

Attarakih, Menwer; Hlawitschka, Mark W.; Abu-Khader, Mazen; Al-Zyod, Samer; Bart, Hans-Jörg

CFD-population balance modeling and simulation of coupled hydrodynamics and mass transfer in liquid extraction columns. (English) [Zbl 1443.76008](#)

Appl. Math. Modelling 39, No. 17, 5105-5120 (2015).

Summary: A hierarchical approach for modeling and simulation of coupled hydrodynamics and mass transfer in liquid extraction columns using detailed and reduced bivariate population balance models is presented. The hierarchical concept utilizes a one-dimensional CFD model with detailed bivariate population balances. This population balance model is implemented in the PPBLAB software which is used to optimize the column hydrodynamics. The optimized droplet model parameters (droplet breakage and coalescence) are then used by a two-dimensional CFD reduced population balance model. As a reduced bivariate population balance model, OPOSPM (One Primary and One Secondary Particle Method) is implemented in the commercial FLUENT software to predict the coupled hydrodynamics and mass transfer of an RDC extraction column with 88 compartments. The simulation results show that the coupled two-dimensional-OPOSPM model produces results that are very close to that of the one-dimensional PPBLAB detailed population balance model. The advantages of PPBLAB are the ease of model setup, implementation and the reduced simulation time (order of minutes), when compared to the computational time (order of weeks) and computational resources using FLUENT software. The advantages of the two-dimensional CFD model is the direct estimation of the turbulent energy dissipation using the $k - \epsilon$ model and the local resolution of continuous phase back mixing.

MSC:

76-10 Mathematical modeling or simulation for problems pertaining to fluid mechanics

76T10 Liquid-gas two-phase flows, bubbly flows

Keywords:

liquid extraction; OPOSPM; CFD; population balance; PPBLAB; fluent

Software:

FLUENT; PPBLAB; LLECMOD

Full Text: [DOI](#)

References:

- [1] Gerstlauer, A.; Gahn, C.; Zhou, H.; Rauls, M.; Schreiber, M., Application of population balances in the chemical industry—current status and future needs, *Chem. Eng. Sci.*, 61, 205-217 (2010)
- [2] Tiwari, S.; Drumm, C.; Attarakih, M. M.; Kuhnert, J.; Bart, H.-J., Coupling of the CFD and the Droplet population balance equation with finite poinset method, (Griebel, M.; Schweitzer, M. A., *Lecture Notes in Computational Science and Engineering: Meshfree Methods for Partial Differential Equations IV*, vol. 65 (2008), Springer Verlag: Springer Verlag Heidelberg), 315-334
- [3] Attarakih, M.; Bart, H.-J.; Faqir, N., Numerical solution of the bivariate population balanced equation for the interacting hydrodynamics and mass transfer in liquid-liquid extraction columns, *Chem. Eng. Sci.*, 61, 113-133 (2006)
- [4] Kalem, M.; Buchbender, F.; Pfennig, A., Simulation of hydrodynamics in RDC extraction columns using the simulation tool “ReDrop”, *Chem. Eng. Res. Des.*, 89, 1-9 (2011)
- [5] Attarakih, M.; Bart, H.-J.; Steinmetz, T.; Dietzen, M.; Faqir, N., LLECMOD: A bivariate population Balance simulation tool for liquid-liquid extraction columns, *Open Chem. Eng. J.*, 2, 10-34 (2008)
- [6] Attarakih, M.; Jildeh, H. B.; Mickler, M.; Bart, H.-J., The OPOSPM as a nonlinear autocorrelation population balance model for dynamic simulation of liquid extraction columns, *Comput. Aided Chem. Eng.*, 31, 1216-1220 (2012)
- [7] Attarakih, M.; Al-Zyod, S.; Abu-Khader, M.; Bart, H.-J., PPBLAB: A new multivariate population balance environment for particulate system modelling and simulation, *Procedia Eng.*, 42, 1574-1591 (2012)
- [8] Attarakih, M., Integral formulation of the population balance equation: application to particulate systems with particle growth, *Comput. Chem. Eng.*, 48, 1-13 (2013)
- [9] Attarakih, M.; Albaraghtli, T.; Abu-Khader, M.; Al-Hamamre, Z.; Bart, H.-J., Mathematical modeling of high- pressure

