Josh Whitehead
ChE-3853

HW 8

1.) ~~Wilson~~

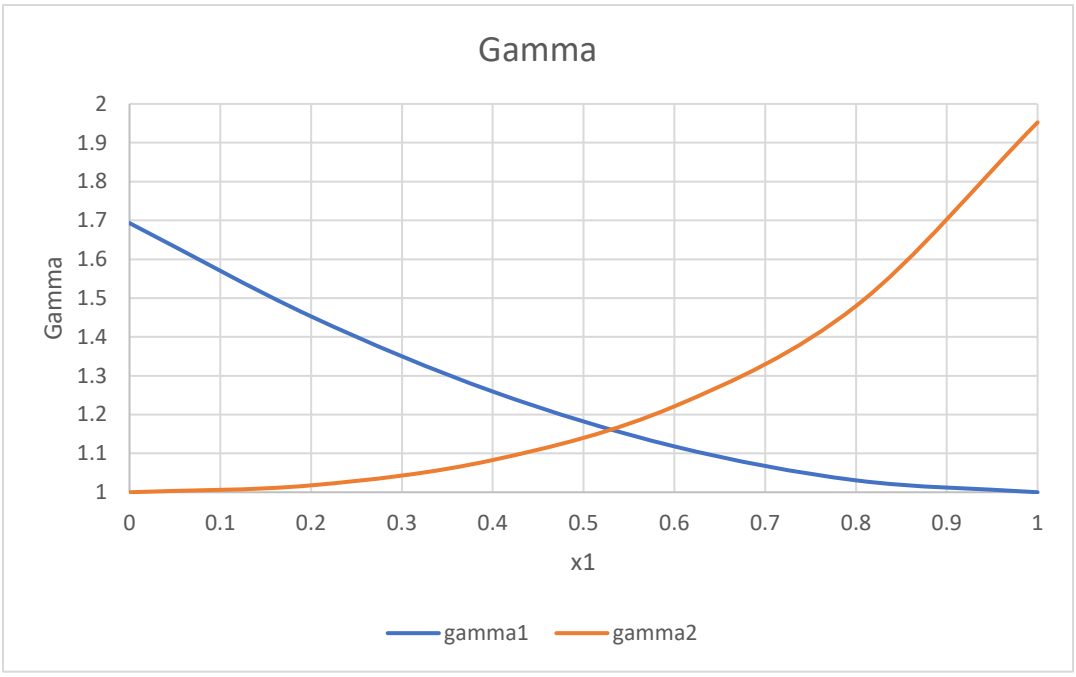
1) guess A_{12}, A_{21} and solve for γ_1, γ_2 with

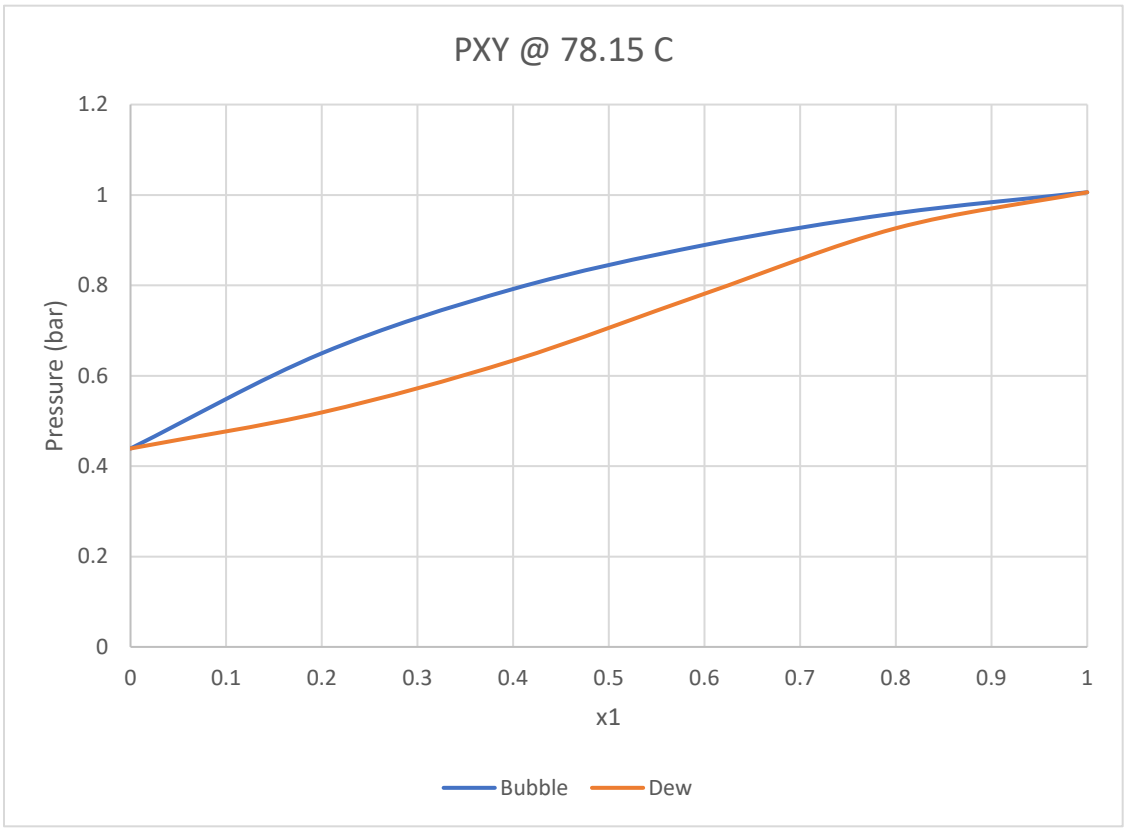
$$\gamma_1 = \exp\left(x_2^2 \left(A_{12} + 2\left(A_{21} - A_{12}\right)x_1\right)\right)$$

