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Discussion

Reply to "Comments on the 'classical equations' given in J. Chromatogr. A 1024 (2004) 195–207", by L.S. Ettre

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We agree with Ettre [1], unfortunately we made two mistakes. In spite of the fact that all six authors *carefully* checked the text, none of us found the mistakes in the formulas of the average peak width and the calculation of the separation number: this means that we were not careful enough, and we do apologise for the oversight. We have rechecked our results and confirmed that they are correct and were calculated with the correct formulas, i.e. the error in the average peak width is a typing mistake while the reported SN formula lacks the -1 term.

The separation number was calculated on E10–E12 methyl esters and not on *n*-alkanes in agreement with Grob et al.'s original articles on the Grob test [2,3]. We know that the separation number was introduced by Kaise and Rieder [4] with *n*-alkanes, but it is now common also to consider the values obtained with methyl esters (in particular when calculated for the Grob test), provided that the use of esters is clearly mentioned in the text (as it is in our text page 199, second column, line 5).

Maximum number of peaks. We agree with the fact that the text may be ambiguous: Δt is the interval of time considered over the chromatographic run. If possible, we suggest an *errata corrige* adding a short sentence defining Δt as $t_2 - t_1$, i.e. the interval of time between the first peak considered (in our case, *n*-dodecane, see the table below) and the last peak considered in the chromatogram (in our case E12 or 2,6-dimethylphenol, see the table below).

We took peak widths as a constant and as a consequence the corresponding standard deviations are also taken as constants, because the time interval $(t_2 - t_1)$ considered is all under programmed temperature and the system operated in constant flow: as a consequence, the peak width is constant, as is clear from the table enclosed, where the peak widths of dodecane and E12 for SE52 and OV1701, and dodecane and 2,6-dimethylphenol (P) are very similar to each other.

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Appendix to Table 3: First and last eluted peak widths in Grob test

GC approach	C-GC	S-GC	F-GC	UFM-GC	UFM-GC
Stationary phase	SE 54				
Column number	I	II	III	IV	IV
First peak width (Wb 1—*n*-dodecane, s)	4.398	1.32	0.828	0.18	0.12
Last peak width (Wb 2—E12, s)	4.042	1.3	0.792	0.17	0.116
Stationary phase	OV 1701				
Column number	V	VI	VII	VIII	VIII
First peak width (Wb 1—*n*-dodecane, s)	4.398	1.68	0.87	0.162	0.108
Last peak width (Wb 2—E12, s)	4.382	1.28	0.784	0.132	0.092
Stationary phase	PEG 20M				
Column number	IX	X	XI	XII	XII
First peak width (Wb 1—*n*-dodecane, s)	4.47	1.56	0.912	0.168	0.126
Last peak width (Wb 2—2,6-dimethylphenol, s)	5.05	1.7	0.802	0.126	0.094

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