- oil-splitting reactor using a reduced population balance model, *Chem. Eng. Sci.*, 84, 276-291 (2013)
- [10] Mohanty, S., Modelling of liquid-liquid extraction column: a review, *Rev. Chem. Eng.*, 16, 199-248 (2000)
- [11] Silva, L. F.L. R.; Lage, P. L.C., Development and implementation of a polydispersed multiphase flow model in OpenFOAM, *Comput. Chem. Eng.*, 35, 2653-2666 (2011)
- [12] Drumm, C.; Attarakih, M. M.; Bart, H.-J., Coupling of CFD with DPBM for an RDC extractor, *Chem. Eng. Sci.*, 64, 721-732 (2009)
- [13] Drumm, C.; Attarakih, M.; Hlawitschka, M. W.; Bart, H.-J., One-group reduced population balance model for cfd simulation of a pilot-plant extraction column, *Ind. Eng. Chem. Res.*, 49, 3442-3451 (2010)
- [14] Hlawitschka, M. W.; Jaradat, M.; Chen, F.; Attarakih, M. M.; Kuhnert, J.; Bart, H.-J., A CFD-Population balance model for the simulation of Kühni extraction column, *Comput. Aided Chem. Eng.*, 29, 2011, 66-70 (2011)
- [15] Hlawitschka, M. W.; Bart, H. J., Determination of local velocity, energy dissipation and phase fraction with LIF- and PIV-measurement in a Kühni miniplant extraction column, *Chem. Eng. Sci.*, 69, 138-145 (2013)
- [16] Hlawitschka, M. W.; Bart, H.-J., CFD-Mass transfer simulation of an RDC column, *Comput. Aided Chem. Eng.*, 31, 920-924 (2013)
- [17] Buffo, A.; Vanni, M.; Marchisio, D. L., Multidimensional population balance model for the simulation of turbulent gas-liquid systems in stirred tank reactors, *Chem. Eng. Sci.*, 70, 31-44 (2012)
- [18] Modes, G.; Bart, H.-J., CFD simulation of nonideal dispersed phase flow in stirred extraction columns, *Chem. Eng. Tech.*, 24, 1342-1345 (2001)
- [19] Drumm, C.; Bart, H.-J., Hydrodynamics in a RDC extractor: single and two-phase PIV measurements and CFD simulations, *Chem. Eng. Tech.*, 29 (2006), 1397-1302
- [20] Drumm, C.; Tiwari, S.; Kuhnert, J.; Bart, H.-J., Finite Pointset Method for simulation of the liquid-liquid flow field in an extractor, *Comput. Chem. Eng.*, 32, 2946-2957 (2008)
- [21] Attarakih, M. M.; Drumm, C.; Bart, H.-J., Solution of the population balance equation using the sectional quadrature method of moments (SQMOM), *Chem. Eng. Sci.*, 64, 742-752 (2009)
- [22] Godfrey, J. C.; Slater, M. J., *Liquid-Liquid Extraction Equipment* (1994), John Wiley & Sons: John Wiley & Sons Chichester
- [23] Kislik, V. S., *Solvent Extraction: Classical and Novel Approaches* (2011), Elsevier: Elsevier Amsterdam
- [24] Wang, F.; Mao, Z.-S., Numerical and experimental investigation of liquid-liquid two-phase flow in stirred tanks, *Ind. Eng. Chem. Res.*, 44, 5776-5787 (2005)
- [25] Schmidt, S. A.; Simon, M.; Attarakih, M. M.; Lagar, G.; Bart, H.-J., Droplet population balance modelling—hydrodynamics and mass transfer, *Chem. Eng. Sci.*, 61, 246-256 (2006)
- [26] Brennen, C. E., *Fundamentals of Multiphase Flows* (2005), Cambridge University Press: Cambridge University Press New York
- [27] Attarakih, M. M.; Jaradat, M.; Drumm, C.; Bart, H.-J.; Tiwari, S.; Sharma, V. K.; Kuhnert, J.; Klar, A., A multivariate population balance model for liquid extraction columns, *Comput. Aided Chem. Eng.*, 26, 1339-1344 (2009)
