DETERMINATION OF ELUTION TIME PREDICTION MODEL OF HYDRODYNAMIC CHROMATOGRAPHY THROUGH DIMENSIONAL ANALYSIS

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1. Introduction

Hydrodynamic chromatography (HDC) is one of the many techniques for particle size determination in the nanometer range. It will work for both solid and soluble samples, which are eluted according to their decreasing size (Revillon, 2000).

As the need to develop a model for predicting behavior of a system arises in a number of disciplines. Most of the models were for solving prediction, control, diagnosis and design problems. It is also possible to develop a model for predicting behavior of HDC as a physical system. The model is considered may lead to economical benefits such as reduce chemist working time and materials needed for analysis.

Several models to predict retention time have been proposed and tested using artificial neural network in ion chromatography (Bolanca *et al*, 2006). This study presents the development of elution time prediction model of HDC using dimensional analysis technique.

2. Theoretical Background

According to Buckingham Pi Theorem, any physical system can be expressed by a dimensionally homogeneous relationship simplified in Eq. (1). The application of this technique involves the identification of variables which requires insights on the natural phenomena and the formation of the complete set of dimensionless products of the variables.

$$\pi_d = k\, f(\pi_1)\, f(\pi_2)\, f(\pi_3) \dots f(\pi_n) \quad \text{.......................} \quad (1)$$

where, Π_d = dependent dimensionless Π term; Π_1, Π_2, Π_3, Π_n = independent dimensionless Π term; and k = coefficient.

The Buckingham's Pi theorem provides the basis for generating a set of dimensionless products that satisfy these constraints, which in one form can be stated as follows: If a physical situation is characterised by n variables and r basic dimensions occur in the dimensional representations of these variables, then there are $n-r$ independent dimensionless products that are sufficient to describe the situation.

The dimensionless products, referred to as the π terms, can be arrived at by using a number of different methods, depending on the type of information available. In the present work, the products are formed by partitioning the variable set into basis (r) and performance variables ($n-r$), and then forming products, in turn, of each of the performance variables with the basis variables. The exponents for the basis variables are selected to make these products dimensionless.

3. Elution Time Prediction Model

Dimensional analysis might be a useful tool to study the characteristic of chromatography. Retention time is an example. We expect the factors that will have an effect on the elution time, t, are flow rate (Q), column length (l), diameter of analyte (d_a), and diameter of particle in separation column (d_s). Thus we can express the function as:

$t = f(Q, l, d_a, d_s)$ .... (2)

Those 5 variables cover two numbers of reference dimensions, i.e. L, and T. Therefore, its yield 3 numbers of pis and a set of dimensionless products (pi terms) as follow:

$$\Pi_1 = \phi(\Pi_2, \Pi_3) \quad \text{...} \quad (3)$$

Selecting d_a and Q as the repeating variables, we can get:

$$\Pi_1 = \frac{tQ}{d_a} \; ; \; \Pi_2 = \frac{l}{d_a} \; ; \; \Pi_3 = \frac{d_s}{d_a}$$

Therefore, we can express the result of the dimensional analysis as:

$$\frac{tQ}{d_a} = \phi\left(\frac{l}{d_a}, \frac{d_s}{d_a}\right) \quad \text{..} \quad (4)$$

Learning data for this empirical model was gathered from experimental work using column, Hipresica FQ N2N (3.1 μm and 1.9 μm, 250 x 4.6 mm i.d), flow rate 0.3 mL/min, and colloid size 5 to 78 nm. Fig. 4 and Fig. 5 present the plotting data of Π_1 versus Π_2 and Π_1 versus Π_3 respectively. The data was obtained from previous experiment on hydrodynamic chromatography of silica colloids. The relationship between Π_1 and Π_2 as expressed in equation below:

$$\Pi_1 = 6 * 10^{-5} \Pi_2^{3.03} \quad \text{...} \quad (5)$$

and the relationship between Π_1 and Π_3 is as follow:

