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Liquid Biphasic Systems: Principles and Potential for Wastewater Treatment

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INTRODUCTION

Clean water is vital to all forms of life. However, rising global consumption and the resulting pollution have made effective **wastewater treatment** a major challenge. Consequently, developing sustainable and efficient methods for water purification has become urgent.

Liquid Biphasic Systems (LBSs) are a promising green liquid-liquid extraction technique in which a mixture of three components forms two distinct liquid phases, enabling the extraction of a target compound through a preferential phase [1,2], showing significant potential for the purification of water.

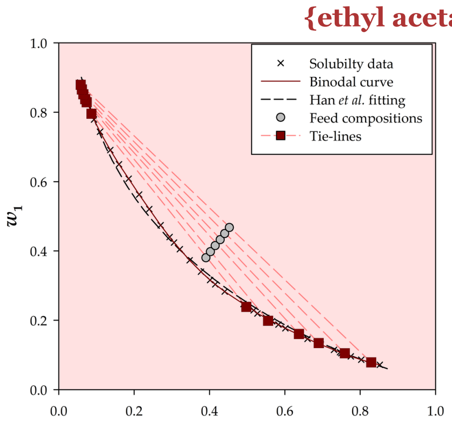
In this work, the **liquid-liquid equilibria** (LLE) of two new LBSs were studied at 298.15 K and 0.1 MPa: {ethyl acetate (1) + propan-1-ol or ethyl lactate (2) + water (3)}. The solubility data were determined by the cloud-point method and correlated using the Han *et al.* equation [3]. The homogeneous regions were described through third-degree polynomials of liquid density (ρ) and refractive index (n_D) data and the compositions of 6 tie-lines were then obtained using these polynomials. Finally, the Othmer-Tobias [4] and Bancroft-Hubard [5] correlations, and the UNIversal QUAsi-Chemical (UNIQUAC) [6] model were applied to describe tie-line composition data.

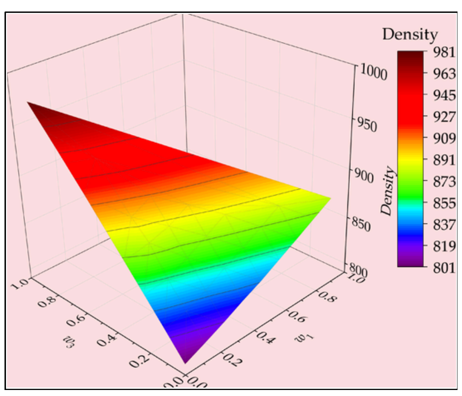
METHODOLOGY

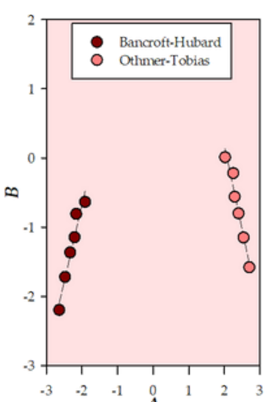
Solubility curve determination → **Phase characterisation through thermophysical property data** → **Phase separation and tie-line composition determination** → **Application of UNIQUAC modelling**

RESULTS AND DISCUSSION

{ethyl acetate (1) + propan-1-ol (2) + water (3)}







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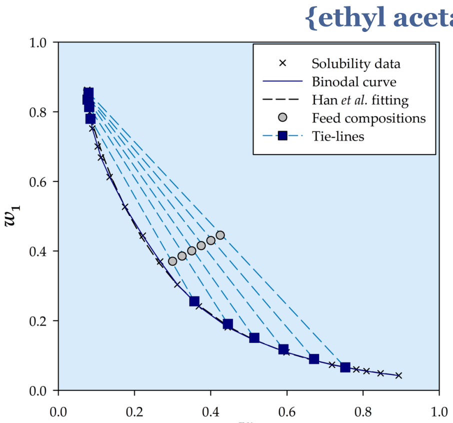

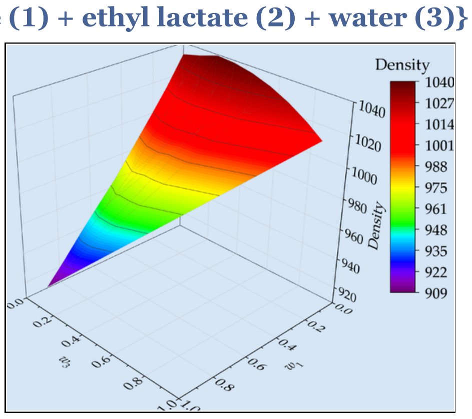

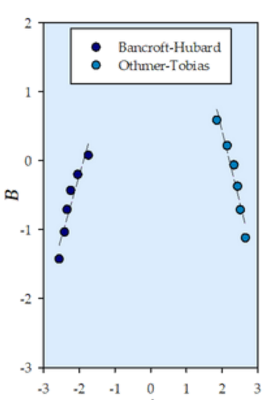

Othmer-Tobias [4]: $A = \log\left(\frac{1-w_{2,\mathrm{II}}}{w_{2,\mathrm{II}}}\right)$ and $B = \log\left(\frac{1-w_{1,\mathrm{I}}}{w_{1,\mathrm{I}}}\right)$ **Bancroft-Hubard** [5]: $A = \log\left(\frac{w_{2,\mathrm{I}}}{w_{1,\mathrm{I}}}\right)$ and $B = \log\left(\frac{w_{2,\mathrm{II}}}{w_{3,\mathrm{II}}}\right)$

Polynomials for ρ and n_D

$$\rho \text{ or } n_D = \sum_{i=1}^{3}\left(a_i w_1^i + b_i w_2^i + c_i w_3^i\right)$$

Tie-line determination

$$\mathrm{O.F.} = \alpha \cdot \sqrt{\frac{\left(\rho_{\mathrm{corr}}(w_i) - \rho_{\mathrm{exp}}\right)^2}{\rho_{\mathrm{exp}}}} + \beta \cdot \sqrt{\frac{\left(n_{D\mathrm{corr}}(w_i) - n_{D\mathrm{exp}}\right)^2}{n_{D\mathrm{exp}}}}$$

UNIQUAC model

$$\frac{G_C^E}{RT} = \sum_{i=1}^{n_{\mathrm{species}}} x_i \ln\left(\frac{\phi_i}{x_i}\right) + 5 \sum_{i=1}^{n_{\mathrm{species}}} q_i x_i \ln\left(\frac{\theta_i}{\phi_i}\right)$$

$$\frac{G_R^E}{RT} = -\sum_{i=1}^{n_{\mathrm{species}}} q_i x_i \ln\left(\sum_{j=1}^{n_{\mathrm{species}}} \theta_j \tau_{ji}\right) \qquad \tau_{ji} = e^{\frac{-(u_{ji}-u_{ii})}{RT}}$$

$$\mathrm{IC} = \frac{\sum_{i=1}^{n_{\mathrm{points}}} \sum_{j=1}^{n_{\mathrm{species}}} \left(x_{ij}^{\mathrm{model,I}} \gamma_{ij}^{\mathrm{I}} - x_{ij}^{\mathrm{model,II}} \gamma_{ij}^{\mathrm{II}}\right)}{n_{\mathrm{points}} \cdot n_{\mathrm{species}}} = 0$$

CONCLUSIONS

- The LBS containing propan-1-ol presented a smaller immiscible zone, due to its higher solubility in both water and ethyl acetate;
- UNIQUAC was successfully applied to describe tie-line composition data.

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