2) Minimize $\dfrac{\left(\gamma_1^{mod} - \gamma_1^{exp}\right)}{\left(\gamma_1^{exp}\right)^2}$

to find A_{12}, A_{21}

3) use New A_{12}, A_{21} to find new γ_1, γ_2


Gamma
2
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
Gamma
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
gamma1
gamma2


PXY @ 78.15 C
1.2
1
0.8
0.6
0.4
0.2
0
Pressure (bar)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
Bubble
Dew

A13

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1					Exp				Model										
2	x1	x2	P	P	gam1	gam2	P1sat	P2sat	g1	g2		A12	A21						
3	0	1	0.439	0.439	1.6931		1.006	0.439	1.6931	1		0.526561	0.669008						
4	0.2	0.8	0.649747	0.51886					1.45276	1.0178									
5	0.4	0.6	0.792008	0.6338					1.259339	1.082953									
6	0.6	0.4	0.889303	0.781511					1.118065	1.221181									
7	0.8	0.2	0.959358	0.926339					1.030639	1.479492									
8	1	0	1.006	1.006		1.9523			1	1.9523									
9																			
10																			
11	err1	err2																	
12	1.54061E-14	3.89E-17																	
13																			
14																			
15																			
16																			
17																			
18																			
19																			
20																			
21																			
22																			
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HW 8

2.4) $A = \frac{\ln(\gamma_1)}{x_2^2} = 0.991 \rightarrow \gamma_1 = \exp(x_2^2 A)$

b) $\gamma_1 = \frac{y_1 P}{x_1 P_1^{sat}} = 1.43$

$\gamma_2 = \frac{y_2 P}{x_2 P_2^{sat}} = 1.18$

$\gamma_1 = \frac{y_1 P}{x_1 P_1^{sat}}$

$A_{12} = \left(2 - \frac{1}{x_2}\right)\frac{\ln(\gamma_1)}{x_2} + \frac{2\ln(\gamma_2)}{x_1}$

$A_{12} = 1.03$ $A_{21} = 0.982$

$\gamma_1 = \exp\left(x_2^2\left(A_{12} + 2(A_{21} - A_{12})x_1\right)\right)$

$\gamma_2 = \exp\left(x_1^2\left(A_{21} + 2(A_{12} - A_{21})x_2\right)\right)$

3) a) $\gamma_1 = \frac{P y_1}{x_1 P_1^{sat}} = 1.35$ $\gamma_2 = \frac{P y_2}{x_2 P_2^{sat}} = 1.02$

