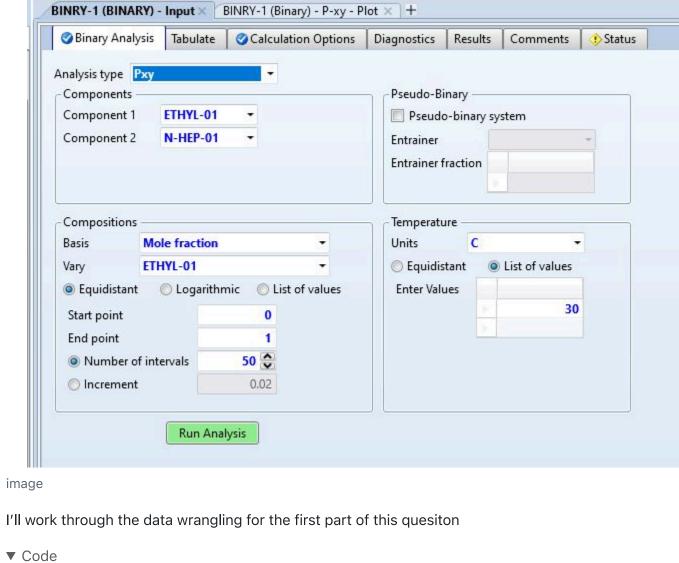
SIS 10.2-1

AUTHOR k.wodehouse & s.blough

part a

using IDEAL model in aspen and going to binary analysis here's what my analysis page looked like when running these different models



import pandas as pd import matplotlib.pyplot as plt

from scipy.interpolate import interp1d

▼ Code

8.0

0.6

import numpy as np

df = pd.read_csv('ideal.tsv', sep='\t') pres = df['TOTAL PRES'] xe, xh, ye, yh = np.array(df['LIQUID1 MOLEFRAC ETHYL-01']), np.array(df['LIQUID1 MOLEFRAC interp_p = interp1d(xe, pres, kind='linear', fill_value="extrapolate") interp_e = interp1d(xe, ye, kind='linear', fill_value="extrapolate") interp_h = interp1d(xh, yh, kind='linear', fill_value="extrapolate") df.head(3)

TOTAL TOTAL LIQUID1 LIQUID2 LIQUID2 TOTAL KVL2 KVL **TOTAL** GAMMA GAMMA GAMMA KVL2 ETHYL- N-HEP- ETHYL- N-HEP-**MOLEFRAC TOTAL** ETHYL- HEP-ETHYL-KVL N-TEMP ETHYL-01 PRES HEP-01 01 01 01 01 01 NaN NaN NaN NaN

NaN

NaN

NaN

NaN

NaN

NaN

TO

ΒE

1

1

1

D & 0 X

Search Aspen Knowledge

8.0

1.0

NaN

NaN

0 30 0.00 0.077455 9.709034 1.000000 1 1 30 0.01 0.084201 8.931212 0.919887 1 1 2 30 0.02 0.090947 8.268773 0.851658 1

mixture comp

fig, ax = plt.subplots(dpi=300)ax.grid(alpha=0.3) ax.plot(xe,ye, label='ethyl') ax.plot(xh,yh, label='n-heptane') ax.plot(xe, xe, ':', c='black') ax.set(xlim=0, ylim=0, xlabel='\$x_e\$, \$x_h\$', ylabel='\$y_e, y_h\$') ax.vlines(0.4723, 0,1, color='green', label='mixture comp') ax.legend(); 1.0 ethyl n-heptane

0.4 0.2 0.0 0.6 0.0 0.2 0.4 8.0 1.0 X_e , X_h **▼** Code print('---- vapor composition ----') print(f'ethyl bromide: {interp_e(0.4723):.4f}') print(f'n-heptane: $\{interp_h(0.4723):.4f\}'\}$ print('---- pressure ----') print(f'{interp_p(0.4723):.4f} bar') ---- vapor composition ----ethyl bromide: 0.8968 n-heptane: 0.0844 sum: 0.9812

I'll make a convenience function to call for the other reports that need generated

