7.9 Isothermal Flash and the Rachford-Rice Equation

Summary

This Jupyter notebook illustrates the use of the Rachford-Rice equation solve the material balances for an isothermal flash of an ideal mixture. The video is used with permission from learnCheme.com, a project at the University of Colorado funded by the National Science Foundation and the Shell Corporation.

Derivation of the Rachford-Rice Equation

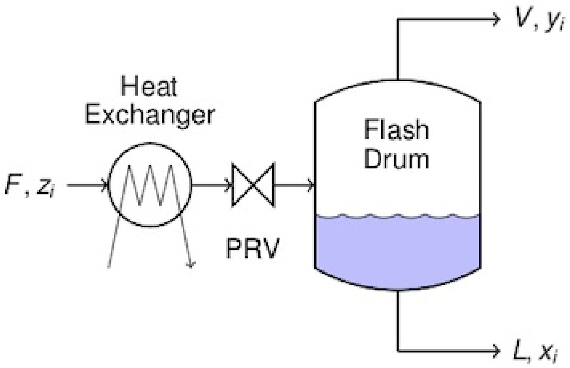
The derivation of the Rachford-Rice equation is a relatively straightford application of component material balances and Raoult's law for an ideal solution.

In [1]:

```
from IPython.display import YouTubeVideo
YouTubeVideo("ACxOiXWq1SQ",560,315,rel=0)
```

Out[1]:

The quantities, definitions, and equations are summarized in the following figure.



$$\phi = \frac{V}{F}$$

$$(1-\phi) = \frac{L}{F}$$

$$x_i = \frac{z_i}{1+\phi(K_i-1)}$$

$$y_i = K_i x_i$$

$$0 = \sum_{i=1}^{N} \frac{(K_i-1)z_i}{1+\phi(K_i-1)}$$

To sketch the derivation, we begin with the overall constraint on the liquid phase and vapor phase mole fractions $x_1 + x_2 + \cdots + x_N = 1$ and $y_1 + y_2 + \cdots + y_N = 1$. Subtracting the first from the second we find

$$\sum_{n=1}^{N}(y_n - x_n) = 0$$

This doesn't look like much, but it turns out to be the essential trick in the development.

Next we need expressions for y_n and x_n to substitute into terms in the sum. We get these by solving the component material balance and equilibrium equations for y_n and x_n. For each species we write a material balance

$$Lx_n + Vy_n = Fz_n$$

Dividing through by the feedrate we get a parameter $\phi = \frac{V}{L}$ denoting the fraction of the feedstream that leaves the flash unit in the vapor stream, the remaining fraction $1-\phi$ leaving in the liquid stream. With this notation the material balance becomes

$$(1-\phi)x_n + \phi y_n = z_n$$

for each species.

The second equation is

$$y_n = K_n x_n$$

where the 'K-factor' for an ideal solution is given by Raoult's law

$$K_n = \frac{P_n^{sat}(T)}{P}$$

The K-factor depends on the operating pressure and temperature of the flash unit. Solving the material balance and equilibrium equations gives

$$x_n = \frac{z_n}{1+\phi(K_n-1)}$$
$$y_n = \frac{K_n z_n}{1+\phi(K_n-1)}$$

so that the difference $y_n - x_n$ is given by

$$y_n - x_n = \frac{(K_n-1)z_n}{1+\phi(K_n-1)}$$

Substitution leads to the Rachford-Rice equation

$$\sum_{n=1}^{N}\frac{(K_n-1)z_n}{1+\phi(K_n-1)} = 0$$

This equation can be used to solve a variety of vapor-liquid equilibrium problems as outline in the following table.

