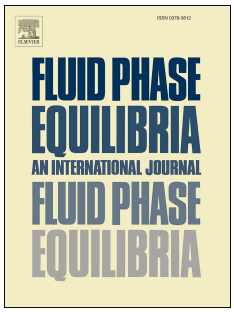

From Wilson to F-SAC: A comparative analysis of correlative and predictive activity coefficient models to determine VLE and IDAC of binary systems

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PII: S0378-3812(18)30064-5

DOI: 10.1016/j.fluid.2018.02.010

Reference: FLUID 11759

To appear in: *Fluid Phase Equilibria*

Received Date: 19 October 2017

Revised Date: 19 December 2017

Accepted Date: 11 February 2018

Please cite this article as: C. Luiz da Silveira, Nina.Paula.Gonç. Salau, From Wilson to F-SAC: A comparative analysis of correlative and predictive activity coefficient models to determine VLE and IDAC of binary systems, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2018.02.010.

From Wilson to F-SAC: A comparative analysis of correlative and predictive activity coefficient models to determine VLE and IDAC of binary systems

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ABSTRACT

Several activity coefficient models are available in literature nowadays, special attention must be given to the recently developed COSMO-SAC and F-SAC models. This work used isothermal data for 11 different binary systems, a total of 1818 experimental points, plus 129 IDAC experimental points of the same systems, to compare the accuracy of 10 activity coefficient models – Wilson, Wilson (literature), NRTL, NRTL (literature), UNIQUAC, UNIQUAC (literature), UNIFAC, UNIFAC (literature), F-SAC, and COSMO-SAC. Amongst the correlative models, the UNIQUAC and NRTL had the best performances, either with literature parameters or with the optimized parameters. When comparing the predictive models, both UNIFAC (with estimated parameters) and COSMO-SAC presented the most accurate results, with total vapor-phase composition residuals of 25.9953 and 25.2157, respectively. However, the F-SAC model was particularly good to predict infinite-dilution activity coefficients, outperforming both COSMO-SAC and UNIFAC, with residuals of 22.1765.

Keywords: vapor-liquid equilibria, COSMO-SAC, F-SAC, binary systems, infinite-dilution activity coefficient, thermodynamic models.

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