

Application of CFD in the Study of Supercritical Fluid Extraction with Structured Packing: Pressure Drop Calculations

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Abstract

Supercritical fluid extraction (SFE) from the liquid phase is usually carried out in packed columns with structured packings, particularly those of the gauze type. Structured packing performs very well for SFE, mainly because of their relatively large surface area and free volume. Nevertheless, it also has important disadvantages such as high cost, low capacities at high flow rates, premature flooding, and entrainment of the liquid phase due to low density differences. The assessment of the real efficiencies of structured packings poses extreme difficulties related to the moderately high pressures involved in SFE processes.

Recently, Computational Fluid Dynamics (CFD) has been used to characterize the complex multi-phase flow inside packed columns and to evaluate the influence of packing shape and geometry on the hydrodynamics and mass and heat transfer rates. Here, we present and discuss two different geometrical models that represent the structured gauze packing (Sulzer EX) that fills our pilot-scale SFE column.

The first model consists of two contacting corrugated sheets enclosed in a box; this model focuses on the space between two packing sheets. The presence of neighboring packing sheets is accounted for by applying periodic conditions on the boundaries perpendicular to the main flow direction.

The second geometric model consists of thirteen contacting packing sheets enclosed in a cylinder. In this case, the model tries to mimic a full packing element, even though we only simulate one third of the height of the actual packing element due to computational constraints. Periodicity is imposed on the flow in order to determine the fully developed flow field and estimate pressure drops for the whole column.

For both models, the flow field is computed using a standard $k - \epsilon$ turbulence model. Our CFD models are validated by comparing simulation results and the pressure-drop data sets of Stockfleth and Brunner, Meyer (carbon dioxide at temperatures ranging from 313 to 393K and pressures ranging from 10.1 to 30 MPa) and Olaño et al (data obtained with air at ambient pressure).

The final objective of our work is to model the complex multi-phase transport phenomena present in SFE columns with structured packing in order to predict exchange rates and to optimize the process. The first stage, presented here, consists in an accurate modeling of the hydrodynamics inside the relatively complex geometry of the structured packing.

Keywords: Pressure drop, CFD modeling, structured packing, supercritical fluids

References

- [1] G. Brunner, *Industrial process development in Countercurrent multistage gas extraction (SFE) processes*, J. Supercrit.Fluids , Vol. 12, 283, 1998.
- [2] F. Haghshenas, M. Zivdar, R. Rahimi, M. N. Esfahany, A. Afacan, K. Nandakumar, K. T. Chuang, *CFD simulation of mass transfer efficiency and pressure drop in a structured packed distillation column*, Chem. Eng. Technol., Vol. 30(7), 854-861, 2007.
- [3] Jens-Torge Meyer, *Druckverlust um Flutpunkte im Hochdruckgegenstromkolonnen mit berkritischen Kohlendioxid*, PhD Dissertation, Technische Universitt Hamburg-Harburg, Germany, 1998.
- [4] S. Olao, S. Nagura, H. Kosuge, K. Asano, *Mass transfer in binary and ternary distillation by a packed column with structured packing*, J. Chem. Eng. Japan, Vol. 28(6), 1995.
- [5] M. McHugh, V. Krukonis, *Supercritical Fluid Extraction: Principles and Practice*, Butterworths, Stoneham.
- [6] R. Stockfleth, G. Brunner, *Hydrodynamics of a packed countercurrent column for the gas extraction*, Ind. Eng. Chem., Vol. 38, 1999.
- [7] R. Stockfleth, G. Brunner, *Holdup, pressure drop and flooding in packed countercurrent columns for the gas extraction*, Ind. Eng. Chem., Vol. 40, 2001.