Problem Classification

Problem Type	z_i's	T	P	ϕ	Action
Bubble Point	✓	unknown	✓	0	Set $x_i = z_i$. Solve for T and y_i's
Bubble Point	✓	✓	unknown	0	Set $x_i = z_i$. Solve for P and y_i's
Dew Point	✓	unknown	✓	1	Set $y_i = z_i$. Solve for T and x_i's
Dew Point	✓	✓	unknown	1	Set $y_i = z_i$. Solve for P and x_i's
Isothermal Flash	✓	✓	✓	unknown	Solve for ϕ, x_i's, and y_i's

Isothermal Flash of a Binary Mixture

Problem specifications

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

In [2]:

```
A = 'acetone'
B = 'ethanol'

P = 760
T = 65

z = dict()
z[A] = 0.6
z[B] = 1 - z[A]
```

Compute the K-factors for the given operating conditions

In [3]:

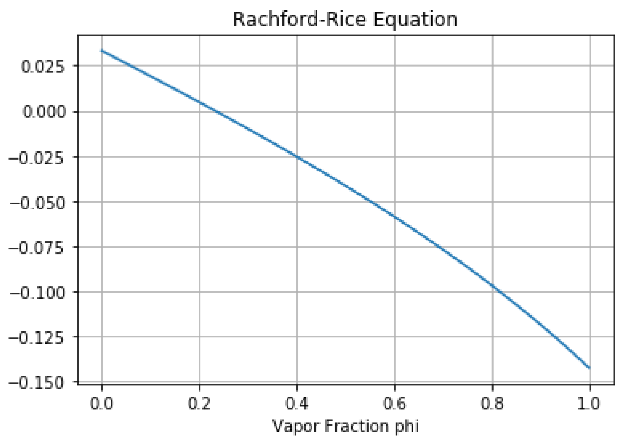
```
# Antoine's equations. T [deg C], P [mmHg]
Psat = dict()
Psat[A] = lambda T: 10**(7.02447 - 1161.0/(224 + T))
Psat[B] = lambda T: 10**(8.04494 - 1554.3/(222.65 + T))

# Compute K-factors
K = dict()
K[A] = Psat[A](T)/P
K[B] = Psat[B](T)/P

print("Pressure     {:6.2f} [mmHg]".format(P))
print("Temperature  {:6.2f} [deg C]".format(T))
print("K-factors:")
for n in Psat:
    print("   {:s}   {:7.3f}".format(n,K[n]))
```

```
Pressure      760.00 [mmHg]
Temperature    65.00 [deg C]
K-factors:
   acetone     1.338
   ethanol     0.576
```

Rachford-Rice equation

In [4]:

```
def RR(phi):
    return (K[A]-1)*z[A]/(1 + phi*(K[A]-1)) + (K[B]-1)*z[B]/(1 + phi*(K[B]-1))

phi = np.linspace(0,1)
plt.plot(phi,[RR(phi) for phi in phi])
plt.xlabel('Vapor Fraction phi')
plt.title('Rachford-Rice Equation')
plt.grid();
```



Finding roots of the Rachford-Rice equation

In [5]:

```
from scipy.optimize import brentq

phi = brentq(RR,0,1)

print("Vapor Fraction  {:6.4f}".format(phi))
print("Liquid Fraction {:6.4f}".format(1-phi))
```

```
Vapor Fraction  0.2317
Liquid Fraction 0.7683
```

Compositions

In [6]:

```
x = dict()
y = dict()

print("Component    z[n]    x[n]    y[n]")

for n in [A,B]:
    x[n] = z[n]/(1 + phi*(K[n]-1))
    y[n] = K[n]*x[n]
    print("{:10s} {:6.4n}  {:6.4f}  {:6.4f}".format(n,z[n],x[n],y[n]))
```

```
Component    z[n]    x[n]    y[n]
acetone       0.6  0.5565  0.7444
ethanol       0.4  0.4435  0.2556
```

Multicomponent Mixtures

In [7]:

```
P = 760
T = 65

z = dict()
z['acetone'] = 0.6
z['benzene'] = 0.01
z['toluene'] = 0.01
z['ethanol'] = 1 - sum(z.values())
```