- [28] Wesselingh, J. A.; Bollen, A. M., Single particles, bubbles and drops: their velocities and mass transfer coefficients, *Trans. Inst. Chem. Eng.*, 77, 89-96 (1999)
- [29] Ribeiro, L. M.; Regueiras, P. F.R.; Guimaraes, M. M.L.; Madureira, C. M.N.; Cruz-Pinto, J. J.C., The dynamic behavior of liquid-liquid agitated dispersions II. Coupled hydrodynamics and mass transfer, *Comput. Chem. Eng.*, 21, 543-558 (1997)
- [30] Coulaloglou, C. A.; Tavlarides, L. L., Description of interaction processes in agitated liquid-liquid dispersions, *Chem. Eng. Sci.*, 32, 1389-1397 (1977)
- [31] Shinnar, R.; Church, J. M., Predicting particle size in agitated dispersions, *Ind. Eng. Chem.*, 52, 253-256 (1960)
- [32] Liao, Y.; Lucas, D., A literature review on mechanisms and models for the coalescence process of fluid particles, *Chem. Eng. Sci.*, 65, 2851-2864 (2010)
- [33] Wegener, M.; Paschedag, A. R.; Kraume, M., Mass transfer enhancement through marangoni instabilities during single drop formation, *Int. J. Heat Mass Transfer*, 52, 2673-2677 (2009)
- [34] Attarakih, M.; Abu-Khader, M.; Bart, H.-J., Modelling and dynamic analysis of a rotating disc contactor (RDC) extraction column using One Primary and One Secondary Particle Method (OOSPM), *Chem. Eng. Sci.*, 91, 180-196 (2013)
- [35] Kumar, A.; Hartland, S., Correlations for prediction of mass transfer coefficients in single drop systems and liquid-liquid extraction columns, *Chem. Eng. Res. Des.*, 77, 372-384 (1999)
- [36] Amanabadi, M.; Bahmanyar, H.; Zarkeshan, Z.; Mousavian, M. A., Prediction of effective diffusion coefficient in rotating disc columns and application in design, *Chin. J. Chem. Eng.*, 17, 366-372 (2009)
- [37] Zhang, S. H.; Yu, S. C.; Zhou, Y. C.; Su, Y. F., Model for liquid-liquid extraction column performance - the influence of drop size distribution on extraction efficiency, *Canad. J. Chem. Eng.*, 63, 213-226 (1985)
- [38] Young, C. H.; Korchinsky, W. J., Modelling drop-side mass transfer in agitated polydispersed liquid-liquid systems, *Chem. Eng. Sci.*, 44, 2355-2361 (1989)
- [39] Handlos, A. E.; Baron, T., Mass and heat transfer from drops in liquid-liquid extraction, *AIChE J.*, 3, 127-136 (1957)
- [40] Kronig, R.; Brink, J., On the theory of extraction from falling droplets, *Appl. Sci. Res.*, A2, 142-154 (1950)
- [41] Alopaeus, V.; Koskinen, J.; Keskinen, K. I.; Majander, J., Simulation of the population balances for liquid-liquid systems in a nonideal stirred tank: Part 2- parameter fitting and the use of multiblock model for dense dispersions, *Chem. Eng. Sci.*, 57,

1815-1825 (2002)

This reference list is based on information provided by the publisher or from digital mathematics libraries. Its items are heuristically matched to zbMATH identifiers and may contain data conversion errors. It attempts to reflect the references listed in the original paper as accurately as possible without claiming the completeness or perfect precision of the matching.