

Notes

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A simple method for the calculation of the minimum number of theoretical plates required for a chromatographic separation

In earlier publications¹⁻⁴ the planning of chromatographic separations of inorganic and organic substances on ion-exchange columns has been reported. Using complex forming agents in the eluent, the most convenient pH and concentration of the solution were calculated by means of equations, which formulated the relation between the distribution coefficient of the substance and the pH of the eluent at a given concentration.

Now an attempt has been made to provide a simple formula for calculating the minimum value of the number of theoretical plates necessary to obtain a clear separation of two components of similar behaviour.

The following symbols are used:

- a = void fraction of the column;
- B, A = substances to be separated;
- $c_{\max, B}$ = the maximum concentration of component B in the effluent;
- D_B = volume distribution coefficient of substance B;
- m_B = total amount of substance B (mmole);
- N = number of theoretical plates;
- v_B = the base line of the triangle in the chromatogram (ml) (see Fig. 1);
- $v_{\max, B}$ = total eluent volume (ml) (see Fig. 1);
- X = total volume of the column (ml).

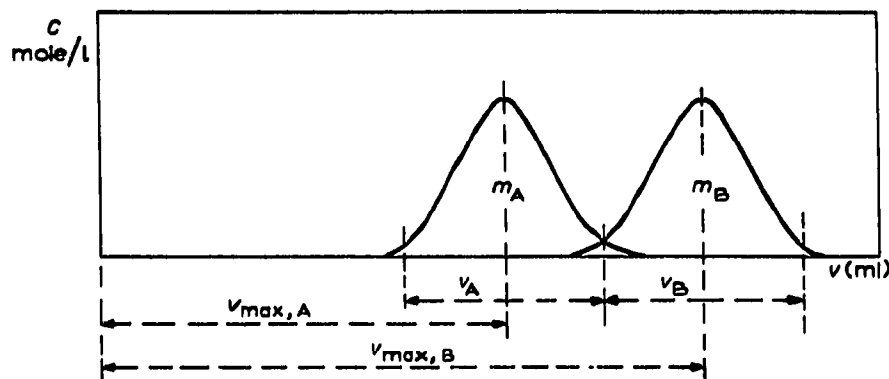


Fig. 1. Elution diagram of two components of similar behaviour.

Let us consider first an ideal chromatogram of two components (see Fig. 1). To obtain a clear separation of the two substances, the distance between the two peaks must be greater than the sum of the two half base lines. Thus,

$$\left(\frac{v_{\max, B}}{v_{\max, A}} - 1 \right) v_{\max, A} \geq \frac{1}{2} v_A + \frac{1}{2} v_B \quad (1)$$

Using the fundamental equation deduced by GLUECKAUF⁵

$$c_{\max} = \frac{m}{v_{\max}} \sqrt{\frac{N}{2\pi}} \quad (2)$$

considering that

$$m_B \approx \frac{1}{2} v_B \cdot c_{\max, B} \quad (3a)$$

$$m_A \approx \frac{1}{2} v_A \cdot c_{\max, A} \quad (3b)$$

we obtain for v_B

$$v_B \approx 2 \cdot v_{\max, B} \sqrt{\frac{2\pi}{N}} \quad (4)$$

and a very similar equation for v_A .

Since v_{\max} can be expressed in terms of the distribution coefficient and column data

$$v_{\max} = X(D + a) \quad (5)$$

eqn. 1 can be transformed:

$$\frac{v_{\max, B}}{v_{\max, A}} - 1 \geq \frac{\frac{1}{2}(v_A + v_B)}{v_{\max, A}}$$

$$\frac{D_B + a}{D_A + a} - 1 \geq \frac{(D_A + a) + (D_B + a)}{(D_A + a)} \sqrt{\frac{2\pi}{N}}$$

$$N \geq 2\pi \left[\frac{\frac{D_B + a}{D_A + a} + 1}{\frac{D_B + a}{D_A + a} - 1} \right]^2 \quad (6)$$

If the distribution coefficients of the two substances to be separated are known, the number of theoretical plates necessary can be calculated. Eqn. 6 differs fundamentally from equations of similar form recommended in the literature^{6,7} for calculation, since the ratio of the $(D + a)$ values corresponding to the ratio of the real eluent volumes (v_{\max}) and not the ratio of the distribution coefficients (*i.e.* separation factor) corresponding to the ratio of net eluent volumes is used.

