

# ChEn 3603 Homework #11

You can load the  $Txy$  data into python easily with the following:

```
# Load the csv data using Pandas then grab numpy arrays for the Txy data
import pandas as pd
data = pd.read_csv('Txy.csv')
Teq = data['T'].values
xeq = data['x'].values
yeq = data['y'].values
```

## Problem 1 (16 pts)

A mixture of 10 kmol of 70 mol% benzene in toluene is distilled at atmospheric pressure using differential distillation with constant boilup rate of 10 mol/min. The tabulated equilibrium data are given in the csv file provided.

1. (1 pts) From the data, determine average values of  $K$  and  $\alpha$ . Plot  $K(T)$  and  $\alpha(T)$  as well as the averages on the same plot.
2. When 50% (by mole) has been vaporized, report the residue composition, the average vapor composition, the temperature of the still, and how long the process takes using:
  - (a) (2 pts) Constant  $K$  assumption, using the average you calculated in part 1.
  - (b) (3 pts) Constant  $\alpha$  assumption, using the average you calculated in part 1.
  - (c) (6 pts) The  $Txy$  data directly

Comment on your findings.

3. (4 pts) Plot  $W/W_0$ ,  $x$  and  $y^{\text{avg}}$  as functions of time for the constant  $K$  and constant  $\alpha$  approximations for 95 mole% vaporized. Comment on the difference between the two methods in predicting  $x(t)$  and  $y^{\text{avg}}(t)$ .

In part 2c, you'll find that you need to solve a nonlinear equation. This can be a bit tricky with some of the python hoops. Here is a template of what I did:

```
def resfun(xlovals):
    # Given an array of lower bounds on the integral (xlovals),
    # this returns an array of residual values.
    # Alternatively, given a scalar for the lower bound, it returns a scalar residual value.

    scalar_input = False

    # make this function work for scalar or array inputs.
    # For scalars, we detect that and then convert them to arrays
    xlovals = np.asarray(xlovals)
```

```

if xlovals.ndim==0:
    scalar_input = True
    xlovals = xlovals[None] # make into a 1D array

results = np.zeros_like(xlovals)
for i in range(len(xlovals)):
    x = ??? # create an appropriate range of x values to carry the integration out

    # 'integrand_fun' calculates the integrand value
    results[i] = np.log( ? ) - np.trapz( integrand_fun(x), x )

if scalar_input:
    return np.squeeze(results) # turn back into a scalar
return results

```

## Problem 2 (16 pts)

Revisit the system from problem 1 for a batch system with a rectifying section that has a *constant reflux ratio*, the same boilup rate as problem 1 (this is  $V$ ) and three equilibrium stages. Given that  $L/V = 0.9$ , do the following:

- (8 pts) Determine the residue composition and average distillate composition when 50% of the original moles remain in the still.
- (2 pts) Show the McCabe-Thiele diagrams for the original mixture and the final mixture for the conditions of part 1.
- (4 pts) Plot  $\frac{W}{W_0}(t)$ ,  $x_W(t)$  and  $x_D^{avg}(t)$ .
- (2 pts) Compare the results from problem 1 part 2 with problem 2 and comment on them. Specifically, create a table like the following:

Method	$x(\text{residue})$	$y^{avg}$ (average distillate)	Time required (hours)
Simple batch			
Batch with rectifying section			

The `batch_constant_r.py` file I provided will be a *lot* of help to you.