

Figure 11: Comparison of the simulation and the optimization mole fraction profiles of water

The other profile (given in Figure 11) considered in this work was that of the water given as the by-product of the process. According to the figure, the mole fraction of water obtained from the initial simulated process was found to be higher than that of the optimized one. This was an indication that less water was being produced in the reaction section of the column of the optimized process than in the initial simulated one.

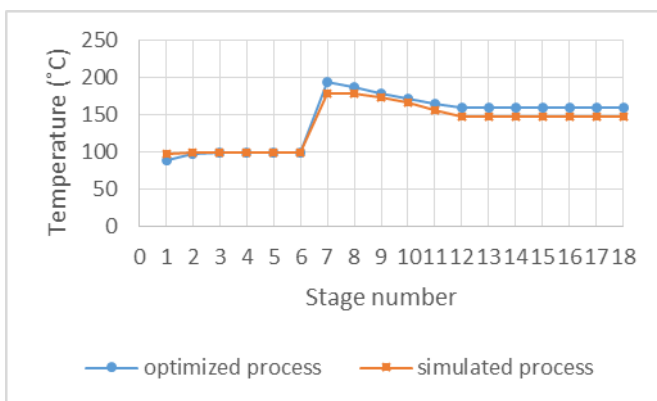


Figure 12: Comparison of the simulation and the optimization temperature profiles of the process

Shown in Figure 12 is the comparison between the temperature profiles of the optimized and the simulated process. From the figure, it was found that the highest temperatures of both of the processes occurred at the reaction section of the column, as discussed earlier in the case of the simulated process. Also noticed was that the temperatures of the optimized process (using Box algorithm), especially from the reaction section down to the reboiler, were higher than those of the simulated one. This could be seen from the higher reboiler duty of the optimized process than that of the simulated one.

4. Conclusion

The results obtained from the simulation of the reactive distillation process used to produce methyl palmitate (a fatty acid methyl ester (FAME)) carried out in this work revealed that FAME can be produced successfully using reactive distillation process because the developed model was able to converge when simulated to give a FAME product having a mole fraction of 0.648. Furthermore, the optimization of the

process revealed that higher purity than that (0.648) could be obtained using Box optimization algorithm because the result of the objective function, which was the maximization of the mole fraction of the FAME obtained from the bottom section of the column was achieved to be 0.7995. The results given by the simulation of the process using the optimum values (reflux ratio of 1.5, feed ratio of 1.181, and reboiler duty of 2.626e+06 kJ/hr) obtained showed that they were theoretically valid. Finally, it has been seen that the Aspen HYSYS model developed in this research work can be used to represent, simulate and optimize a reactive distillation process successfully. It is recommended that, at least, an experiment should be carried out to experimentally validate the optimum values of the manipulated parameters obtained in this work.

5. Acknowledgement

Special thanks go to Aare Afe Babalola (SAN), The Founder, and the Management of Afe Babalola University, Ado-Ekiti, Ekiti State, Nigeria for providing a very conducive environment to carry out this research.

6. Nomenclature

Bottom Bottom product
 FAME Fatty acid methyl ester
 M-palmitate Methyl palmitate
 Q_C Condenser duty (kJ/hr)
 Q_R Reboiler duty (kJ/hr)
 RD Reactive Distillation
 SQP Sequential Quadratic Programming
 Top Top product

References

- [1] Aspen. 2012. Aspen HYSYS V8.0 [27.0.0.38]. Aspen Technology, USA.
- [2] Giwa, A. 2012. Steady-State Modeling of n-Butyl Acetate Transesterification Process Using Aspen PLUS: Conventional versus Integrated. *ARPN Journal of Engineering and Applied Sciences*, 7(12), 1555-1564.
- [3] Giwa, A. 2013. Sensitivity Analysis of ETBE Production Process Using Aspen PLUS. *International Journal of Advanced Scientific and Technical Research*, 3(1), 293-303.
- [4] Giwa, A. and Giwa, S. O. (2012). Optimization of Transesterification Reaction Integrated Distillation Column Using Design Expert and Excel Solver. *International Journal of Advanced Scientific and Technical Research*, 2(6), 423-435.
- [5] Giwa, A. and Giwa, S. O. (2013). Isopropyl Myristate Production Process Optimization Using Response Surface Methodology and MATLAB. *International Journal of Engineering Research and Technology*, 2(1), 1-10.
- [6] Giwa, A., Bello, A. and Giwa, S. O. (2014). Performance Analyses of Fatty Acids in Reactive Distillation Process for Biodiesel Production. *International Journal of Scientific & Engineering Research*, 5(12), 529-540.