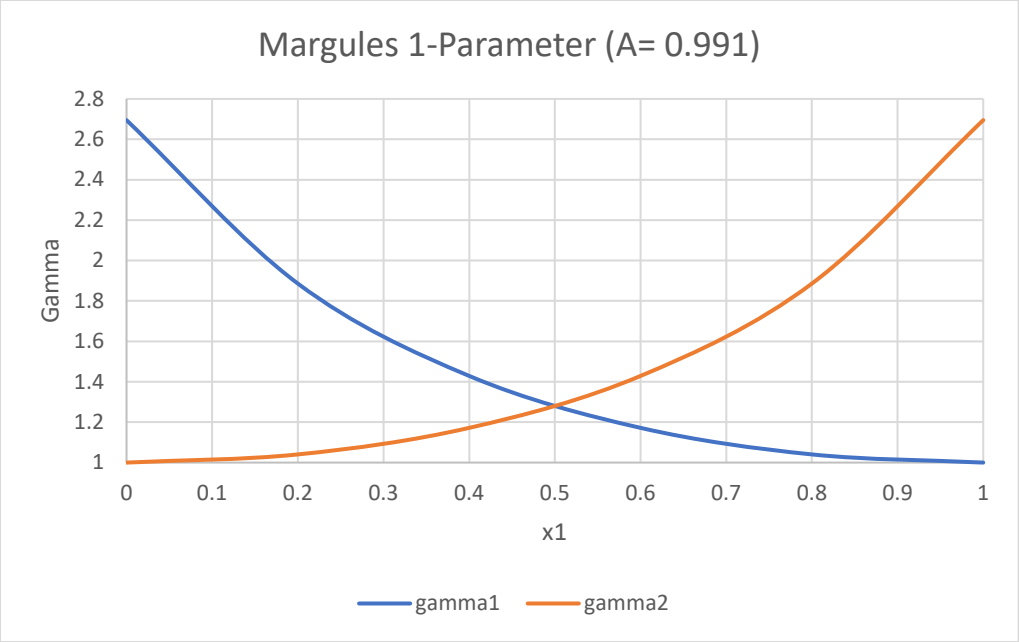
$A = \frac{\ln \gamma_1}{x_2^2} = 0.474$

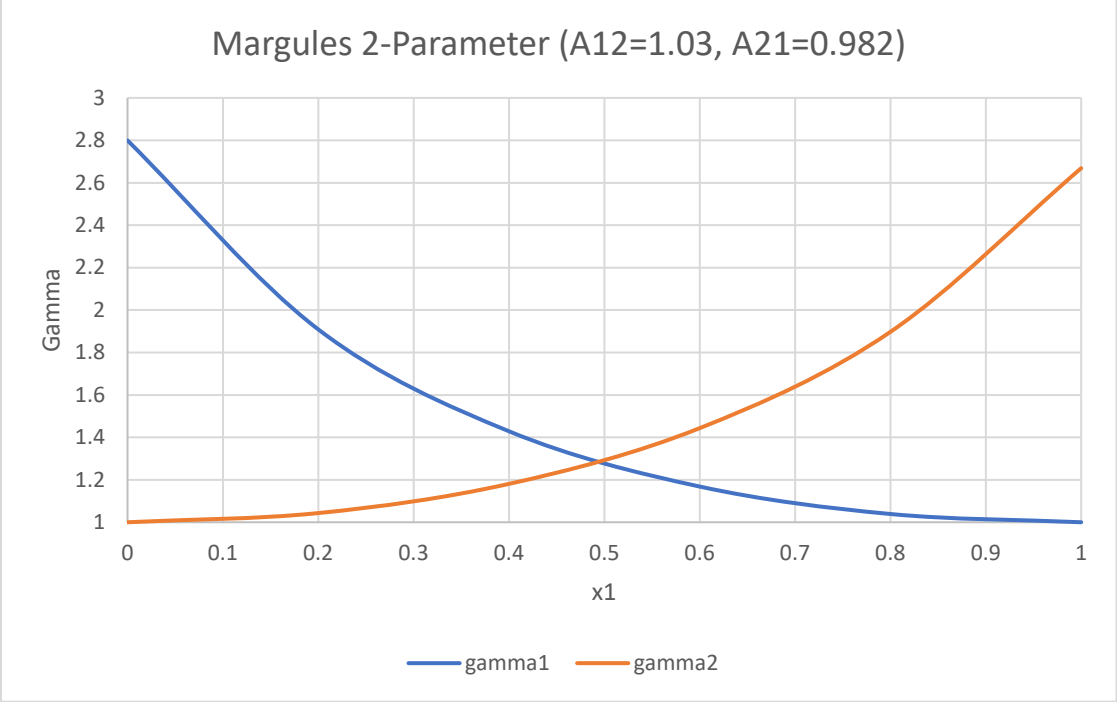
model:

$\gamma_1 = \exp(x_2^2 A)$, $\gamma_2 = \exp(x_1^2 A)$

$P_{dew} = \frac{1}{\frac{y_1}{P_1^{sat}\cdot\gamma_1} + \frac{y_2}{P_2^{sat}\cdot\gamma_2}}$

@ 0.6:


Margules 1-Parameter (A= 0.991)
Gamma
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
gamma1
gamma2


Margules 2-Parameter (A12=1.03, A21=0.982)
Gamma
3
2.8
2.6
2.4
2.2
2
1.8
1.6
1.4
1.2
1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
x1
gamma1
gamma2