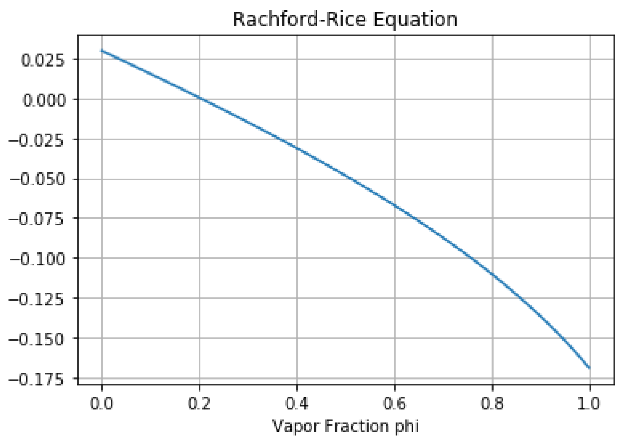
In [8]:

```
Psat = dict()
Psat['acetone'] = lambda T: 10**(7.02447 - 1161.0/(224 + T))
Psat['benzene'] = lambda T: 10**(6.89272 - 1203.531/(219.888 + T))
Psat['ethanol'] = lambda T: 10**(8.04494 - 1554.3/(222.65 + T))
Psat['toluene'] = lambda T: 10**(6.95805 - 1346.773/(219.693 + T))

K = {n : lambda P,T,n=n: Psat[n](T)/P for n in Psat}

print("Pressure     {:6.2f} [mmHg]".format(P))
print("Temperature  {:6.2f} [deg C]".format(T))
print("K-factors:")
for n in K:
    print("    {:s}   {:7.3f}".format(n,K[n](P,T)))
```

```
Pressure     760.00 [mmHg]
Temperature   65.00 [deg C]
K-factors:
   acetone    1.338
   benzene    0.613
   ethanol    0.576
   toluene    0.222
```

In [9]:

```
def RR(phi):
    return sum([(K[n](P,T)-1)*z[n]/(1 + phi*(K[n](P,T)-1)) for n in K.keys()])

phi = np.linspace(0,1)
plt.plot(phi,[RR(phi) for phi in phi])
plt.xlabel('Vapor Fraction phi')
plt.title('Rachford-Rice Equation')
plt.grid();
```



In [10]:

```
from scipy.optimize import brentq

phi = brentq(RR,0,1)

print("Vapor Fraction  {:6.4f}".format(phi))
print("Liquid Fraction {:6.4f}".format(1-phi))
```

```
Vapor Fraction  0.2033
Liquid Fraction 0.7967
```

In [11]:

```
x = {n: z[n]/(1 + phi*(K[n](P,T)-1)) for n in z}
y = {n: K[n](P,T)*z[n]/(1 + phi*(K[n](P,T)-1)) for n in z}

print("Component    z[n]    x[n]    y[n]")

for n in z.keys():
    print("{:10s} {:6.4f}  {:6.4f}  {:6.4f}".format(n,z[n],x[n],y[n]))
```

```
Component    z[n]    x[n]    y[n]
acetone     0.6000  0.5615  0.7511
benzene     0.0100  0.0109  0.0067
toluene     0.0100  0.0119  0.0026
ethanol     0.3800  0.4158  0.2396
```

Experiments suggest the bursting pressure of a 2 liter soda bottle is 150 psig.

Exercises

Design of a Carbonated Beverage

The purpose of carbonating beverages is to provide a positive pressure inside the package to keep out oxygen and other potential contaminants. The burst pressure of 2 liter soda bottles has been measured to be 150 psig (approx. 10 atm). For safety, suppose you want the bottle pressure to be no more than 6 atm gauge on a hot summer day in Arizona (say 50 °C,) and yet have at least 0.5 atm of positive gauge pressure at 0 °C. Assuming your beverage is a mixture of CO_2 and water, is it possible to meet this specification? What concentration (measured in g of CO_2 per g of water) would you recommend?

In [ ]:

```

```