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## TRANSVERSE TEMPERATURE DISTRIBUTIONS IN ISOTACHOPHORESIS COLUMNS OF RECTANGULAR CROSS-SECTION

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### SUMMARY

An analysis of the transient and steady state heat conduction problem in isotachophoresis columns of rectangular cross-section is given, based on a linear variation in electrical conductivity with temperature and accounting for the effects of wall thickness. The predictions are qualitatively similar to those obtained for circular cross-section columns in an earlier paper. The importance of the rectangular column lies in its potential for greater productivity in preparative applications.

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### INTRODUCTION

In an earlier paper<sup>1</sup> we have discussed the problem of radial temperature distribution in isotachophoretic columns of circular cross-section. Here the corresponding problem for a column of rectangular cross-section is discussed.

A detailed discussion of the assumptions made has been given previously<sup>1</sup> and will not be repeated here. Let it suffice that we neglect temperature dependence of properties except for a linear dependence of electrical conductivity on temperature over the range of interest and further assume that convective effects are negligible (our primary interest being in space processing applications<sup>2</sup>).

The resolution of the isotachophoretic process (inter-species front thickness<sup>3</sup>) depends upon the applied electrical field strength which cannot therefore be chosen arbitrarily. Clearly the heat generated per unit volume of the supporting medium also depends upon the electrical field strength and it has been shown<sup>1</sup> that there is thus a maximum size (radial) of column which may be used if the column has circular cross-section.

Similar considerations lead to the determination of a maximum permissible spacing between parallel plates forming the walls of a column of rectangular cross-section. However, the width of the plates may (in principle) be extended indefinitely without altering the thermal balance. It follows that the total volume of sample processed may be increased many times over that for a similar process conducted in a circular column.

Although the conclusions to be drawn from the present analysis will be similar

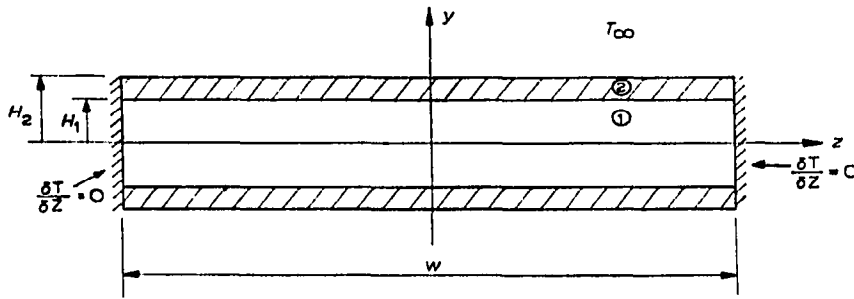


Fig. 1. Geometry of the isotachophoretic column.  $w$  = Width.

to those obtained previously<sup>1</sup>, the quantitative results presented here should be useful to those concerned with the design of isotachophoretic columns.

#### STATEMENT OF THE PROBLEM

The physical arrangement is depicted in Fig. 1. The side walls of the column are supposed to be perfectly insulated ( $\partial T / \partial z = 0$ ) so that we have a conduction problem in the  $y$  direction only provided that the region is sufficiently removed from any separation front. By symmetry we need consider only the upper half plane. Then the statement of the problem in terms of appropriate dimensionless variables is as follows\*:

$$\frac{\partial^2 \theta_1}{\partial \eta \tau} = \frac{\partial \theta_1}{\partial \tau} - S(1 + a\theta_1), \quad 0 \leq \eta \leq \eta_1, \tau > 0$$

$$\frac{\partial^2 \theta_2}{\partial \eta^2} = \frac{K_1}{K_2} \frac{\partial \theta_2}{\partial \tau}, \quad \eta_1 \leq \eta \leq 1, \tau > 0$$

The following conditions must be satisfied:

$$\text{at } \eta = 0, \frac{\partial \theta_1}{\partial \eta} = 0, \theta_1 \text{ is finite.}$$

$$\text{at } \eta = \eta_1, \theta_1 = \theta_2, k_1 \frac{\partial \theta_1}{\partial \eta} = k_2 \frac{\partial \theta_2}{\partial \eta}$$

and

$$\text{at } \eta = 1, \frac{\partial \theta_2}{\partial \eta} + \gamma \theta_2 = 0$$