Since in liquid chromatographic separations the first substance is always eluted with an eluent volume comparable with the dead volume of the column, in calculations the latter may not be neglected.

Another advantage of eqn. 6 is that the ratio and not the difference of the terms is used, the latter being more common⁸; the ratio is more characteristic for the expression of the effectiveness of separations.

The values obtained at various $(D_B + a)/(D_A + a)$ ratios were calculated and compared with the data of the diagram of GLUECKAUF⁵, which is based on rigorous mathematical treatment of the overlapping ratio of the two curves. The values calculated by eqn. 6 correspond to separations with an impurity of less than 0.3%, if the ratio of the amount of the two components is 1:1. Since the real form of the curves always differs from the ideal one, and therefore the calculations are in any way

only approximative, eqn. 6 may be proposed for informatory calculations in the planning of liquid chromatographic separations.

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- 1 J. INCZÉDY, P. KLATSMÁNYI-GÁBOR AND L. ERDEY, *Acta Chim. Acad. Sci. Hung.*, 61 (1969) 261; *ibid.*, 62 (1969) 1.
- 2 J. INCZÉDY AND L. GLÓSZ, *Acta Chim. Acad. Sci. Hung.*, 62 (1969) 241.
- 3 J. INCZÉDY, *Acta Chim. Acad. Sci. Hung.*, in press.
- 4 J. INCZÉDY, *Planning of Ion-Exchange Chromatographic Separations using Complex Equilibria*, Soc. Chem. Ind., London, 1969, p. 204.
- 5 E. GLUECKAUF, *Principles of Operation of Ion-exchange Columns*, Soc. Chem. Ind., London, 1954, p. 34.
- 6 J. J. VAN DEEMTER, F. J. ZUIDERWEG AND A. KLINKENBERG, *Chem. Eng. Sci.*, 5 (1956) 271.
- 7 R. DYBCZYŃSKI, *J. Chromatog.*, 31 (1967) 155.
- 8 J. BEUKENKAMP, W. RIEMAN AND S. LINDENBAUM, *Anal. Chem.*, 26 (1954) 505.

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Imbrication patterns

WALRAVEN, LADON and KEULEMANS have recently described¹⁻³ imbrication plots or roofing tile patterns as an aid in the tentative identification of organic compounds. Isomers of homologous compounds were shown to form staggered parallel plots depending on the carbon number when examined on two stationary phases. It is shown that the series of parallel linear relationships representing isomeric compounds that are produced when logarithmic expressions of retention on two stationary phases are plotted according to carbon number are simply a particular extension of established homologous plots. The overlapping plots are parallel only when the structural parameters of the isomers are non-interacting or where interactions are present these are independent of the structures of the variable portions of the isomers. An example of the plots is shown in Fig. 1a, using data of methyl esters of monocarboxylic acids⁴.

Linear relationships of homologous compounds on two stationary phases are well known. JAMES⁵ with aliphatic amines plotted relative retention on a polar and a non-polar stationary phase to produce linear plots radiating from the origin for each homologous series. With hydrocarbons a series of parallel lines were produced by JAMES AND MARTIN⁶ using the logarithm of retention obtained on two phases. Concurrently primary, secondary and tertiary alkanols, alkanones and *n*-alkanes were shown to produce parallel linear plots using two polar phases⁷. Similar results have been achieved with fatty esters by the use of a "new" and an "aged" polyester stationary phase⁸. Differences in behaviour of these esters have also been observed by the use of a single polar column using two temperatures⁹ while plots of isomeric alkanes C₅-C₉ have been reported using squalane at 30° and 70° (ref. 10).

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