Simulation 1 - Aspen Plus V12 - aspenONE

0.075 0.000 0.025 0.050 0.075 0.100 0.125 0.150 0.175 0.200 0.225 0.250 0.275 0.300 0.325 0.350 0.375 0.400 0.425 0.450 0.475 0.500 0.525 0.550 0.575 0.600 0.625 0.650 0.675 0.700 0.725 0.750 0.775 0.800 0.825 0.850 0.875 0.900 0.925 0.950 0.975 1.000

here's what the p-x-y plot looked like for the GRAYSON model

BINRY-1 (BINARY) - Input × BINRY-1 (Binary) - P-xy - Plot × +

▲ 🔯 BINRY-1 Results

<section-header> Safety Analysis

anged Check Status

0.2

0.0

part c

0.0

0.2

mixture comp

0.2

0.4

0.6

 x_e, x_h

8.0

1.0

- ∂ ×

Search Aspen Knowledge

Solubility A Ternary Diag

Next Run Reset Control Panel Report & Mixture PT Envelope A Residue Curves

Swap Search BIP Completeness

Component i To Component j To Source To Temp. Units To AU To AU To BU To BU To BU To CU To DU TO TLOW TO THIGH TO

8.0

0.6

0.4

0.2

0.0

0.0

gamma ethyl bromide: 1.2108 gamma n-heptane : 1.0691

Customize

These can be fed into aspen by noticing $A_{12}=lpha$ and $A_{21}=eta$

Lostomize Draw Structure ↑ Retrieve Parameters ₩ DIPPR ★ Regression

⊘Input Databanks Comments

Temperature-dependent binary parameters

Parameter VANL

Binary Interaction - VANL-1 (T-DEPENDENT) × BINRY-1 (Binary) - P-xy - Plot × BINRY-1 (BINARY) × +

Help Data set 1

alpha: 0.67529999 beta: 0.30524933

File Home View

Properties

Components Methods

> ▲ Parameters Pure Components

→ : Simulation 🕍 Safety Analysis Energy Analysis

0.6

filler

☑ Specifications▷ ☑ Selected Methods

ANDKIJ-1
ANDMIJ-1
HENRY-1 MLQKIJ-1 MUKIJ-1 MULIJ-1 ☑ RKTKIJ-1 ☑ VANL-1 Electrolyte Pair Electrolyte Ternary UNIFAC Groups Results Routes NC Props

0.4

0.6

 X_e, X_h

Data Estimation

Properties All Items ⊳ 词 Setup Components

Methods

Specifications

---- pressure ----

0.3961 bar

► Code

part b

P-xy Merge Plot Pressure bar

Parameters
Routes
NC Props

Tabpoly

Chemistry
Property Sets

File Home View Customize Resources Design Format

0.725

0.675

0.625

0.575

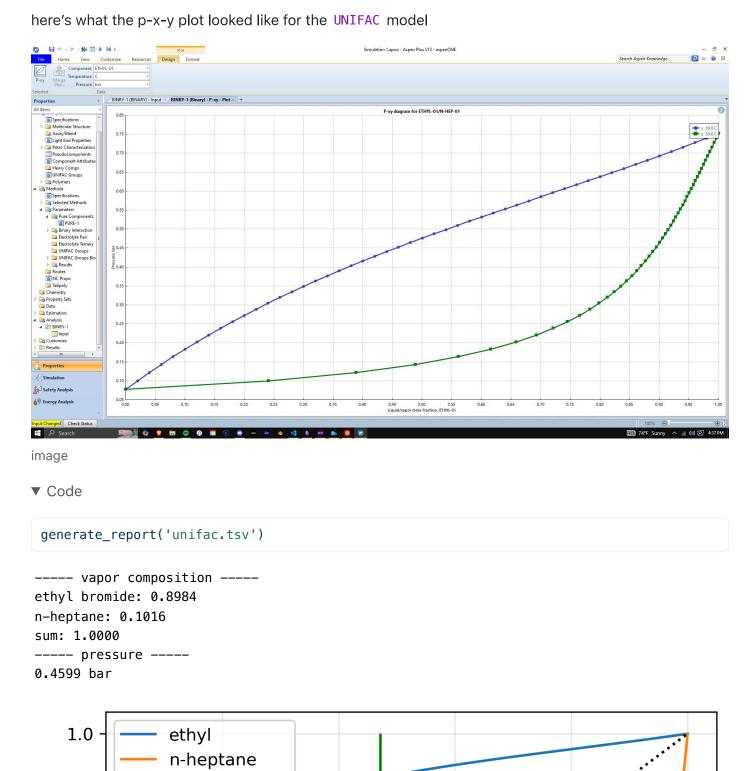
0.525

0.475

0.425

0.375 0.325 0.275 0.250 0.225 0.175 0.150 0.125

image ▼ Code generate_report('ptb.tsv') ---- vapor composition ----ethyl bromide: 0.8903 n-heptane: 0.1097 sum: 1.0000 ---- pressure ----0.4558 bar 1.0 ethyl n-heptane mixture comp 8.0 0.6 0.4



