Critical Assessment of Using Ionic Liquid as Entrainer via Extractive Distillation

Supporting Information

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This text file is the supporting information for the paper "Critical Assessment of Using Ionic Liquid as Entrainer via Extractive Distillation."

Detailed Information of Estimated PLXANT model

Detailed Information of Economic Analysis

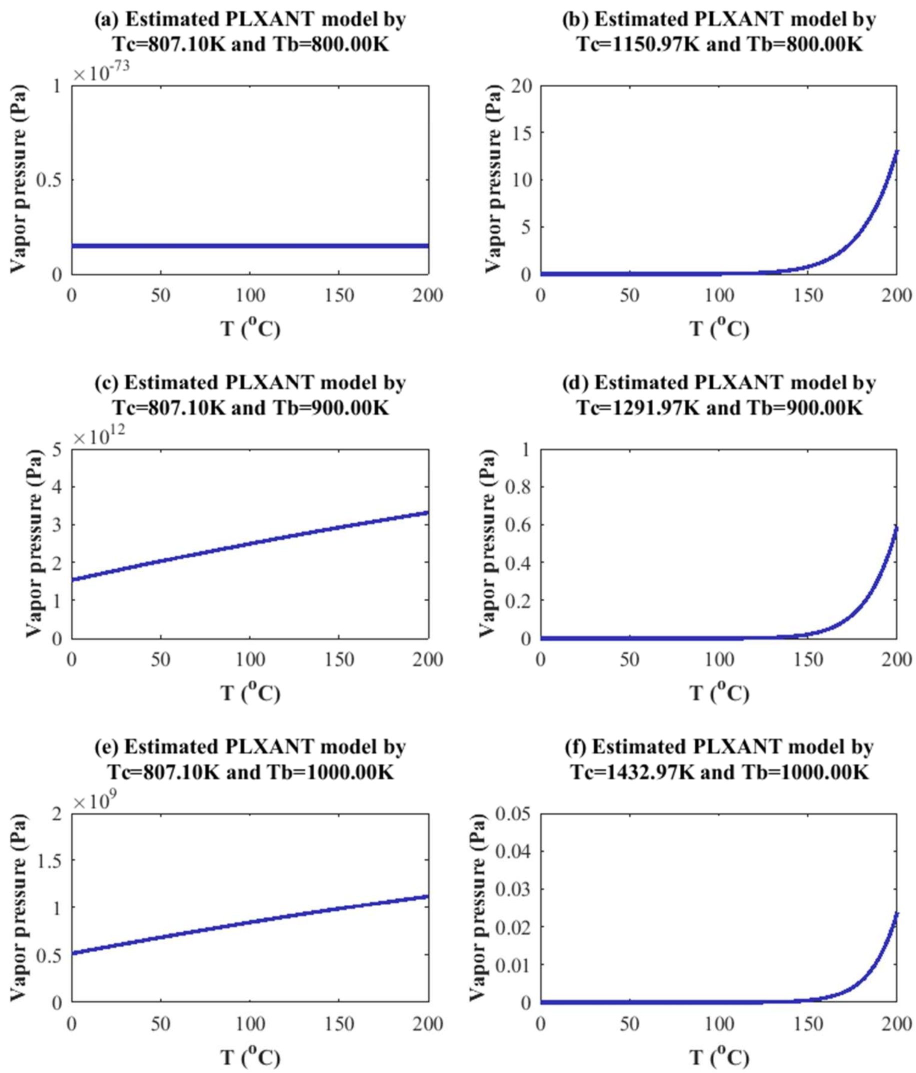
Retrofitted or Duplicate Process Flowsheet for Separation

Sensitivity Analysis to Impurity in IL Recover Stream

Figure S7. Sensitivity analysis of how E/F, NE, NF and NT influence Xwmax for 99.99 mol% IPA case.

Supporting Information I: Estimated PLXANT model

Figure S1. Estimated PLXANT model of [EMIM][OAC] by the critical temperature from the group contribution method and Klincewicz method.