#### SOLUTIONS

Following methods described elsewhere<sup>1,4</sup> we write

$$\theta(\eta, \tau) = \theta^s(\eta) + \theta^t(\eta, \tau)$$

\* A list of symbols is given on page 49.

where superscripts  $s$  and  $t$  denote steady state and transient components of the solution. Omitting the formal details, the results obtained are given below.

$$\theta_1^s = A_1 \cos(\beta\eta) - \frac{1}{\alpha}, \quad 0 \leq \eta \leq \eta_1$$

$$\theta_2^s = A_2 \left[ (\eta - 1) - \frac{1}{\gamma} \right], \quad \eta_1 \leq \eta \leq 1$$

$$A_1 = \frac{1}{\alpha \left\{ \cos(\beta\eta_1) + \frac{k_1}{k_2} \beta \sin(\beta\eta_1) \left[ (\eta_1 - 1) - \frac{1}{\gamma} \right] \right\}}$$

$$A_2 = -\frac{k_1}{k_2} \beta \sin(\beta\eta_1) A_1$$

$$\theta_j^t = \sum_{r=1}^{\infty} A_r X_{jr}(\eta) e^{-\alpha_j \beta_{jr}^2 \tau} \text{ in region } j, j = 1, 2$$

where

$$\alpha_1 = 1, \alpha_2 = \frac{K_2}{K_1}$$

$$X_{1r} = \cos(\lambda_{1r}\eta)$$

$$X_{2r} = B_r [\cos(\beta_{2r}\eta) + C_r \sin(\beta_{2r}\eta)]$$

$$\lambda_{1r}^2 = \beta_{1r}^2 + \beta^2$$

The Eigenvalues  $\beta_{1r}$  and  $\beta_{2r}$  are related by

$$\beta_{1r}^2 = \alpha_2 \beta_{2r}^2$$

and may be determined from the relationship

$$k_1 \lambda_{1r} \sin(\lambda_{1r} \eta_1) = k_2 \beta_{2r} B_r [\sin(\beta_{2r} \eta_1) - C_r \cos(\beta_{2r} \eta_1)]$$

The coefficients in the above are

$$C_r = \frac{\beta_{2r} \sin(\beta_{2r}) - \gamma \cos(\beta_{2r})}{\beta_{2r} \cos(\beta_{2r}) + \gamma \sin(\beta_{2r})}$$

$$B_r = \frac{\cos(\lambda_{1r} \eta_1)}{\cos(\beta_{2r} \eta_1) + C_r \sin(\beta_{2r} \eta_1)}$$

$$A_r = \frac{\int_0^{\eta_1} [-\theta_1^s] X_{1r} d\eta + \left( \frac{K_1 k_2}{K_2 k_1} \right) \eta_1 \int_{\eta_1}^1 (-\theta_2^s) X_{2r} d\eta}{\int_0^{\eta_1} X_{1r}^2 d\eta + \left( \frac{K_1 k_2}{K_2 k_1} \right) \eta_1 \int_{\eta_1}^1 X_{2r}^2 d\eta}$$

