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Publisher *Taylor & Francis*

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Separation Science and Technology

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713708471>

The Equivalent Gaussian Sample Inlet Profile

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To cite this Article De Clerk, K. , Buys, T. S. and Pretorius, Victor(1971) 'The Equivalent Gaussian Sample Inlet Profile', Separation Science and Technology, 6: 5, 733 — 736

To link to this Article: DOI: 10.1080/00372367108057966

URL: <http://dx.doi.org/10.1080/00372367108057966>

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NOTE

The Equivalent Gaussian Sample Inlet Profile

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Summary

The applicability of the equivalent Gaussian (EG)-inlet profile for the prediction of bandwidths is evaluated by comparison of the elution profiles with those resulting from a plug inlet. Gas compressibility is taken into account.

The response of a chromatographic column operating in the linear part of the distribution isotherm to a δ -sample input profile is known (1) to be Gaussian. In situations where finite sample inlet volumes are important, the response may be calculated by means of Laplace transform techniques (2) or by considering the actual sample as a stack of δ -inputs (3). These methods provide information on the concentration distribution itself. However, this information is often unnecessarily detailed for chromatographic purposes. For instance, one is usually only interested in the lower moments of the distribution. The second moment, which relates to the plate height, is of particular significance. The purpose of the present note is to show that a good approximate description is obtained by replacing the actual input profile, when this is assumed to be a double step (plug), by an equivalent Gaussian

(EG)-inlet. This EG-inlet is defined as that Gaussian concentration profile which has the same maximum height and area as that of the actual inlet concentration distribution (see Fig. 1).

If compressibility of the mobile phase is taken into account, the expression for $C_p(x)$ resulting from a plug input of width w is found (3) as

$$C_p(x) = \frac{C_i}{p} \left\{ Z^* \left[\xi \left(X + \frac{p\sqrt{2\pi}}{2} \right) \right] - Z^* \left[\xi \left(X - \frac{p\sqrt{2\pi}}{2} \right) \right] \right\} \quad (1)$$

where C_i = initial concentration, $p = P_i/P_0$ = ratio of inlet to outlet pressures,

$$X = \frac{x - x_2 - (pw/2)}{\sigma_{ii}}$$

x_2 = position of second step, x = axial coordinate, σ_{ii}^2 = inlet variance of EG-inlet, $w = \sigma_{ii}\sqrt{2\pi}$, $\xi = \sigma_{ii}/\sigma_c$, σ_c^2 = variance produced by the column, and $Z^*(x) = 0.5[1 + \text{erf}(x/\sqrt{2})]$.

The response of the column to the EG-inlet may be written down directly since the input is already a solution of the basic differential equation describing the axial migration of the sample. The inlet and

TABLE 1

Comparison of Bandwidths at Half Maximum Peak Height for Plug- and EG-Inlets

p	ξ	Bandwidth at half-height (cm)		W_s/W_p	Height (cm)	
		Plug, W_p	EG W_s		Plug	EG
1	2	1.60	1.60	1	12.50	11.34
	1.5	1.75	1.80	1.028	11.85	10.55
	1	1.82	2.10	1.153	10.00	8.90
1.5	2	2.55	2.40	0.941	8.55	8.06
	1.5	2.40	2.50	1.041	8.40	7.70
	1	2.50	2.70	1.080	7.90	7.00
2	2	3.18	3.00	0.943	6.65	6.20
	1.5	3.23	3.25	1.006	6.65	6.00
	1	3.25	3.40	1.046	6.30	5.68

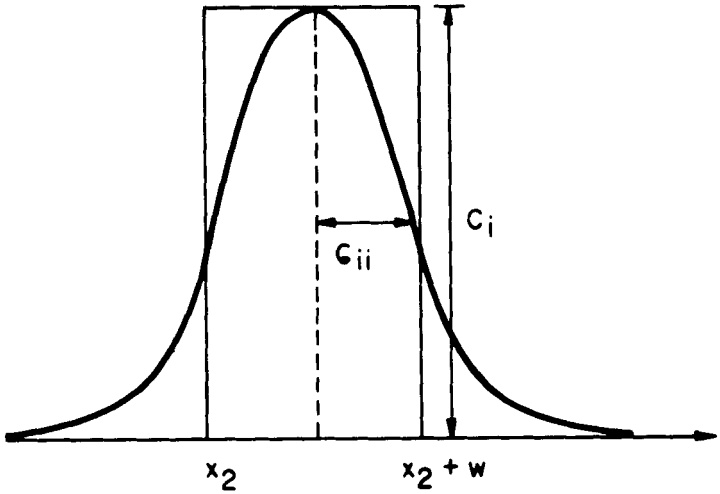


FIG. 1. Definition of the EG inlet in terms of a plug inlet.

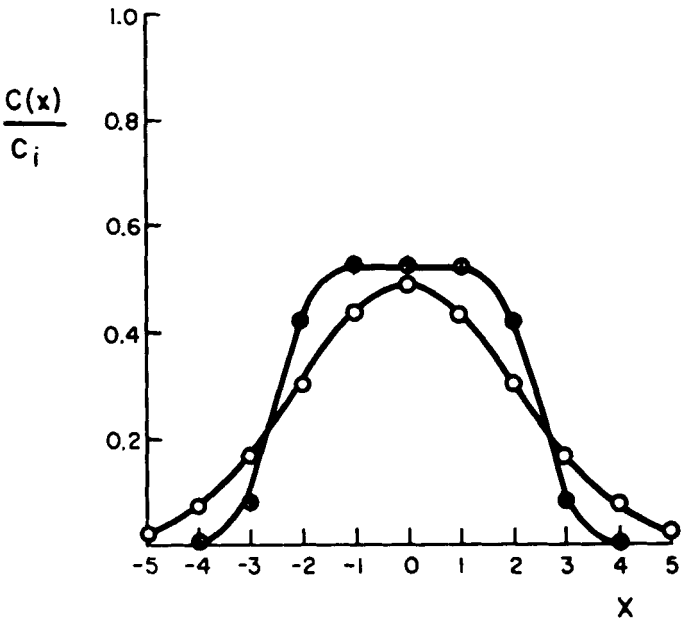


FIG. 2. Comparison of typical elution curves resulting from plug and EG inlets. $p = 2$, $\xi = 2$.

column variances are simply additive so that

$$C_e(x) = \frac{C_i \xi}{(1 + p^2 \xi)^{1/2}} \exp \left\{ -\frac{X^2}{2[(\xi^2)^{-1} + p^2]} \right\} \quad (2)$$

where $C_i = m_i/\sigma_{ii}\sqrt{2\pi}$, and $m_i \equiv$ mass of component i in sample. The presence of p in Eq. (2) takes the compressibility of the input sample into account. The effect of the pressure gradient on σ_c^2 is assumed to be included in σ_c^2 itself.

Equations (1) and (2) have been compared numerically for different values of the parameters ξ and p . The results are summarized in Table 1 and Fig. 2 from which it is seen that the ratios of the bandwidths at half-height are close to unity. Figure 2 shows a typical pair of response functions. Application of the EG-inlet has been found to simplify the description of preparative chromatography considerably (4).

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Received by editor February 16, 1971