$$\Pi_1 = 2 * 10^{11} \Pi_3^{2.86} \quad \text{..} \quad (6)$$

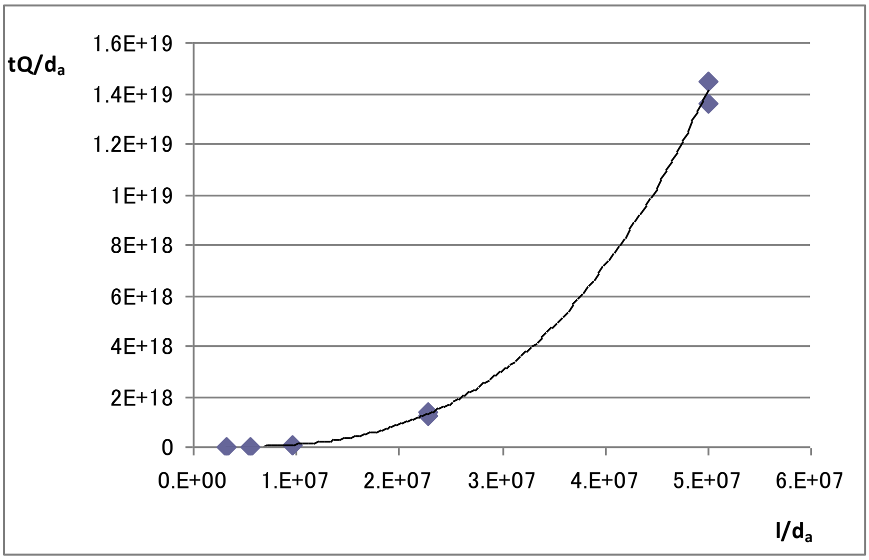

Fig. 4 Relationship between Π_1 and Π_2

Hence, an empirical equation to predict the elution time as follow:

$$t = 2289 \frac{d_a^3}{Q} \left(\frac{l}{d_a}\right)^{1.54} \left(\frac{d_s}{d_a}\right)^{1.45} \quad \text{or} \quad t = \frac{2289 l^{1.54} d_s^{1.45}}{Q d_a^{0.01}}$$

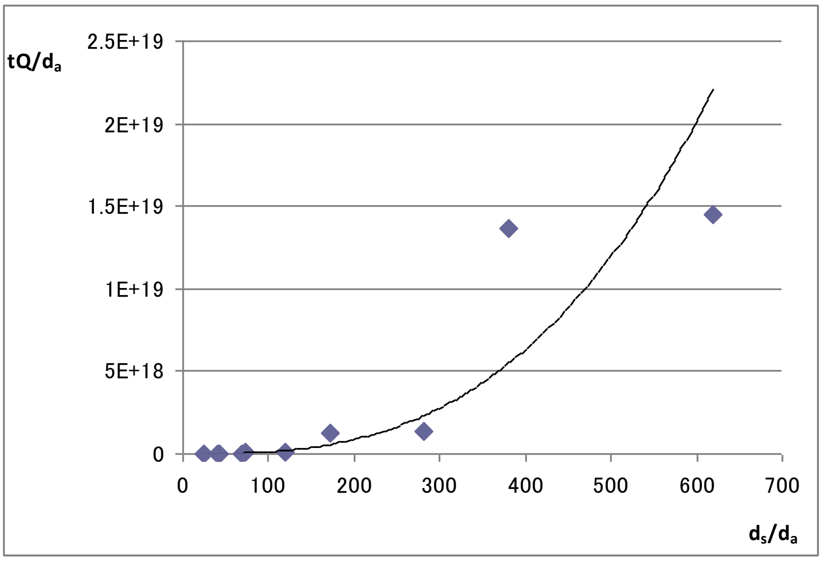

Fig. 5 Relationship between *Π1* and *Π3*

Under 95% confidence limit, it is can be said that there is no significant difference between predicted and observed elution time (Fig. 6). However, it was suggested to add more learning data to reduce error of the prediction model. Data from different column dimensions are required to make the prediction model better.

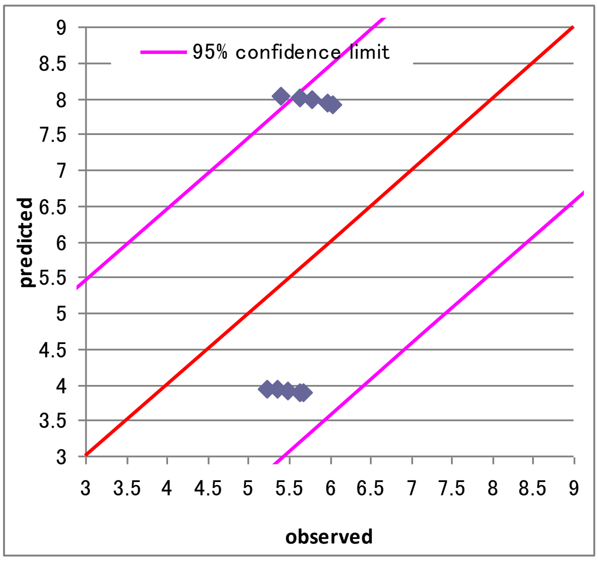

Fig. 6. Comparison of predicted and observed elution time

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