

Prediction of surface tension of solvent mixtures at various temperatures

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Background and Aims: Mixed solvents are employed in many pharmaceutical processes and their physico-chemical properties including the surface tension are the crucial information for the process designer. The aim of this presentation is to propose a global model to predict the surface tension of binary solvents at various temperatures using a combination of the Jouyban-Acree model and Abraham solvation parameters.

Methods: Available surface tension data of binary solvents at various temperatures were collected from the literature. The Abraham parameters of the solvents were computed using Pharma-Algorithm and the data were analyzed using SPSS 11. The mean relative deviations (MRDs) between experimental and predicted surface tensions were used to evaluate the accuracy of the proposed model.

Results: The trained version of the proposed model is:

$$\begin{aligned} \log \sigma_{m,T} = & x_1 \log \sigma_{1,T} + x_2 \log \sigma_{2,T} \\ & + \frac{x_1 x_2}{T} \left[-14.168 - 24.252(S_1 - S_2)^2 - 3.872(A_1 - A_2)^2 + 8.396(V_1 - V_2)^2 \right] \\ & + \frac{x_1 x_2 (x_1 - x_2)}{T} \left[104.555(E_1 - E_2)^2 + 30.723(S_1 - S_2)^2 + 26.715(V_1 - V_2)^2 \right] \\ & + \frac{x_1 x_2 (x_1 - x_2)^2}{T} \left[40.702 - 257.571(E_1 - E_2)^2 - 12.271(A_1 - A_2)^2 - 70.553(V_1 - V_2)^2 \right] \end{aligned}$$

where $\sigma_{m,T}$, $\sigma_{1,T}$, and $\sigma_{2,T}$ are the surface tensions of the mixed solvents and the mono-solvents 1 and 2 at temperature (T), x denotes the fraction of the solvents, E is the excess molar refraction, S is dipolarity/polarizability of the solvents, A denotes the solvents hydrogen-bond acidity and V is the McGowan volume of the solvents, and subscripts 1 and 2 means solvents 1 and 2. The model was statistically significant with the F value of 1326 ($p < 0.0005$) and covered the $\sigma_{m,T}$ range of 15.32 to 74.27 mN·m⁻¹ with the overall MRD (\pm SD) of 6.1 (\pm 6.2) % (N=5327).

Conclusions: The proposed model provides reasonably accurate predictions and the only required data for prediction of the surface tension of the binary mixtures are the surface tensions of the solvents 1 and 2.

Key words: Surface tension, Jouyban-Acree model, Binary solvent mixtures, Abraham solvation parameters