



NOTE

Three Dimensional Plottings of Characteristic Equations and Optimization of Micellar Electrokinetic Capillary Chromatography

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There are two characteristic equations obtained from the resolution equations of Terabe and Ghowsi. These characteristic equations are plotted three dimensionally for the first time. Optimum conditions for these characteristic equations are discussed from three dimensional plots.

Key Words: Micellar electrokinetic capillary chromatography, Optimization, Resolution equation, Terabe's and Ghowsi's characteristic equation.

The first pioneering work on optimization of characteristic equation of micellar electrokinetic capillary chromatography were done by Foley¹ and Ghowsi *et al.*². In column chromatography the resolution equation is given as³

$$R_s = \frac{N^{1/2}}{4} \cdot \frac{(\alpha-1)}{\alpha} \cdot \frac{k'}{(1+k')} \quad (1)$$

where k' is the capacity factor, α is the selectivity and N is the number of theoretical plates. Terabe *et al.*⁴ proposed the micellar electrokinetic capillary chromatography (MECC) for the first time and they proposed the resolution equation for MECC:

$$R_s = \frac{N^{1/2}}{4} \cdot \frac{\alpha-1}{\alpha} \cdot \frac{k'}{k'+1} \cdot \frac{1-t_0/t_{mc}}{1+(t_0/t_{mc})k'} \quad (2)$$

where N, α and k' were already defined a new term is appearing in equation (2) for resolution is $\frac{1-t_0/t_{mc}}{1+(t_0/t_{mc})k'}$. In

this term k' is the capacity factor and t_0 and t_{mc} are retention times of the aqueous and micellar phases respectively. The characteristic equation for MECC to optimize is from equation (2):

$$f(k', t_0/t_{mc}) = \frac{k'}{(k'+1)} \cdot \frac{(1-t_0)/t_{mc}}{1+(t_0/t_{mc})k'} \quad (3)$$

This characteristic equation has two variables k' and the ratio t_0/t_{mc} for optimization the three dimensional plots using

DPlot software were obtained. In a recent work a new model for the MECC using a model based on effective length migrated on a similar to tread mill ease were proposed. Based on this model

$$R_s = \frac{1}{4} [(D_{ep})_B RT/4]^{\frac{1}{2}} (N_{pseudo}^{\frac{1}{2}}) \left[\frac{\alpha-1}{\alpha} \right] \left[\frac{k'}{k'+1} \right]^{\frac{3}{2}} \frac{1-(t_0/t_{mc})}{1+(t_0/t_{mc})k'} \quad (4)$$

Variables of this equations were defined in the previous work⁵. In present work the new characteristic equation is optimized using three dimensional plot using DPlot software. The characteristic equation of R_s for equation (4) is the last two terms

$$f(k', t_0/t_{mc}) = \left(\frac{k'}{k'+1} \right)^{3/2} \cdot \left(\frac{(1-t_0)/t_{mc}}{1+(t_0/t_{mc})k'} \right) \quad (5)$$

This new characteristic equation has also two variables k' and t_0/t_{mc} which can be plotted three dimensional.

Three dimensional plots

In previous work⁶ the characteristics equations were obtained. In the same work approximations are used to obtain the optimized analytical solution. In present work by the help of modern technology of computer and three dimensional software of DPlot direct access to the plots of characteristics equations (3,5) are possible.

Fig. 1 shows the three dimensional plot of characteristic equation (3) obtained by Terabe *et al.*⁴. In this work $f(k', t_0/t_{mc})$ is a function of two independent variables k' and t_0/t_{mc} . k' is

changing between 1 to 10 and t_0/t_{mc} changes between 0.1 to 1. In Fig. 1 the surface of the three dimensional plot shows maximums. The greater maximum occurs at $f(k'_{max}, t_0/t_{mc} max) = 0.51$. These maximums are local maximums.

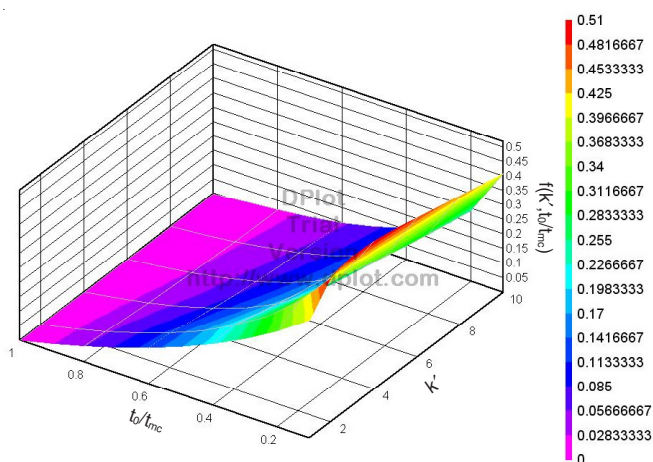


Fig. 1. Three dimensional plot of Terabe's characteristic equation (3)

In Fig. 2 the characteristic equation (5) based on proposed thread mill model⁵ is plotted.

This plot shows no local maximums but there is a single maximum occurs at $t_0/t_{mc} = 0$, $k' = 10$ where $f(k', t_0/t_{mc}) = 2.25$.

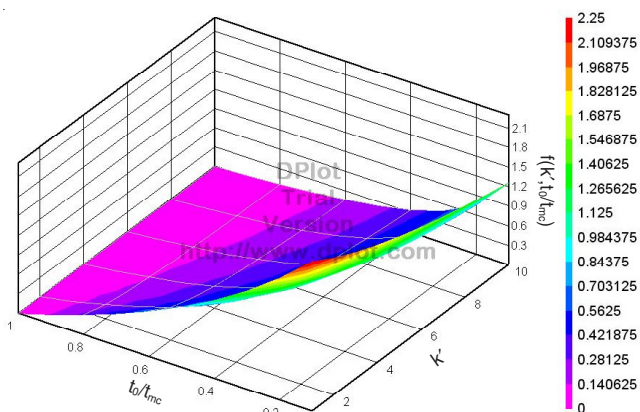


Fig. 2. Three dimensional plot of Ghowsi's characteristic equation (5)

Conclusion

In present work the three dimensional plots of the characteristic equations are obtained. This method of optimization is more accurate than previous work⁶. Because the three dimensional plots are actually visualized. It is very interesting observation that the Terabe's *et al.* characteristic equation shows local maximums in three dimension plots (Fig. 1), but the three dimensional plot of characteristic equation obtained by us based on thread mill model⁶, Fig. 2, shows no local maximums on the surface of three dimensional plot.

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