;+\; \bar{n}\, Q \Delta L \Delta T$

Generation rate of population : 0

Accumulation rate of population : 0

Then,

$$n_1 V G_1 \Delta T = n_2 V G_2 \Delta T + n Q \Delta L \Delta T$$

$$\frac{n_2 G_2 - n_1 G_1}{\Delta L} = -\frac{Q}{V}\bar{n}$$

As $\Delta L \rightarrow 0$,

$$\frac{dnG}{dL} = -\frac{Q}{V} n$$

By McCabe's ΔL law,

$$\frac{1}{n}\frac{dn}{dL} = -\frac{1}{G\tau}$$

where

$$\tau = V/Q$$

Solution,

$$n = n^0 \exp(-\frac{L}{G\tau})$$

Boundary condition

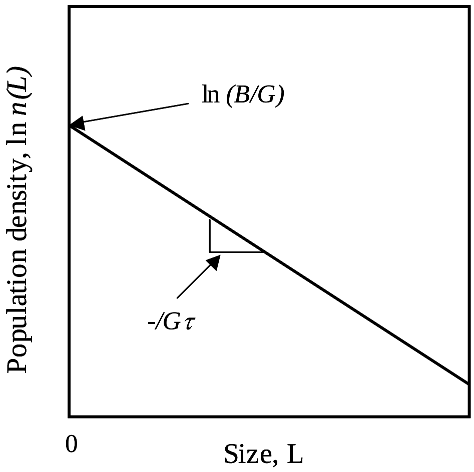
$n(L) = n^0$ at $L=0$

Definition of nucleation rate (B)

$$B \equiv \left.\frac{dN(L)}{dt}\right|_{L=0} = \left.\frac{dN}{dL}\right|_{L=0} \left.\frac{dL}{dt}\right|_{L=0} = n^0 G$$

Therefore,

$$n = \frac{B}{G} \exp(-\frac{L}{G\tau})$$




***- Other distributions***

Total population of crystals

$$N_T = \int_0^\infty n dL = \int_0^\infty \frac{B}{G} \exp(-\frac{L}{G\tau}) dL = B\tau$$

Total length of crystals

$$L_T = \int_0^\infty L n dL = \int_0^\infty L \frac{B}{G} \exp(-\frac{L}{G\tau}) dL = BG\tau^2$$

Total area of crystals

$$A_T = \int_0^\infty \beta L^2 n dL = \int_0^\infty \beta L^2 \frac{B}{G} \exp(-\frac{L}{G\tau}) dL = 2\beta B G^2 \tau^3$$

Total mass of crystals (=magma density)

$$M_T = \rho_{cry} \int_0^\infty \alpha L^3 n dL = \int_0^\infty \alpha L^3 \frac{B}{G} \exp(-\frac{L}{G\tau}) dL = 6\alpha B G^3 \tau^4$$

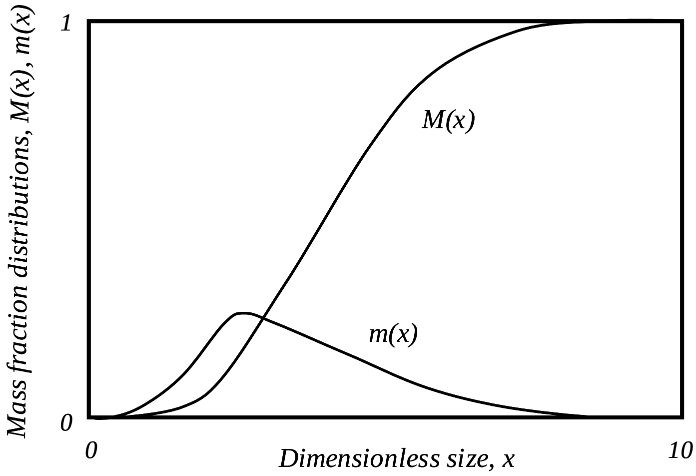
Cumulative mass fraction distribution (*M(x)*)

$$M(x) = \frac{M(L)}{M_T} = \frac{\int_0^x x^3 \exp(-x) dx}{\int_0^\infty x^3 \exp(-x) dx} = 1 - (1 + x + \frac{x^2}{2!} + \frac{x^3}{3!}) \exp(-x)$$

where $x = L/G\tau$.

Differential mass fraction distribution (*m(x)*)

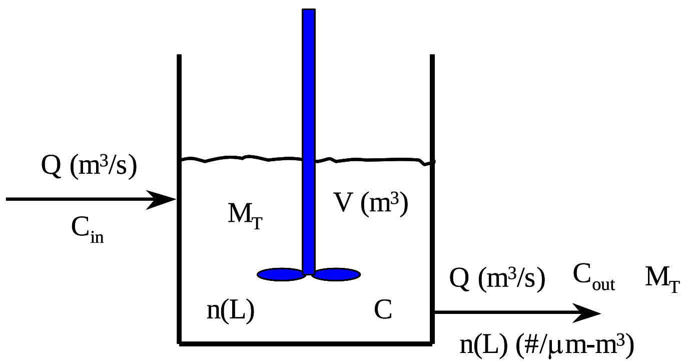
$$m(x) \equiv \frac{dM(x)}{dx} = \frac{x^3}{3!} \exp(-x)$$



The median (at $x$=*0.5*) ; $\overline{x_M} \equiv \frac{\overline{L_M}}{G\tau} = 3.67$

$$\overline{L}_{4,3} = \left[ \frac{\int_0^\infty L^4 n dL}{\int_0^\infty L^3 n dL} \right] = 4G\tau$$

***- The mass balance***




Input rate : $QC_{in}$

Output rate : $QC_{out} + QM_T$

Generation rate : 0

Accumulation rate : 0

$QM_T$ is equal to amount of solute transformed to solid state.

$$QM_T = 3\rho_{cry}\frac{\alpha}{\beta}GA_T V = Q(C_{in} - C_{out})$$

Then,

$$G = K\frac{(C_{in} - C_{out})}{\tau A_T}$$

Since $G \propto \Delta C$,

$$\Delta C = K_1 \frac{(C_{in} - C_{out})}{\tau A_T}$$