part d we can start by calculating the activity coefficents using this equation $\gamma_i = rac{y_i P_{ ext{total}}}{x_i P_i^{ ext{vap}}}$ the van laar parameters using these equations from the textbook in chapter 9 $lpha = \left(1 + rac{x_2 \ln \gamma_2}{x_1 \ln \gamma_1}
ight)^2 \ln \gamma_1$ (9.5-10) $eta = \left(1 + rac{x_1 \ln \gamma_1}{x_2 \ln \gamma_2}
ight)^2 \ln \gamma_2$ where 1 is ethyl bromide and 2 is n-heptane **▼** Code ye = 0.815yh = 1 - yexe = 0.2843xh = 1 - xe $pvap_e = 0.7569$ $pvap_h = 0.0773$ Ptotal = 0.3197 T = 273.15 + 30.0gammae = ye * Ptotal / (xe * pvap_e) $gammah = yh * Ptotal / (xh * pvap_h)$ print(f'gamma ethyl bromide: {gammae:.4f}') print(f'gamma n-heptane : {gammah:.4f}\n') alpha = (1 + (xh * np.log(gammah))/(xe * np.log(gammae)))**2 * np.log(gammae)print(f'alpha: {alpha:.8f}') beta = (1 + (xe * np.log(gammae))/(xh * np.log(gammah)))**2 * np.log(gammah)print(f'beta: {beta:.8f}')

Results Available Check Status 允 🐌 😍 🐷 🧧 🚷 📶 🖫 🗤 image □ □ □ · ○ · N→ □ → □ ▼ - ∂ × Simulation 1 - Aspen Plus V12 - aspenONE Design Format Search Aspen Knowledge 🔎 a 🕡 🛭 Component ETHYL-01
Temperature C Pressure bar Selected Binary Interaction - VANL-1 (T-DEPENDENT) × BINRY-1 (Binary) - P-xy - Plot × BINRY-1 (BINARY) × + Properties All Items 0 P-xy diagram for ETHYL-01/N-HEP-01 Setup ◆ x 30.0 C ◆ y 30.0 C 0.90 Specifications ▶ Selected Methods 0.85 0.80 Pure Components 4 Binary Interaction 0.75 ANDKIJ-1
ANDMIJ-1
HENRY-1 0.70 0.65 MLQKIJ-1 0.60 MULIJ-1 호 0.55 NRTL-1
RKTKIJ-1 e 0.50 VANL-1 0.45 Electrolyte Pair 0.35 UNIFAC Groups Bin Routes 0.25 NC Props 0.15 0.05 Safety Analysis 0.00 0.02 0.04 0.06 0.08 0.10 0.12 0.14 0.16 0.18 0.20 0.22 0.24 0.26 0.28 0.30 0.32 0.34 0.36 0.38 0.40 0.42 0.44 0.46 0.48 0.50 0.52 0.54 0.56 0.58 0.60 0.62 0.64 0.66 0.68 0.70 0.72 0.74 0.76 0.78 0.80 0.82 0.84 0.86 0.88 0.90 0.92 0.94 0.96 0.98 1.00 69 Energy Analysis Liquid/vapor mole fraction, ETHYL-01 Results Available Check Status 9 요^R 🔈 😍 🐷 🧧 🖇 📶 🖫 (v)) 10:2 3/6/ image ▼ Code

generate_report('vanlaar.tsv') ---- vapor composition ethyl bromide: 0.8895 n-heptane: 0.1105 sum: 1.0000 ---- pressure -0.4224 bar ethyl 1.0 n-heptane mixture comp 8.0

 y_e, y_h 0.4 0.2 0.0 0.2 0.4 0.0 0.6 8.0 1.0 X_e, X_h ▼ Code