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THE EFFECTS OF COLUMN WALLS ON CONCENTRATION AND TEMPERATURE PROFILES FOR SOLUTES WITH HIGH ADSORPTION HEAT

Mateusz Przywara, Marcin Chutkowski, Krzysztof Kaczmariski

Department of Chemical and Process Engineering,
Rzeszow University of Technology, Poland

INTRODUCTION

Modeling of the chromatography process has been an indispensable tool in predicting concentration profiles and understanding the retention phenomena for many years. Recently the authors of papers [1,2] demonstrated theoretically that non-zero adsorption enthalpy and nonlinearity of the adsorption isotherm may be the sources of significant deformations of concentration profiles in HPLC.

However, in these works, the calculations were performed for columns operating in adiabatic conditions, without taking into account the presence of the column wall and, as well as the temperature gradients in the radial direction resulting from the transport of heat. In this work, an extension of the theoretical research presented in the above papers was undertaken to analyze the effects of: (1) the column wall presence and the properties of column wall material (steel, PEEK), (2) the thermal conditions of the column operation (natural convection, water bath), (3) variable column diameter (4) heat of adsorption values on the resulting concentration profiles. Our mathematical model is two-dimensional (z, r direction) which takes into account mass balance for the mobile phase (EDM - Equilibrium Dispersive Model) coupled with heat balance for packing and column wall, and pressure distribution model. The solutions were obtained by the Orthogonal Collocation on Finite Element (OCFE) numerical procedure.

RESULTS OF MODEL SOLUTIONS

Effects of column wall presence, column wall material (stainless steel, PEEK), and the column thermal conditions (adiabatic, natural convection, water bath) on peak profiles were shown in figures.

As can be seen, ignoring the column wall can completely change the outlet concentration profiles. On the other hand, when a wall is taken into account, the peak profiles are similar and slightly depend on the column thermal conditions. Concentration band profiles for $k = 0.001 \text{ W/m}^2/\text{deg}$ (heat is practically not transferred to the surrounding air) and for $k = 10 \text{ W/m}^2/\text{deg}$ (natural convection conditions) are almost identical. When the column wall has higher heat conductivity (steel vs. PEEK), the peaks are slightly broader. Moreover, increasing the column diameter results in lowering the height and increasing the width of the concentration profiles.

CONCLUSION

The obtained solutions confirmed that the listed above process factors (1) - (4) cannot be ignored in prediction of the concentration profiles.

REFERENCES

- [1] Qamar et al., Ind. Eng. Chem. Res. 2018, 57, 2287–2297.
- [2] Khan et al., Ind. Eng. Chem. Res. 2021, 60, 12592–12601.

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