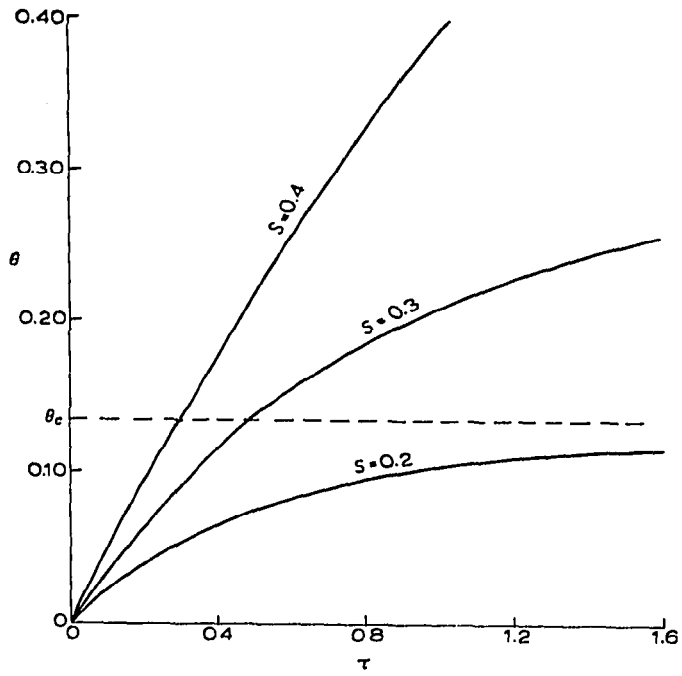


Fig. 2. Centerline transient temperature response for  $\eta_1 = 2/3$ ,  $\gamma = \infty$ ,  $\eta = 0$ .  $\theta_e =$  Maximum permissible  $\theta$ .

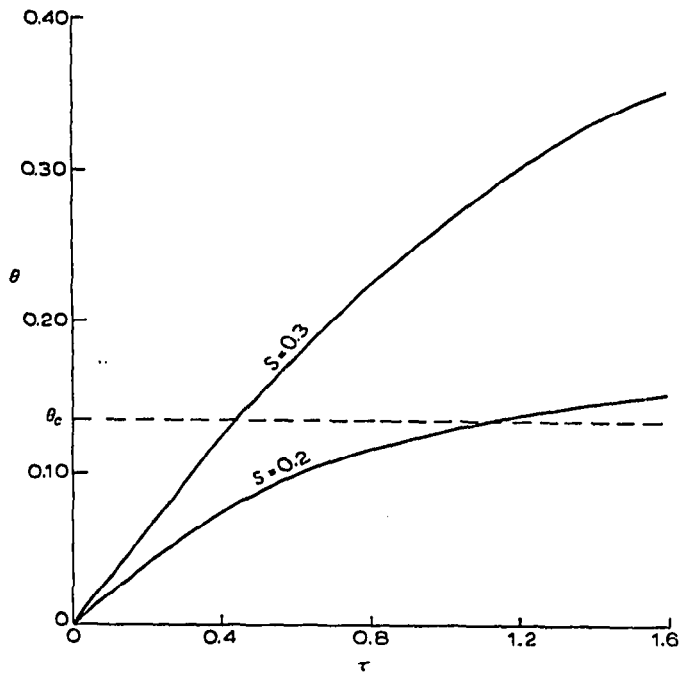


Fig. 3. Centerline transient temperature response for  $\eta_1 = 4/5$ ,  $\gamma = \infty$ ,  $\eta = 0$ .  $\theta_e =$  Maximum permissible  $\theta$ .

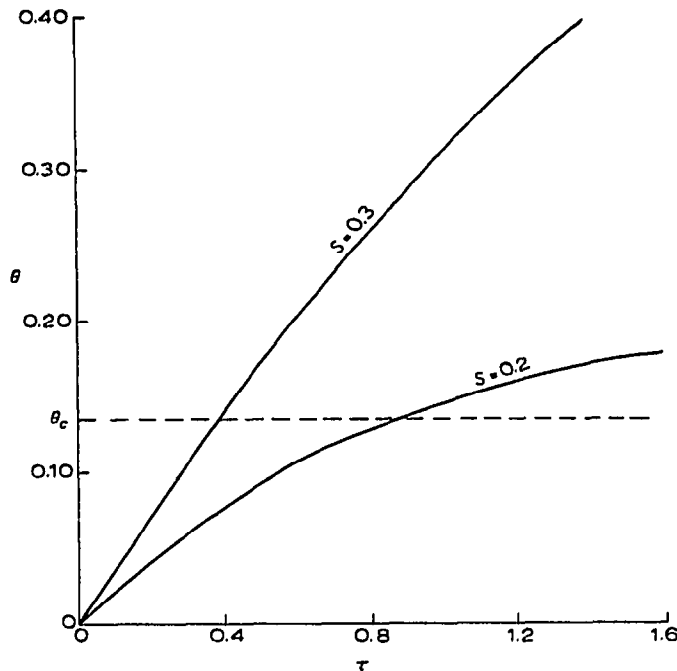


Fig. 4. Centerline transient temperature response for  $\eta_1 = 9/10$ ,  $\gamma = \infty$ ,  $\eta = 0$ .  $\theta_c =$  Maximum permissible  $\theta$ .