Supporting Information II: detailed information of economic analysis

Table S1 Basis of economics and equipment sizing

Column diameter (D): Aspen tray sizing

Column length (L): NT trays with 2-ft spacing plus 20% extra length

Column and other vessel (D and L are in meters)

  Capital cost = $17{,}640(D)^{1.066}(L)^{0.802}$

Condensers (area in m^2)

  Heat-transfer coefficient = 0.852 kW/K-m^2

  Differential temperature = reflux-drum temperature – 315 K

  Capital cost = $7296(\text{area})^{0.65}$

Reboilers (area in m^2)

  Heat-transfer coefficient = 0.568 kW/K-m^2

  Differential temperature = steam temperature – base temperature ($\Delta T > 20$ K)

  Capital cost = $7296(\text{area})^{0.65}$

Vacuum system

  Steam ejector

    Size factor (S): flow rate (lb/hr)/suction pressure (torr)

    Cost multiplying factor (C_M):

      One-stage: 1.0, two-stages: 1.8, three-stages: 2.1

    Capital cost = $1690(C_M)(S)^{0.41}$

    Steam used amount is assumed to be 10 times of flowrate.

    Operating cost = (Steam consumption) * (LP steam cost)

  Liquid-ring pump

    Size factor (S): flow rate (ft^3/min)

    Capital cost $8250(S)^{0.35}$

  Screw compressor

    Size factor (S): flow rate (ft^3/min)

    Capital cost $9590(S)^{0.38}$

Energy cost

  HP steam = \$9.88/GJ (41 barg, 254 ºC)

  MP steam = \$8.22/GJ (10 barg, 184 ºC)

  LP steam = \$7.78/GJ (5 barg, 160 ºC)

  Cooling water (320K) = \$0.354/GJ

  Chilled water (15 ^{o}C) = \$4.43/GJ

  Refrigerant at -50 ^{o}C = \$13.11/GJ

  Refrigerant at -67.78 ^{o}C = \$17.97/GJ

Refrigerant at -101.11 ^{o}C = $26.71/GJ
Electricity = $16.9/GJ

Chemical cost
Acetone = $3.40/kg
IPA = $3.87/kg

TAC = (capital cost/payback period) + energy cost;
Payback period = 3 years; Operating hour = 8000 hours/year

Supporting Information III: Retrofitted or Duplicate Process Flowsheet for Separation

Table S2 UNIQUAC model parameters of acetone/methanol/DMSO system.

Component i	Acetone	Acetone	Methanol
Component j	Methanol	DMSO	DMSO
Source	ASPEN VLE-IG	ASPEN VLE-IG	ASPEN VLE-IG
a_{ij}	0	0	0
a_{ji}	0	0	0
b_{ij} (K)	-225.1533	-62.9317	129.3624
b_{ji} (K)	52.7705	-20.3857	23.4854

UNIQUAC activity coefficient model:

$$\ln\gamma_i = \frac{\Phi_i}{x_i} + \frac{z}{2} q_i \ln\left(\frac{\theta_i}{\Phi_i}\right) - q_i^{'} \ln\left(\sum_k \theta_k \tau_{ki}\right) - q_i \sum_j \frac{\theta_j \tau_{ij}}{\sum_j \theta_j \tau_{ji}} + l_i + q_i - \frac{\Phi_i}{x_i} \sum_j x_j l_j \,,$$

where

γ_i is the activity coefficient of component i,

x_i is the mole fraction of component i,

q_i is the pure component area parameter of component i,

r_i is the pure component volume parameter of component i,

$$\Phi_i = \frac{x_i r_i}{\sum_k x_k r_k} \,,$$

$$\theta_i = \frac{x_i q_i}{\sum_k x_k q_k} \,,$$

$$\tau_{ij} = \exp\left(a_{ij} + \frac{b_{ij}}{T}\right),$$

$$l_i = \frac{z}{2}(r_i - q_i) + 1 - r_i \,,$$

$z = 2$.

Table S3 NRTL model parameters of IPA/water/DMSO system.

