

Supporting Information

Phase separation of alcohol (1-propanol, 2-propanol, or *tert*-butanol) from their aqueous solutions in the presence of biological buffer MOPS

Saidah Altway^{1,2}, Mohamed Taha^{1,3}, Ming-Jer Lee*¹

¹ Department of Chemical Engineering, National Taiwan University of Science and Technology, 43 Keelung Road, Section 4, Taipei 106-07, Taiwan

² Department of Chemical Engineering, Institut Teknologi Sepuluh Nopember, Kampus ITS, Keputih, Sukolilo, Surabaya 60111, Indonesia

³ Occupational Health and Safety (OHS) Office, Directorate of Manpower of Beni-Suef, Beni-Suef, Egypt

Corresponding Author:

Ming-Jer Lee; Tel.: +886 2 2737 6626; Fax: +886 2 2737 6644; E-mail:
mjlee@mail.ntust.edu.tw

Table S1. Azeotrope Alcohols with Water^a

Organic solvents	Azeotropic temperature/K	Azeotropic composition/ w_1
1-Propanol	360.80	0.717
2-Propanol	353.25	0.88
<i>tert</i> -Butanol	353.05	0.8824

^a taken from Horsley¹

Table S2. The Average Absolute Deviation (AAD) of NRTL Model for Ternary Systems of Alcohol (1) + Water (2) + MOPS (3)

Phase	Δx_1 AAD	Δx_2 AAD	Δx_3 AAD	Grand AAD ^a
1-Propanol (1) + Water (2) + MOPS (3)				
Aqueous	0.0024	0.0048	0.0060	0.0069
Organic	0.0113	0.0112	0.0058	
2-Propanol (1) + Water (2) + MOPS (3)				
Aqueous	0.0057	0.0035	0.0048	0.0061
Organic	0.0104	0.0073	0.0051	
<i>tert</i> -Butanol (1) + Water (2) + MOPS (3)				
Aqueous	0.0076	0.0078	0.0034	0.0056
Organic	0.0057	0.0059	0.0033	

^a grand AAD = $\left(\sum_{k=1}^N \sum_{j=1}^2 \sum_{i=1}^3 |x_{ijk}^{calc} - x_{ijk}^{expt}| \right) / 6N$; where N is the number of tie-lines.

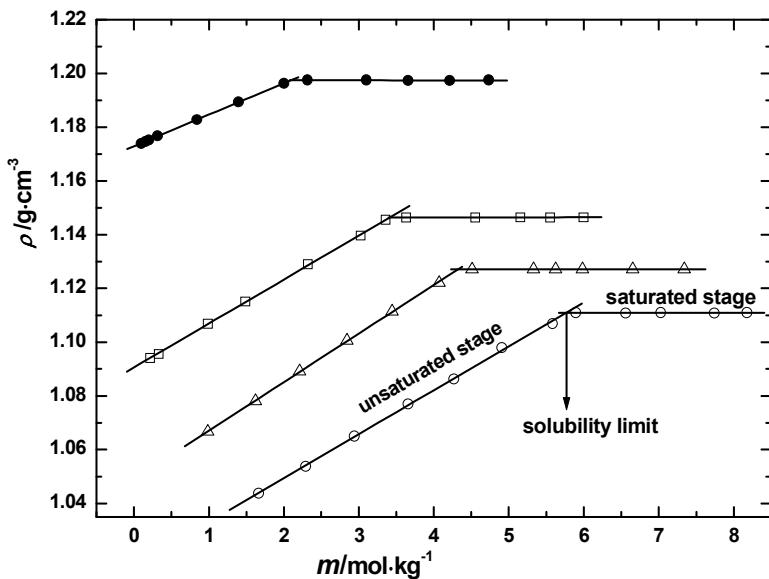


Figure S1. Plot of density against molality to determine the solid solubility²

References

- (1) Horsley, L. H. *Tables of Azeotropes and nonazeotropes*, in: *Azeotropic data-III*; American Chemical Society: Washington DC, 1973.
- (2) Taha, M.; Lee, M. J. Buffers and ionic salts: densities and solubilities of aqueous and electrolyte solutions of tris(hydroxymethyl)aminomethane and N-tris[hydroxymethyl]-4-amino-butanesulfonic acid. *J. Chem. Eng. Data* **2009**, *54*, 2501-2512.