# Efficient numerical methods based on finite volume for handling steep fronts in chromatographic separation processes

Bijan Medi, Mohammad Amanullah*

School of Chemical and Biomedical Engineering, 62 Nanyang Drive, Nanyang Technological University, Singapore-637459
*Corresponding author (E-mail: Aman@ntu.edu.sg)

Steep fronts and shock layers are probable to occur in chromatographic separation processes. As long as there is no analytical solution for the governing differential equation which is most often the case, effective numerical methods must be utilized for speed and accuracy. Literature reports that conventional numerical methods such as ordinary finite difference are not capable of capturing the true effects of steep fronts efficiently (Czok and Guiochon 1990). Therefore, as an alternative, high resolution techniques, e.g. orthogonal collocation on finite elements, have been applied that provide reasonable accuracy (Gu, Truei et al. 1992). However, these methods are computationally expensive which makes their application inconvenient for solving large scale optimization problems, such as using genetic algorithm (Amanullah and Mazzotti 2006), and on-line optimizing control (Grossmann, Amanullah et al. 2008).

Correct estimation of flux terms is critically important in convection dominant (advection) problems including equilibrium theory and more realistic models in adsorption processes. Finite volume technique is conventionally used in the field of computational fluid dynamics to cope with this demand but it is unexplored in the chromatographic separation processes (Vasconcellos, Neto et al. 2003; Cruz, Santos et al. 2005). This method is capable of enforcing the integral form of conservation laws effectively on each discretized cell (Versteeg and Malalasekra 1996). As a result, finite volume appears advantageous over both finite elements and finite difference techniques. Due to its integral form of analysis, one can use a tailor-made scheme for prediction of flux terms at cell boundaries. In contrast, use of a tailor-made scheme is not possible in finite difference for the very nature of this technique. In orthogonal collocation, the goal is to minimize the estimation error by allocating a suitable functional form without considering the realistic convective nature of the problem (Kaczmarski, Mazzotti et al. 1997). Therefore, while finite volume inherits its simplicity from finite difference, it can provide a good level of accuracy and has the prospect of being a unique choice for fast, stable and accurate numerical solutions.

In this paper, a systematic approach based on accuracy, stability, and computational time has been taken to investigate the efficacy of different numerical techniques, including finite volume, for chromatographic separation processes in both convection-dominant and convection-diffusion problems. Simulation results indicate superior speed and accuracy of finite volume comparing to other methods.

Amanullah, M. and M. Mazzotti (2006). "Optimization of a hybrid chromatography-crystallization process for the separation of troger's base enantiomers." Journal of Chromatography A **1107**(1-2): 36-45.

Cruz, P., J. C. Santos, et al. (2005). "Simulation of separation processes using finite volume method." Computers & Chemical Engineering **30**(1): 83-98.

Czok, M. and G. Guiochon (1990). "Comparison of the results obtained with different models for the simulation of preparative chromatography." Computers & Chemical Engineering **14**(12): 1435-1443.

Grossmann, C., M. Amanullah, et al. (2008). "Optimizing control of simulated moving bed separations of mixtures subject to the generalized langmuir isotherm." Adsorption **14**(2-3): 423-432.

Gu, T., Y. H. Truei, et al. (1992). "Modeling of gradient elution in multicomponent nonlinear chromatography." Chemical Engineering Science **47**(1): 253-262.

Kaczmarski, K., M. Mazzotti, et al. (1997). "Modeling fixed-bed adsorption columns through orthogonal collocations on moving finite elements." Computers and Chemical Engineering **21**(6): 641-660.

Vasconcellos, J. F. V., A. J. S. Neto, et al. (2003). "An inverse mass transfer problem in solid-liquid adsorption systems." Inverse Problems in Engineering **11**(5): 391-408.

Versteeg, H. and W. Malalasekra (1996). An introduction to computational fluid dynamics: The finite volume method Prentice Hall.