Component i	Isopropanol	Isopropanol	Water
Component j	Water	DMSO	DMSO
Source	ASPEN VLE-IG	ASPEN VLE-IG	ASPEN VLE-IG
a_{ij}	-1.3115	0	-1.2449
a_{ji}	6.8284	0	1.7524
b_{ij} (K)	426.40	115.28	586.80
b_{ji} (K)	-1483.46	-25.01	-1130.22
c_{ij}	0.30	0.30	0.30

NRTL model:

$$\ln\gamma_i = \frac{\sum_j x_j \tau_{ji} G_{ji}}{\sum_k x_k G_{ki}} + \sum_j \left[\frac{x_j G_{ij}}{\sum_k x_k G_{kj}} \left(\tau_{ij} - \frac{\sum_m x_m \tau_{mj} G_{mj}}{\sum_k x_k G_{kj}} \right) \right],$$

$$G_{ij} = \exp(-c_{ij}\tau_{ij}),$$

$$\tau_{ij} = a_{ij} + \frac{b_{ij}}{T}, \quad \tau_{ii} = 0$$

Figure S2. Retrofitted process flowsheet for acetone/methanol separation based on Luyben's work.

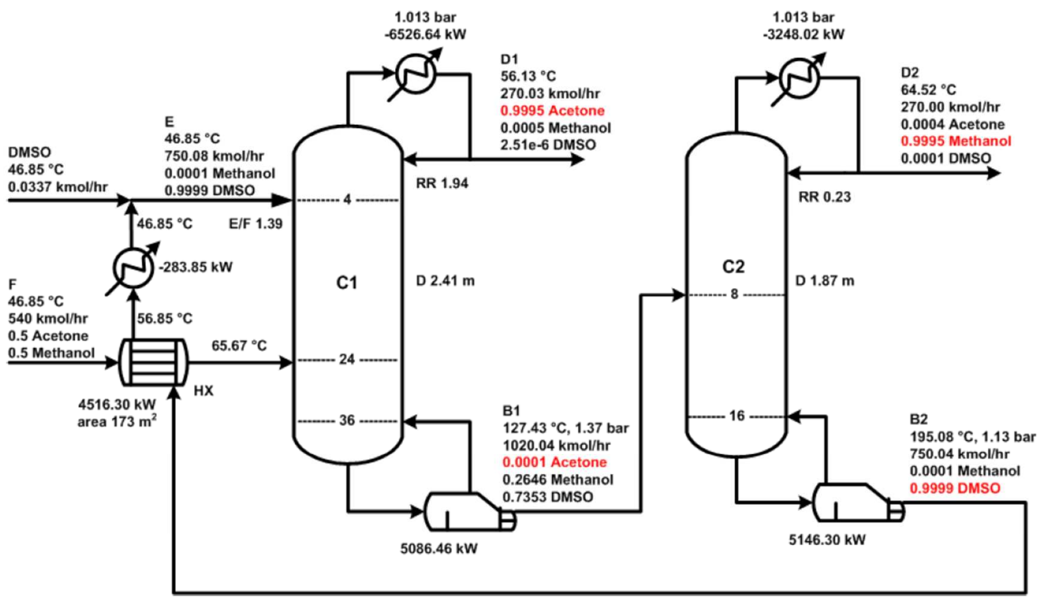


Figure S3. Duplicate process flowsheet for IPA dehydration to 99.9999 mol% from Arifin and Chien's work.

