GC Equations

Adjusted Retention Time (t_R')

An analyte's retention time (t_R) minus the elution time of an unretained peak (t_m).

$$t_R' = t_R - t_m$$

Adjusted retention time is also equivalent to the time the analyte spends in the stationary phase.

Capacity Factor (k)

Expression that measures the degree of retention of an analyte relative to an unretained peak, where t_R is the retention time for the sample peak and t_m is the retention time for an unretained peak. A measurement of capacity will help determine whether retention shifts are due to the column (capacity factor is changing with retention time changes) or the system (capacity factor remains constant with retention time changes).

$$k = \frac{t_R - t_m}{t_m}$$

Thus, the higher the capacity factor, the longer the retention time.

Effective Theoretical Plates (N_{eff})

A measure of a column performance that accounts for the effects of unretained elution time, where t_R' is the adjusted retention time and σ is the standard deviation of the peak.

$$N_{eff} = \left(\frac{t_R'}{\sigma}\right)^2$$

This value also remains constant as retention gaps and guards are used. Depending on the method of peak width calculation, different efficiencies can be reported. This leads to two popular measures:

$$N_{eff} = 16\left(\frac{t_R'}{W}\right)^2$$

Where W is the tangential peak width (13.4% peak height).

$$N_{eff} = 5.54\left(\frac{t_R'}{W}\right)^2$$

Where W is the width measured at half height (50% peak height).

HEEP (H_{eff})

Height Equivalent to an Effective Plate.

$$H_{eff} = L/N_{eff}$$

Where L is the column length. The smaller the N_{eff}, the more efficient the column's performance.

HETP (H)

Height Equivalent to a Theoretical Plate is a measure of column efficiency where L is the column length and N is the number of theoretical plates.

$$H = L/N$$

HETP is based on actual (t_R) rather than adjusted retention times (t_R').

Linear Velocity (u)

Mobile phase flow rate expressed in cm/s and is expressed as:

$$u = L/t_m$$

Where L is the column length and t_m is the breakthrough time of an unretained peak.

Phase Ratio (β)

The ratio of the volume of mobile phase to the stationary phase. An important value when changing the column dimensions in a method.

$$\beta = \frac{\text{column ID (µm)}}{\text{4 x film thickness (µm)}}$$

Resolution

A measure of the separation of two peaks taking into account both the difference in elution time and the peak widths.

$$R_s = \frac{(t_2 - t_1)}{0.5\,(W_1 + W_2)}$$

Where t_2 and t_1 are the two retention times, and W_1 and W_2 are baseline peak widths.

Selectivity (α)

The relative retention of two adjacent peaks. Selectivity can be calculated using capacity factor.

$$\alpha = \frac{k_2}{k_1}$$

Trennzahl Number

A value to describe a separation. The Trennzahl number is calculated from the resolution between two consecutive homologous hydrocarbons. The Trennzahl number represents the number of peaks that can be included between the two hydrocarbon peaks.

$$T_z = \left(\frac{t_{R2} - t_{R1}}{(W_h)_1 + (W_h)_2}\right) - 1$$

Where t_R equals analyte retention time and W_h equals peak width at half height.

van Deemter Equation

This is a relationship that considers the effect of linear velocity on the HETP or H, where A accounts for eddy diffusion, B describes the molecular diffusion of the vapor in the direction of the column axis, C refers to the resistance to transfer from the stationary to mobile phase and u is the linear velocity of the mobile phase.

$$H = A + \frac{B}{u} + Cu$$