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# CHARACTERIZATION OF INJECTED SAMPLE PLUGS IN MICROCHIP CAPILLARY ELECTROPHORESIS

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## INTRODUCTION

Since the capillary electrophoresis was proposed to be run in the chip format, tremendous studies have been performed by covering many different aspects of this technology. One key element is the sample plug generated between the injection and separation process, because it will play a governing role on the final separation performance, i.e., the separation efficiency depends on the initial sample plug and its further dispersion development. In literature, some work has been done previously to generate various sample plugs, or optimize them by means of either channel design or operational control. However, little work has been reported to characterize the sample plug with evaluating parameters. Usually, the well-defined and reproducible sample plug is anticipated for high quality separation. By experience, thin-rectangular sample plugs are normally assumed, but not technically proved yet, to have superior performance in electrophoretic separation. Quantitative study is necessary to be performed to demonstrate the relevant qualitative estimation or analysis. All above stated are the motivation of current work.

## DESIGN OF EVALUATING PARAMETERS

As shown in Fig-1, the boundaries of an injected sample plug are denoted as its half-maximum concentration contour lines. There could be other concerns like alternative values and homogeneity, but this arrangement is just for characterization here. Due to the usual symmetric structure, the top-half can be defined and expressed as an approximate quadratic function. Of course, a higher order curve fit will introduce more accuracy.

$$y = W_{sp}(x) = a_0 + a_1 x + a_2 x^2 = a_0\left(1 + \frac{a_1}{a_0}x + \frac{a_2}{a_0}x^2\right)$$

In this project, the sample plugs are characterized by four designed evaluating parameters in terms of size and shape, which are considered as two important properties influencing the separation performance. The first two parameters are similar to the mean value and the deviation in statistics. The mean width of sample plug reflects the amount of injected species as analytes, and the second, abbreviated as RMS (root-mean-square), shows the boundary roughness of sample plug. In the following definition equations, all the integrals are across a whole vertical channel width ($W$).

$$\bar{W}_{sp} = \frac{\int W_{sp}dx}{\int dx}/W \qquad \in [0, +\infty)$$

$$RMS = \sqrt{\frac{\int (W_{sp} - \bar{W}_{sp})^2 dx}{W}}/\bar{W}_{sp} \qquad \in [0, +\infty)$$

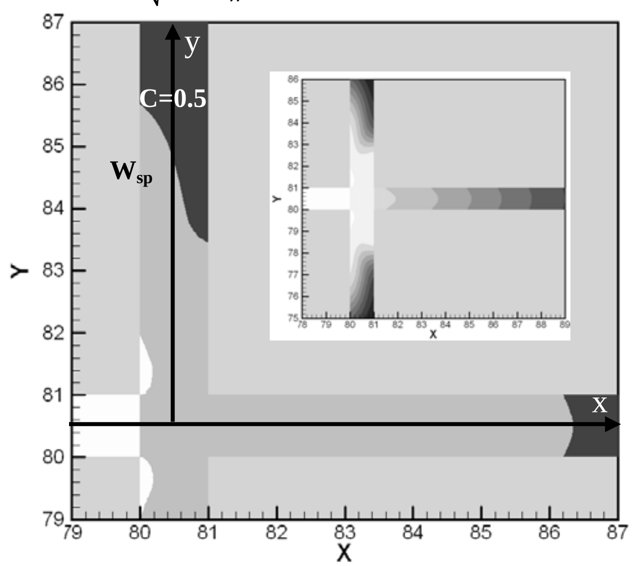


**Fig-1. Schematic diagram of the definition of a sample plug**

The other two parameters (Sy1 and Sy2) are derived from the first-order and second-order moment analysis on the sample plug region. They are proved to be independent and are mainly used as geometric shape factors. For quadratic sample plugs with a known value of $a_0$, there is a unique correspondence between a given sample plug and a combination of these two parameters.

$$Sy1 = \frac{\int W_{sp}x dx}{\int \bar{W}_{sp}dx}/(0.5W) \qquad \in [-1, +1]$$

$$Sy2 = \frac{\int W_{sp}x^2 dx}{\int \bar{W}_{sp}x^2 dx} - 1 \qquad \in [-1, +2]$$

## ANALYSIS ON QUADRATIC SAMPLE PLUGS

In practical situations, the generated sample plugs seldom match the ideal quadratic distribution exactly. However, every sample plug can be approximated with a closest fit by a certain quadratic equation. Plenty of abnormal sample plugs are skipped in this study, because only the 'all-positive' continuous sample plugs are close to the real injections. The valid and invalid sample plugs are determined analytically by the coefficients of $a_1/a_0$ and $a_2/a_0$. The regions for each are divided by several segments in Fig-2, where the portion above the curve refers to valid sample plugs. Cases falling within the rectangular area are mainly studied and examined in current work, because they are close to practice and therefore valuable to be investigated. In Fig-3, five valid (a-e) and two invalid (h-i) sample plugs are shown as typical examples.