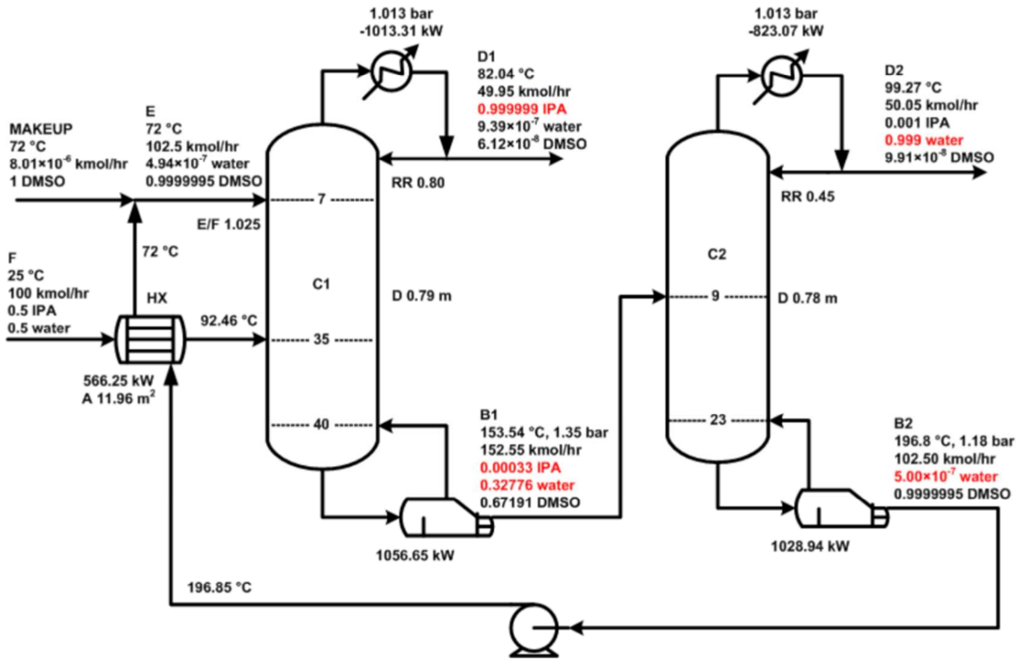
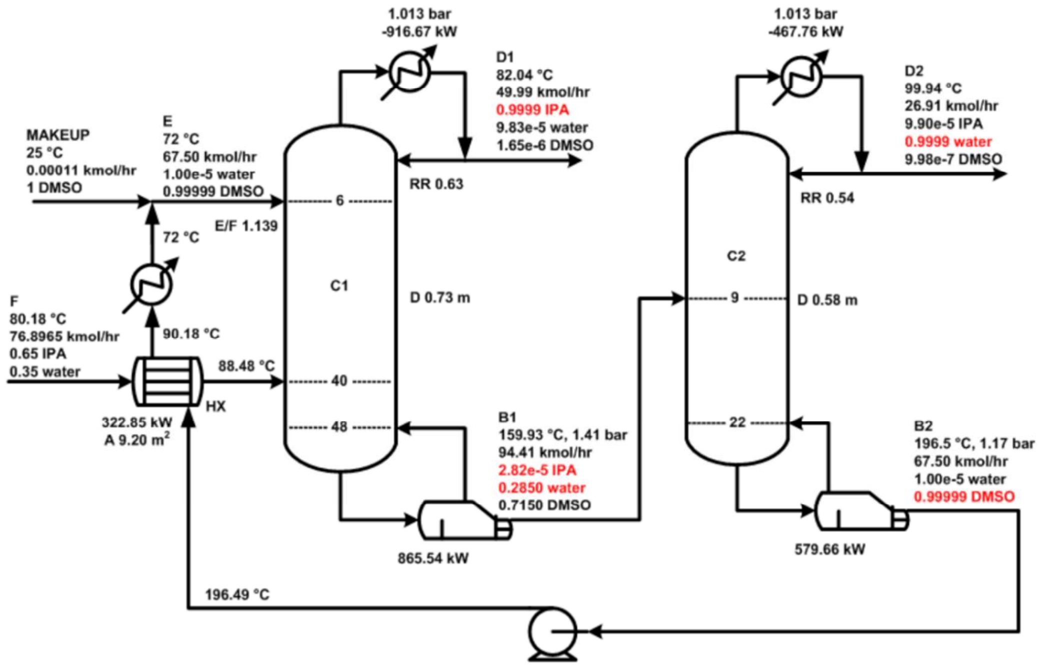


Figure S4. Retrofitted process flowsheet for IPA dehydration to 99.9999 mol% from Liang et al.'s work.



Supporting Information IV: Sensitivity Analysis to Impurity in IL Recover Stream

Figure S5. Sensitivity analysis of how E/F, NE, NF and NT influence Xmmax for acetone/methanol separation..

