



## **Systematic computer aided methods and tools for lipid process technology**

Olivia A. Perederic<sup>1</sup>, Bent Sarup<sup>2</sup>, John M. Woodley<sup>1</sup>, Georgios M. Kontogeorgis<sup>1</sup>

*1 Department of Chemical and Biochemical Engineering, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark; 2 Vegetable Oil Technology Business Unit, Alfa Laval Copenhagen A/S, DK-2860 Søborg;*

\*gk@kt.dtu.dk

### **Highlights**

- State of the art for lipid phase equilibria.
- Systematic identification method for lipid predictive tools improvement.
- Process design and analysis of shea oil fractionation using developed tools.

### **1. Introduction**

Today, chemical engineering methods and tools are widely used for the development and analysis of various processes across different industries. The thermodynamic properties of the involved chemicals, and the models used to describe them, represent the foundation of all the methods and tools used. In recent years, there has been an increasing interest in lipid compounds and their mixtures, which are used in a wide range of applications and industries. A detailed analysis of data and model availability for lipid compounds shows that there is still a need for predictive tools to cover the gaps where experimental data are missing.

The aim of this work is to develop, validate and apply systematic methods and tools for the lipid process technology. Thermodynamic and process aspects of the problem are considered: a systematic method for data analysis and phase equilibria modelling, application of the developed models to lipids processing alongside process modelling, design, analysis and improvement. Particular attention has been given to specialty fats processing using solvent, such as shea oil acetone fractionation. The most important aspects of the process are solvent recovery and product purification of solvent residues.

### **2. Methods**

The detailed analysis of data and models available in the literature for lipid compounds and mixtures was performed and discussed. Further, a systematic method for data analysis and phase equilibria modelling was used for estimate new interaction parameters for lipid compounds. The aim of the method is to improve the quality of phase equilibria prediction for the selected group contribution based methods. The results obtained were used to perform the process modelling, design and analysis for shea oil solvent fractionation process using various tools.

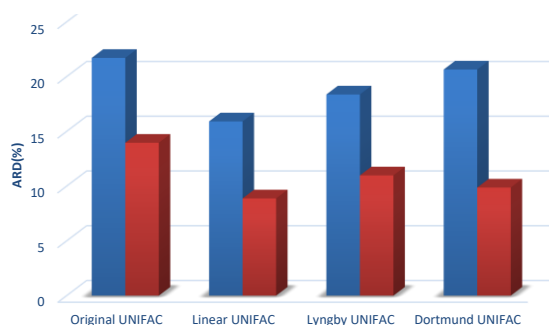
### **3. Results and discussion**

Different models, from EoS to activity and combined models are used to describe lipid phase equilibria. The general trend for increasing deviation of VLE correlation using different activity coefficient models is: NRTL  $\approx$  Wilson < UNIQUAC. The SLE trend for increasing deviation is:

UNIQUAC < Wilson  $\approx$  NRTL. For LLE, NRTL and UNIQUAC prove to have similar performance and both can be used to describe lipid LLE. Although these models provide good predictions, there are a limited number of interaction parameters which cover only a few classes of lipid compounds (e.g: fatty esters, fatty acids). The performance of different UNIFAC variants with their published parameters was tested, and the trend for increasing deviation (ARD%) for VLE description is: Linear UNIFAC < Lyngby UNIFAC < Dortmund UNIFAC < Original UNIFAC. For lipid SLE prediction, the deviation in prediction increase as follows: Original UNIFAC < Dortmund UNIFAC < Linear UNIFAC < Lyngby UNIFAC.

After applying the systematic identification method, the performance of the models using the new lipid-based parameters for describing lipid VLE improves for all the UNIFAC variants, as presented in Figure 1. The extrapolation of the models to SLE prediction using the lipid-based parameters shows little to no improvement compared to the models with the published parameters. Further, Original UNIFAC model with the lipids parameters was used for process modelling, design and analysis of shea oil solvent fractionation.

The shea oil acetone fractionation process consists in three parts: (I) separation by fractional crystallization of shea oil into two products, shea olein and shea stearin; (II) solvent recovery in a series of flash units; and (III) solvent purification and recycling. Improvements of the process (e.g.: heat integration) are performed based on the economic and environmental analysis of the base case scenario.



**Figure 1.** Average relative deviation, ARD(%) for different UNIFAC variants for lipids VLE prediction using published (■) and lipid-based parameters (■).

#### 4. Conclusions

The detailed analysis of available models and data for lipids showed the need of having predictive models to describe lipid systems. By using a systematic identification method, new lipid-based parameters for different UNIFAC variants were estimated and analysed for extrapolation capabilities. Further, the models were used for shea oil acetone fractionation process modelling, design and analysis, and improvements of the process are proposed.

#### References

- [1] D.D. Damaceno, O.A. Perederic, R. Ceriani, G.M. Kontogeorgis, R. Gani, *Fluid Phase Equilib.* 470 (2018), 249-258.
- [2] O.A. Perederic, S. Appel, B. Sarup, J.M. Woodley, G.M. Kontogeorgis, R. Gani, *Comput. Aided Chem. Eng.* 43 (2018) 737-742.
- [3] O.A. Perederic, L.P. Cunico, S. Kalakul, B. Sarup, J.M. Woodley, G.M. Kontogeorgis, R. Gani, *J. Chem. Thermodyn.* 121 (2018) 153-169.