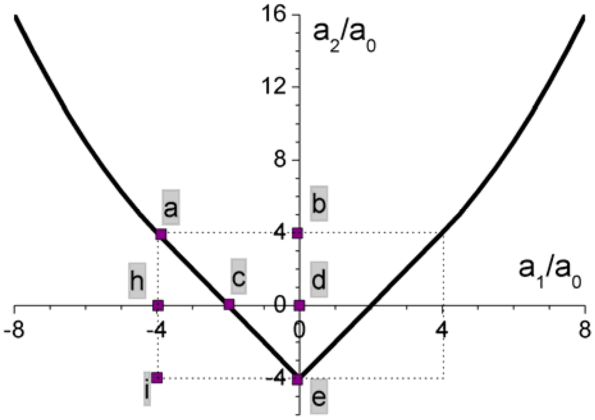


**Fig-2. Regions of valid and invalid quadratic sample plugs**

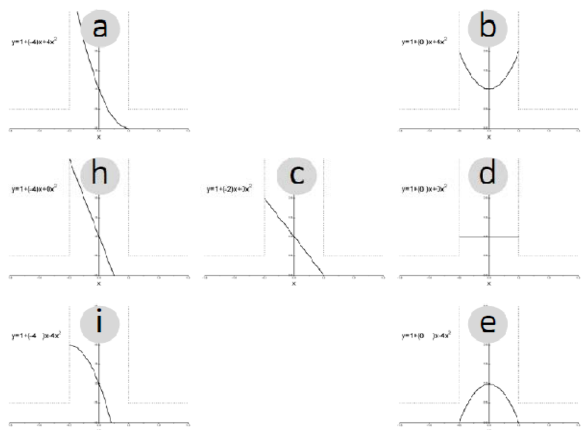


**Fig-3. Demonstration of seven typical sample plugs**

Based on the results of valid sample plugs, the relationship of evaluating parameters and the coefficients of quadratic equations defining sample plugs are revealed by the contour plots in Fig-4 and Fig-5. The plug size has a linear dependence on the coefficient of $a_0$ and $a_2$. The shape of plug with smaller absolute values of evaluating parameters (RMS, Sy1 and Sy2) is more rectangular-like. It was found that the new parameter $Sy12(=\sqrt{(Sy1)^2+(Sy2)^2})$ played a similar role as RMS, but Sy1 and Sy2 cannot be replaced only by RMS. For a given sample plug, it can be characterized by the four evaluating parameters. On the contrary, for a group of pre-determined evaluating parameters, the corresponding quadratic sample plug can be approximated and plotted out visually.

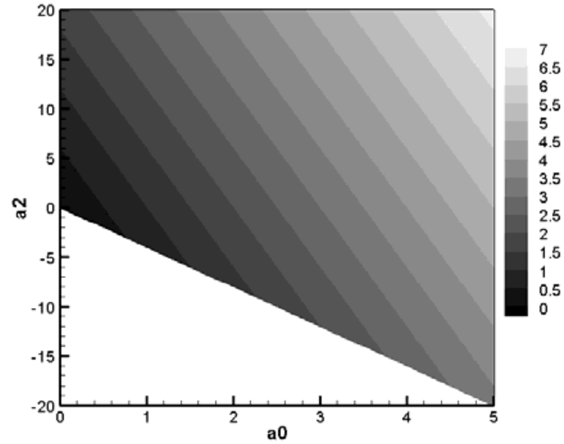


**Fig-4. Relationship of the size evaluating parameter ($\overline{W}_{sp}$) and the coefficients of quadratic equations**

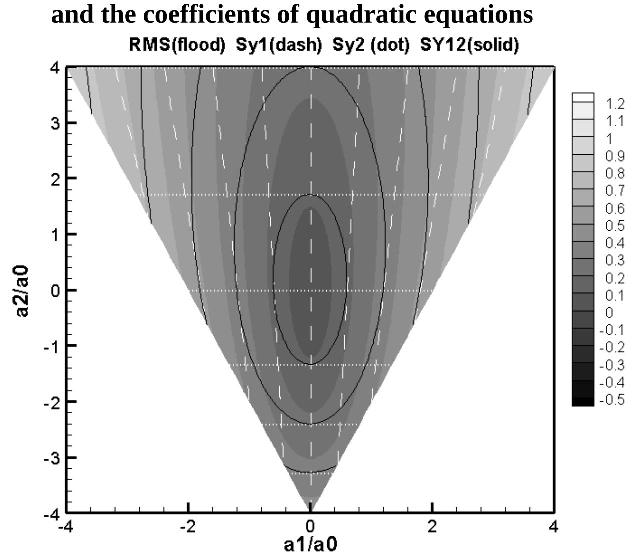


**Fig-5. Relationship of the shape evaluating parameters ($RMS$, $Sy1$, and $Sy2$) and the coefficients**

For future work, we will examine the effectiveness and sensitivity of those parameters on differentiating the overall separation performances. Meanwhile, the results will be validated by experiments and modification will be made based on iterative studies. In a word, the attempts to characterize sample plugs in this study are expected to provide guidance and reference to practical manipulation aiming at producing high quality separations in microchip capillary electrophoresis.

## REFERENCES


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