#### RESULTS AND DISCUSSION

Numerical calculations were performed on the CDC-6400 computer at the University of Arizona Computer Center. Figs. 2, 3, and 4 show centerline transient temperature response for various heating rates for three different values of the wall thickness parameter  $\eta_1$ . In each case, the dimensionless heat transfer coefficient,  $\gamma$ , is infinite (corresponding to a constant outer wall temperature). The values of the properties used in making these calculations are identical to those used in ref. 1. The maximum allowable value of  $\theta$  ( $\theta_c$ ) is again 0.1355, based on a cooling bath temperature of  $0^\circ\text{C}$  and a maximum allowable temperature in the column of  $37^\circ\text{C}$ .

As can be seen from Figs. 2-4, there exists for each value of  $\eta_1$  a value of  $S$  ( $S_{\max.}$ ) for which  $\theta_c$  is approached asymptotically. The variation of  $S_{\max.}$  with  $\eta_1$  is shown in Fig. 5 for  $\gamma = \infty$ . A comparison with the corresponding plot for the case of radial temperature gradients<sup>1</sup> shows that for a given value of wall thickness parameter, the maximum allowable dimensionless heating rate is considerably less for the rectangular column than for the circular column.

Fig. 6 depicts the steady state temperature profile for various values of  $S$  for  $\eta_1 = 0.8$ . Comparison with the corresponding data for the circular cross-section shows that for given values of wall thickness parameter and dimensionless heating rate, the velocity profiles for the rectangular case will be considerably more "bowed" than for the circular case.

Fig. 7 shows steady state temperature distributions for various values of  $\eta_1$  with the heating rate in each case equal to  $S_{\max.}$ . This figure demonstrates that as in

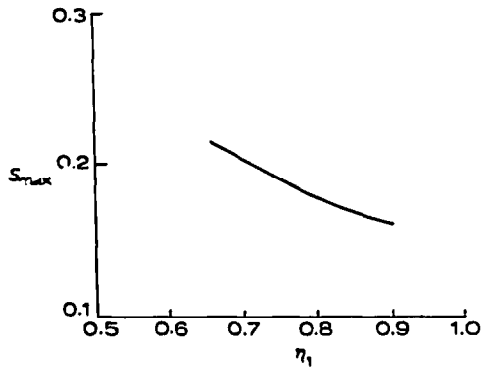


Fig. 5. Variation of maximum heating rate with wall thickness parameter,  $\gamma = \infty$ .

the case of radial temperature gradients, there is an advantage to be gained from the use of thick-walled columns since the total temperature drop within the column (and hence velocity variation or "bowing" effect) is seen to increase considerably with decreasing wall thickness.

The advantage of rectangular over circular cross-section columns is found in their use in preparative applications. The electric field used in either case is determined by resolution requirements<sup>3</sup>, and specification of a given value of wall thickness parameter determines the maximum heating rate allowable in each of the two cases. Specification of both electric field strength and  $S_{max}$ , determines the internal radius for the case of circular cross-section ( $R_1$ ) and the plate spacing for the case of rectangular cross-section ( $2H_1$ ). It is clear from previous discussion that  $R_1 > H_1$ . However, specification of  $R_1$  determines the volume per unit length available for sepa-

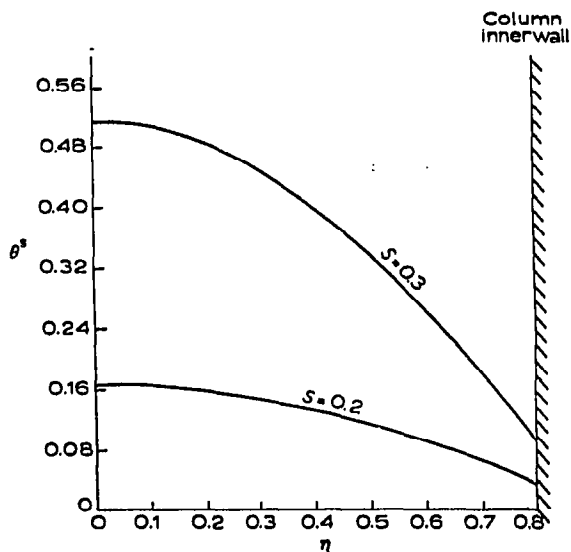


Fig. 6. Steady state temperature profiles based on a linear variation of electrical conductivity with temperature,  $\eta_1 = 0.8$ ,  $\gamma = \infty$ .