- [7] Giwa, A., Giwa, S. O., Bayram, İ. and Karacan, S. (2013). Simulations and Economic Analyses of Ethyl Acetate Productions by Conventional and Reactive Distillation Processes Using Aspen Plus. *International Journal of Engineering Research & Technology*, 2(8), 594-605.
- [8] Karacan, S. and Karacan, F. (2014). Simulation of Reactive Distillation Column for Biodiesel Production at Optimum Conditions. *Chemical Engineering Transactions*. 39, 1705-1710.
- [9] Kusmiyati, K., and Sugiharto, A. (2010). Production of Biodiesel from Oleic Acid and Methanol by Reactive Distillation. *Bulletin of Chemical Reaction Engineering & Catalysis*, 5 (1), 2010, 1-6.
- [10] Martins, M. I., Pires, R. F., Alves, M. J., Hori, C. E., Reis, M. H. and Cardoso, V. L. (2013). Transesterification of Soybean Oil for Biodiesel Production Using Hydrotalcite as Basic Catalyst. *Chemical Engineering Transactions*, 32, 817-822.
- [11] Murat, M.N., Mohamed, A. and Bhatia, S. (2003). Modeling of a Reactive Distillation Column: Methyl Tertiary Butyl Ether (MTBE) Simulation Studies. *IJUM Engineering Journal*, 4(2), 13-30.
- [12] Nwambunwo, S. C. (2015). Modelling, Simulation and Optimization of Fatty Acid Methyl Ester Reactive Distillation Process Using Aspen HYSYS. B.Eng. Thesis (Unpublished). *Afe Babalola University, Ado-Ekiti*, Ekiti State, Nigeria, 1-46.
- [13] Pöpken, T., Steinigeweng, S. and Gmehling, J. (2001). Synthesis and Hydrolysis of Methyl Acetate by Reactive Distillation Using Structured Catalytic Packing: Experimental and Simulation. *Industrial and Engineering Chemistry Resources*, 40, 1566-1574.
- [14] Samakpong, M., Pawit, T. and Apichit, S. (2012). Process Simulation and Optimization of Biodiesel Production using Reactive Distillation from Rubber Seed Oil. *Pure and Applied Chemistry International Conference*, 653-655.
- [15] Seader, J.D. and Henley, E. J (2006). *Separation process principle*. Wiley John Wiley & Sons Incorporation, New Jersey, USA.
- [16] Simasatitkul, L., Siricharnsakunchai, P., Patcharavorachot, Y., Assabumrungrat, S. and Arpornwichanop, A. (2011). Reactive Distillation for Biodiesel Production from Soybean Oil. *Korean Journal of Chemical Engineering*, 28(3), 649– 655.
- [17] Taylor, R. and Krishna, R. (2000). Review: Modeling Reactive Distillation. *Chemical Engineering Science*, 55, 5183-5229.

Author Profile



Samson Chukwufumnanya NWAMBUONWO was born in Lagos State, Nigeria in 1992. He received his Bachelor Degree in Chemical Engineering from Afe Babalola University, Ado-Ekiti, Ekiti State, Nigeria in 2015 with *First Class Honours*. He had his internship programme of his undergraduate programme under Pan Ocean Oil Cooperation University Internship Programme (Scholarship) where he learnt about gas and crude oil processing in the Pan Ocean gas plant processing facility and flow station.



Dr. Abdulwahab GIWA was born in Ile-Ife, Osun State, Nigeria in 1976. He obtained his National Diploma in Chemical Engineering from Kaduna Polytechnic, Kaduna, Nigeria in 1998 with a *Distinction* Grade as the Best Student of the Programme. Furthermore, he received his Bachelor Degree in Chemical Engineering from Federal University of Technology, Minna, Nigeria in 2004 with *First Class Honours* as the Best Student in School of Engineering and Engineering Technology. Moreover, he got his PhD Degree from Ankara University, Ankara, Turkey in 2012, also in the field of Chemical Engineering, with a Cumulative Grade Point Average (CGPA) of *4.00 out of 4.00*. Thereafter, he proceeded to Middle East Technical University, Ankara, Turkey to have his Postdoctoral research experience. He is currently a Senior Lecturer with the Department of Chemical and Petroleum Engineering, Afe Babalola University, Ado-Ekiti, Ekiti State, Nigeria. He is very interested in researches in the areas of Process Modelling, Simulation, Optimization, Design and Control.

Appendix

Table A1: Some basic properties of the process components

Component	Molecular weight (kg/kgmol)	Boiling point (°C)	Density (kg/m ³)
Palmitic acid	256.4	351.0	881.6
Methanol	32.04	64.65	795.7
Methyl palmitate	270.5	326.1	880.0
Water	18.02	100.0	998.0

Source: Aspen, 2012