

Chromatography Equations

Plate Theory

$$p + q = 1$$

p is fraction in mobile phase, q is fraction in stationary phase

$$F_{(r,n)} = \frac{n!}{(n-r)!r!} p^r q^{n-r}$$

Fraction of solute in the r^{th} of n plates.

$$F_{(r,n)} = \frac{(np)^r e^{-np}}{r!} p^r q^{n-r} = \frac{(np)^r e^{-np}}{\sqrt{2\pi r}} \left(\frac{e}{r}\right)^r$$

$$r_{\text{max}} = np$$

r_{max} is the peak, aka the plate with max solute fraction

$$F_{(r_{\text{max}},n)} = \frac{1}{\sqrt{2\pi r_{\text{max}}}}$$

$$Q_{(N,n)} = F_{(N,n)} m = \frac{m}{\sqrt{2\pi N}}$$

Where $r_{\text{max}} = N$, then $Q_{(N,n)}$ is the quantity of material in the Nth plate

$$S_{\text{max}} = Q_{(N,n)} N / t_r$$

S_{max} is the rate of solute escape in mole/unit time

$$S_{\text{max}} = \frac{Nm}{\sqrt{2\pi N}} \frac{1}{t_r}$$

$$N = \frac{2\pi (S_{\text{max}})^2 t_r^2}{m^2}$$

Number of plates

$$m = s k h t_w$$

moles, k is proportionality constant, s is shape constant : 1/2 for triangular

$$S_{\text{max}} \propto h \text{ or } S_{\text{max}} = kh$$

S_{max} (rate of solute escape) proportional to height of peak

$$N = \frac{8\pi t_r^2}{t_w^2}$$

N relates to column efficiency

$$N = 16 \left(\frac{t_R}{W_b}\right)^2$$

Efficiency (For gaussian peak shape)

$$N_{\text{eff}} = 5.54 \left(\frac{t'_R}{W_h}\right)^2$$

Effective efficiency - N using peak width at half height

$$A_s = BC/AC$$

Peak Asymmetry - @10% peak h - AC is distance, from front to ctr, CB back to center

$$TF = AB/2AC = \frac{A_{5\%h} + B_{5\%h}}{2A_{5\%h}}$$

Tailing Factor - measured at 5% h

$$\sigma = 0.3035 h$$

h is peak height

$$N = \left(\frac{t_r}{\sigma}\right)^2 = \frac{2\pi (S_{\text{max}})^2 t_R^2}{m^2}$$

m is # moles

HETP

$$H = L/N$$

plate height is column length divided by # plates

$$H = \frac{L\sigma^2}{t_r^2} = A + \frac{B}{\mu} + C\mu$$

$$\mu_{\text{opt}} = \sqrt{\frac{B}{C}}$$

Optimal mobile phase velocity

$$PC = 1 + \frac{\sqrt{N}}{4} \ln \left(\frac{t_R}{t_M}\right)$$

Peak Capacity - # peaks can be fitted between t_M and t_R w/ 4σ gap

$$H = A + B/u + Cu$$

Van Deemter equation, terms relate to Eddy diff, longit diff,

$$I = 100 \left[n + (N - n) \frac{\log(t_R)_u - \log(t_R)_n}{\log(t_R)_N - \log(t_R)_n} \right]$$

Kovats Index. Where $I/100 = \sim$ # of carbons

\bar{v} = velocity of the retained solute

u is velocity of the mobile phase

$t_0 = t_M$ = Dead time or time of unretained solute

$t'_r = t_r - t_0$	Adjusted retention time is retention time minus dead time
$V'_r = V_r - V_0$	Adjusted
$V_T = V_s + V_0$	Total volume
$\bar{v} = \mu \frac{\text{moles of solute in mobile phase}}{\text{total number of moles}} = \mu \frac{c_M V_M}{c_M V_M + c_S V_S} = \mu \frac{1}{1 + \frac{c_S V_S}{c_M V_M}} = u \frac{1}{1 + \frac{K V_S}{V_M}} = \mu \frac{1}{1 + k'_A}$	
$\bar{v}_A = \mu \frac{1}{1 + k'_A}$	velocity for retained solute A
$k' = \left(\frac{u}{\bar{v}} - 1 \right)$	Retention factor or capacity
$k'_A = \frac{K_A V_M}{V_M} = \frac{t_R - t_M}{t_M} = \frac{t'_R}{t_M}$	Retention factor (capacity) for solute A
$K = \frac{V_M}{V_S} \left(\frac{u}{\bar{v}} - 1 \right) = \frac{V_M}{V_S} k' = \beta k' = \frac{c_S}{c_M}$	Partition Factor / Distribution coefficient
$\alpha = \frac{K_B}{K_A} = \frac{k'_B}{k'_A} = \frac{t'_R(B)}{t'_R(A)}$	separation factor or selectivity
$R_S = 2 \frac{t_{R2} - t_{R1}}{w_{b1} + w_{b2}}$	Resolution (of peaks), w/ w _b being width at base
$R_S = \frac{\sqrt{N}}{4} \frac{\alpha - 1}{\alpha} \frac{k}{k + 1}$	Efficiency * Selectivity * Retention factor
$N = 16 R_S^2 \left(\frac{\alpha}{\alpha - 1} \right)^2 \left(\frac{1 + k'_B}{k'_B} \right)^2$	Efficiency from R _s , selectivity, and retention factor
$A_{UC} = 1.06 * h * w_{0.5}$	Area under a gaussian curve
$\beta = \frac{V_M}{V_S}$	
$V_S = L \pi r_c^2 L$	Vol of SP is $L \pi r_c^2 L$ of column, where r _c is radius of column
$K = \frac{V_R - V_0}{V_S}$	
$V_R = V_0 + K V_S$	
$P' = P'_1 C_1 + P'_2 C_2$	P is polarity index, C is molar concentration
$\frac{k'_2}{k'_1} = 10^{\frac{P'_1 - P'_2}{2}}$	Changing Eluent polarity index affect, Normal phase
$\frac{k'_2}{k'_1} = 10^{\frac{P'_2 - P'_1}{2}}$	Changing Eluent polarity index affect, Reverse phase