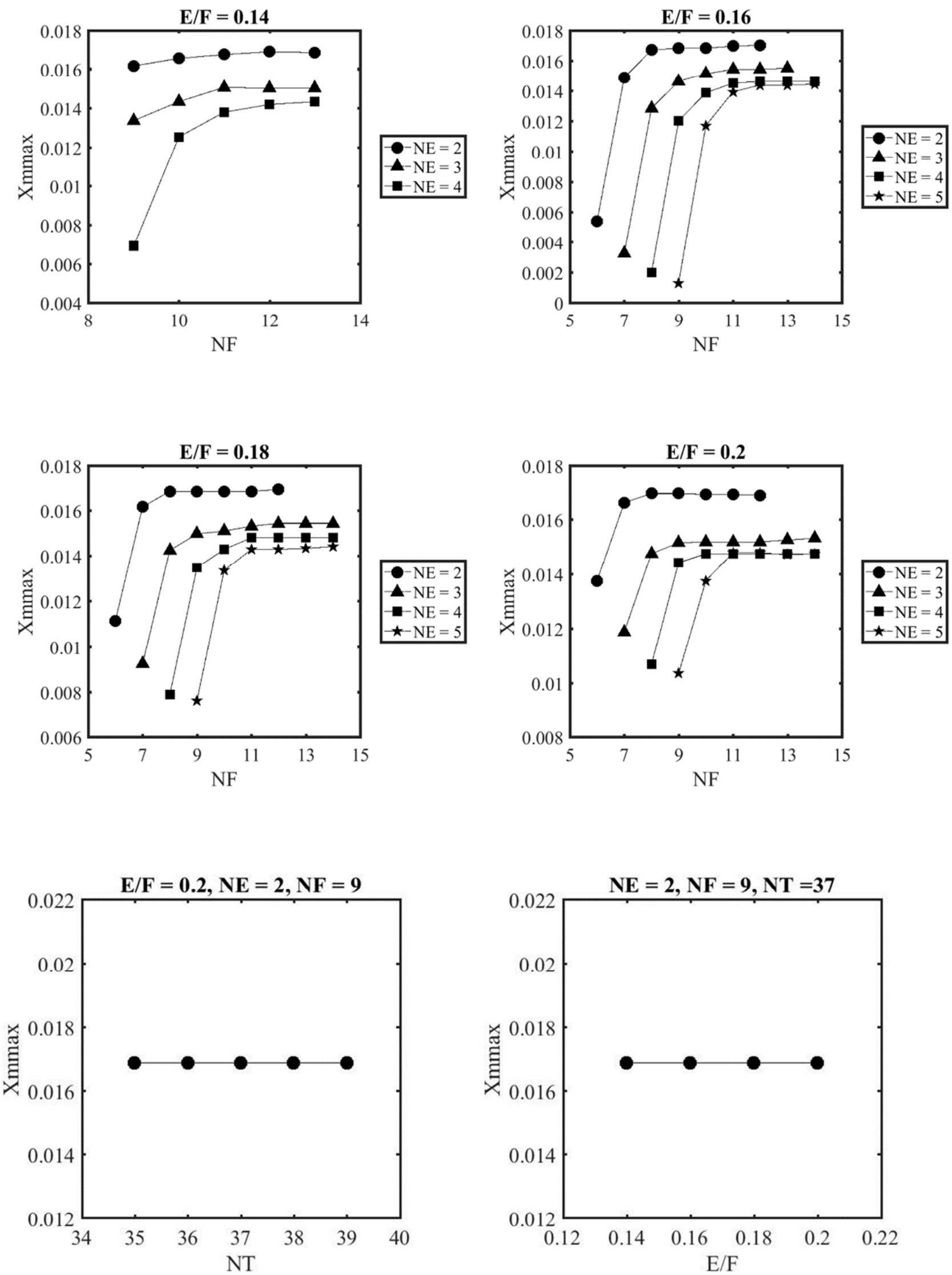


Figure S6. Sensitivity analysis of how E/F, NE, NF and NT influence Xwmax for 99.9999 mol% IPA case.

