

Appendix C. Equations

Equation 1 – HPLC column linear velocity

$$F_{2.1} = \left(\frac{d_{2.1}}{d_{4.5}} \right) \cdot F_{4.6}$$

F = Flow rate

d= Column Diameter

Equation 2 - Van Deemter Equation

$$H = A + \frac{B}{u} + C \cdot u$$

H = Plate height

A = Eddy diffusion

B = Longitudinal Diffusion

C = Mass transfer kinetics

u = Linear Velocity

Equation 3 - Expanded Van Deemter Equation

$$H = 2\lambda d_p + \frac{2GD_m}{\mu} + \frac{\omega(d_p)^2 \mu}{d_m} + \frac{Rd_f^2 \mu}{D_s}$$

λ = particle shape

d_p = particle diameter

D_m = mobile phase diffusion coefficient

D_s = stationary phase diffusion coefficient

d_f = film thickness

G, ω and R are constants

Equation 4 – Sensitivity

$$\text{Sensitivity} = \frac{TP}{TP + FN}$$

TP = Number of True Positives

FN = Number of False Negatives

Equation 5 - Specificity

$$\text{Specificity} = \frac{TN}{TN + FP}$$

TN = Number of True Negatives

FP = Number of False Positives