J16

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	1 Parameter																		
2	T (C)	P (kPa)	x1	x2	y1	y2	p1sat	p2sat	gam1	A	x1	x2	gam1	gam2					
3	45	37	0.398	0.602	0.428	0.572	27.78	29.82	1.432287	0.991359824	0	1	2.694897	1					
4											0.2	0.8	1.886023	1.040451					
5											0.4	0.6	1.428878	1.17189					
6											0.6	0.4	1.17189	1.428878					
7											0.8	0.2	1.040451	1.886023					
8											1	0	1	2.694897					
9																			
10																			
11	2 Parameter																		
12	T (C)	P (kPa)	x1	x2	y1	y2	p1sat	p2sat	gam1 exp	gam2exp	A12	A21	x1	x2	gam1 mod	gam2 mod			
13	45	37	0.398	0.602	0.428	0.572	27.78	29.82	1.432287	1.178945211	1.029474	0.981592	0	1	2.799594	1			
14													0.2	0.8	1.90905	1.043237			
15													0.4	0.6	1.42878	1.180866			
16													0.6	0.4	1.168268	1.443634			
17													0.8	0.2	1.03885	1.897385			
18													1	0	1	2.668701			
19																			
20																			
21																			
22																			
23																			
24																			
25																			
26																			
27																			

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Hw 8

3a) exp:

$$\gamma_i = \frac{y_i P}{x_i P_i^{sat}}$$

$$A = \frac{\ln \gamma_1}{x_2^2} = 0.475$$

guess:

$$P = \frac{1}{\frac{y_1}{P_1^{sat}} + \frac{y_2}{P_2^{sat}}} \rightarrow x_1 = \frac{y_1 \cdot P}{P_1^{sat}} \rightarrow \gamma_1, \gamma_2$$

$$P_{new} = \frac{1}{\frac{y_1}{P_1^{sat} \cdot \gamma_1} + \frac{y_2}{P_2^{sat} \cdot \gamma_2}} \rightarrow \text{Iterate} \rightarrow \boxed{P = 41.0 \text{ kPa}}$$

b) same technique as part (a)

but using

$$\gamma_1 = \exp\left(x_2^2 \left(A_{12} + 2\left(A_{21} - A_{12}\right) x_1\right)\right)$$

$$\gamma_2 = \exp\left(x_1^2 \left(A_{21} + 2\left(A_{12} - A_{21}\right) x_2\right)\right)$$

$$A_{12} = \left(2 - \frac{1}{x_2}\right) \frac{\ln \gamma_1}{x_2} + 2\frac{\ln \gamma_2}{x_1}$$

$$A_{21} = \left(2 - \frac{1}{x_1}\right) \frac{\ln \gamma_2}{x_1} + \frac{2 \ln(\gamma_1)}{x_2}$$

I17

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S
1	1 Parameter																		
2	p1sat	p2sat	x1	x2	y1	y2	P	T	gam1exp	gam2exp	A		Model						
3	46.86	27.3	0.2	0.8	0.363	0.637	34.98	298	1.354859	1.02025	0.474527		P	x1	gam1	gam2			
4													36.42176	0.466348	1.144695	1.108714			
5													40.98205	0.458409	1.149341	1.104858			
6													40.98053	0.456539	1.150448	1.103961			
7													40.98045	0.456098	1.15071	1.10375			
8													40.98044	0.455995	1.150771	1.103701			
9																			
10																			
11																			
12																			
13	2 Parameter																		
14	p1sat	p2sat	x1	x2	y1	y2	P	T	gam1exp	gam2exp	A12	A21		Model					
15	46.86	27.3	0.2	0.8	0.363	0.637	34.98	298	1.354859	1.02025	0.485193	0.458528		P	x1	gam1	gam2		
16														36.42176	0.466348	1.140074	1.111722		
17														40.96597	0.460086	1.143718	1.108664		
18														40.96503	0.45861	1.144586	1.10795		
19														40.96498	0.458261	1.144792	1.107782		
20														40.96497	0.458179	1.14484	1.107742		
21																			
22																			
23																			
24																			
25																			
26																			
27																			

Sheet1 Sheet2 Sheet3 Sheet4

Ready 100%

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HW 8

4) a.) @ Azeotrope: $x_1 = y_1$ $\therefore \gamma_1 = \frac{P}{P_1^{sat}}$

$\gamma_2 = \frac{P_2}{P_2^{sat}}$

$P_1 = P_2 \rightarrow \frac{\gamma_2}{\gamma_1} = \frac{P_1^{sat}}{P_2^{sat}}$

$\frac{\gamma_2}{\gamma_1} = \frac{\exp(x_1^2 A)}{\exp(x_2^2 A)} = \frac{P_1^{sat}}{P_2^{sat}}$

$\rightarrow \ln\left(\frac{P_1^{sat}}{P_2^{sat}}\right) = A\left(x_1^2 - x_2^2\right)$

$A = -0.81$

$\gamma_1 = \exp(x_2^2 \cdot A) = \exp(0.25^2 A) = 0.951$

b)