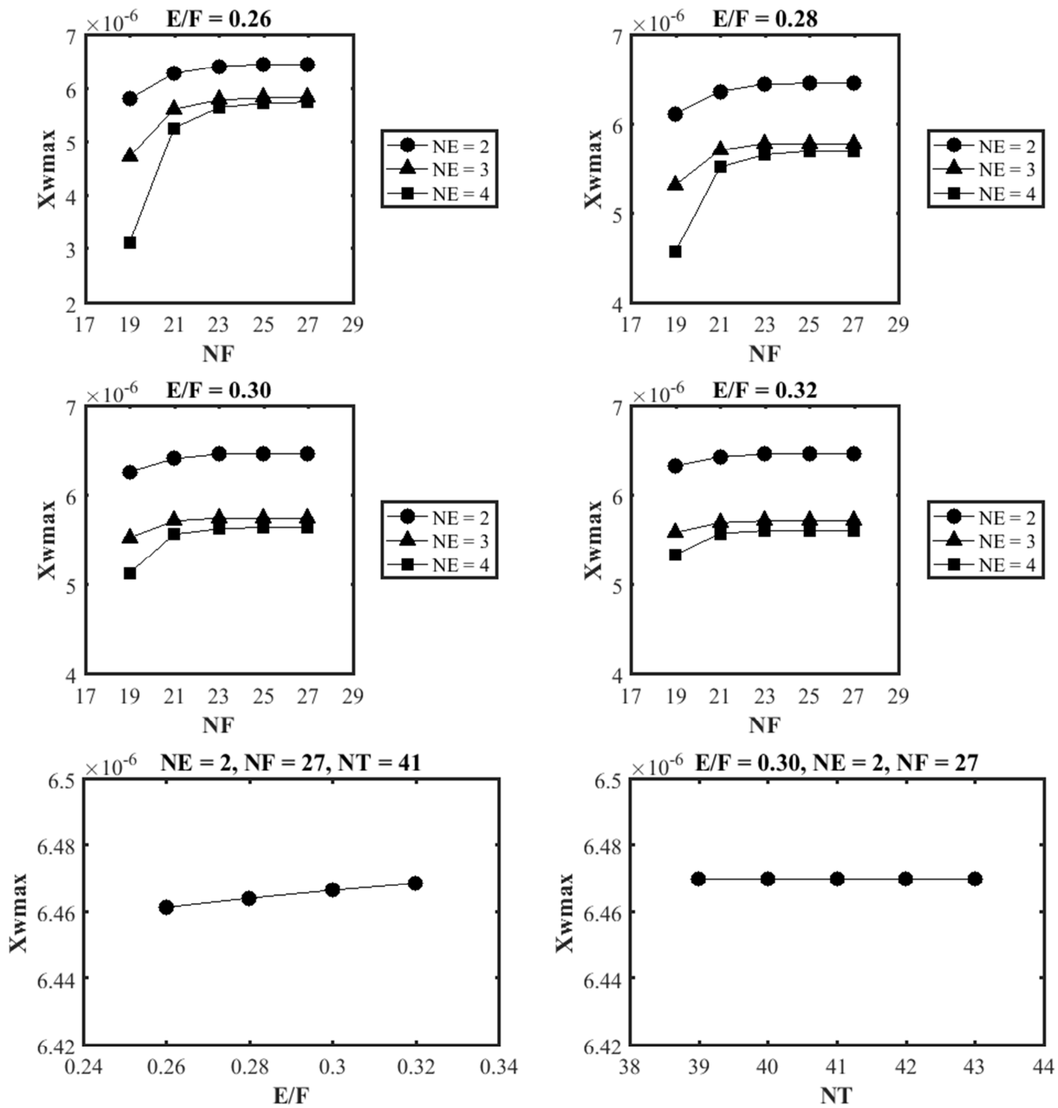


Figure S7. Sensitivity analysis of how E/F, NE, NF and NT influence Xwmax for 99.99 mol% IPA case.