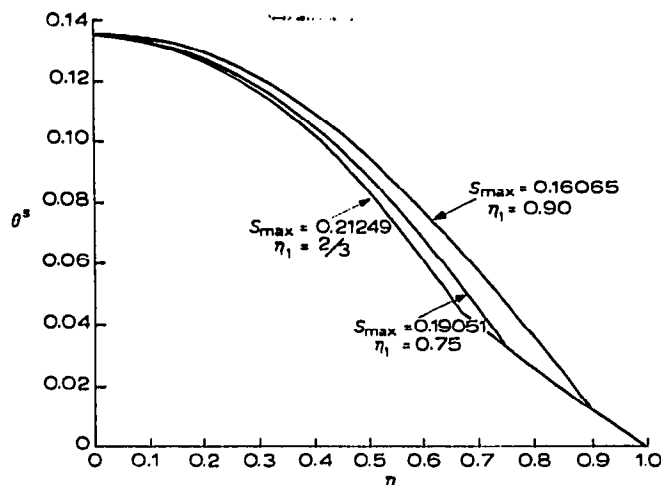


Fig. 7. Steady state temperature profiles for  $S = S_{\max}$ .

ration in a column of circular cross-section whereas the volume per unit length available for separation in a column of rectangular cross-section is dependent not only on  $H_1$ , but also on the width of the plates which may (in principle) be extended indefinitely without altering the thermal balance. It follows that the total volume of sample processed may be increased many times over that for a similar process conducted in a circular column. We hope to be able to provide experimental measurements relevant to this investigation in a future communication.

#### CONCLUSION

An analysis of the transient and steady state heat conduction problem in isotachophoresis columns of rectangular cross-section is seen to produce qualitatively similar results to those obtained for circular cross-section columns. The importance of the rectangular column is seen to lie in its potential for greater productivity in preparative applications.

#### ACKNOWLEDGEMENTS

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#### LIST OF SYMBOLS

- $E$  = Electric field (V/cm)
- $h$  = Heat transfer coefficient [cal/(cm<sup>2</sup> sec °K)]
- $H_1$  =  $y$  coordinate of inside of column wall (cm)

- $H_2$  =  $y$  coordinate of outside of column wall (cm)  
 $J$  = Mechanical equivalent of heat (cal/J)  
 $k$  = Thermal conductivity [cal/(cm sec °K)]  
 $K$  = Thermal diffusivity (cm<sup>2</sup>/sec)  
 $Q_0$  = Heat generation per unit volume evaluated at a  $\theta$  of 0 =  $JE^2\sigma_0$  [cal/(cm<sup>3</sup> sec)]  
 $R_1$  = Internal radius of circular column (cm)  
 $S$  = Dimensionless heating rate =  $Q_0H_2^2/k_1T_\infty$   
 $t$  = Time (sec)  
 $T$  = Temperature (°K)  
 $y$  = Coordinate distance (cm)  
 $z$  = Coordinate distance (cm)  
 $\alpha$  = Dimensionless coefficient of electrical conductivity  
 $\beta$  =  $\sqrt{\alpha S}$   
 $\gamma$  = Dimensionless heat transfer coefficient =  $hH_2/k_2$   
 $\eta$  = Dimensionless coordinate =  $y/H_2$   
 $\eta_1$  = Dimensionless wall thickness parameter =  $H_1/H_2$   
 $\theta$  = Dimensionless temperature =  $(T - T_\infty)/T_\infty$   
 $\sigma_0$  = Electrical conductivity evaluated at  $\theta = 0$  [ $1/(\Omega \text{ cm})$ ]  
 $\tau$  = Dimensionless time =  $K_1t/H_2^2$

### Subscripts

Superscript 1 refers to properties of the electrolyte solution, 2 refers to properties of the column wall and  $\infty$  refers to properties of the cooling bath surrounding the isotachopheresis column.

### Superscripts

Superscript  $s$  refers to steady state conditions and  $t$  refers to transient conditions.

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