

Numerical Method

Dept. Material Science & Engineering
Undergraduate Course (4th year)
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Homework #4

Multicomponent Phase Equilibria -> System of non-linear equations

- Newton's Method

$$P_k = P_{k-1} - \frac{f(P_{k-1})}{f'(P_{k-1})}$$

$$P_{(k)} = P_{(k-1)} - [J(P_{(k-1)})]^{-1} F(P_{(k-1)})$$



$$J(X) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \dots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_2}{\partial x_n} \\ \vdots & \vdots & \dots & \vdots \\ \frac{\partial f_n}{\partial x_1} & \frac{\partial f_n}{\partial x_2} & \dots & \frac{\partial f_n}{\partial x_n} \end{bmatrix}$$

Jacobian Matrix

$$f_1(x_{Ge}^L, x_{Ge}^{dia}) = \Delta G_{Ge}^{dia \rightarrow L} + RT \ln x_{Ge}^L - RT \ln x_{Ge}^{dia}$$
$$f_2(x_{Ge}^L, x_{Ge}^{dia}) = (\Delta G_{Si}^{dia \rightarrow L} + RT \ln(1 - x_{Ge}^{dia}) - RT \ln(1 - x_{Ge}^L))$$

Homework #4

```
void main( )
```

- Initial Temp.
- Initial X_L, X_S
- Interval of Temp.
- Number of loop

File Output

```
FILE *file;  
file = fopen("result.txt", "w");  
  
fprintf(file, "Temp X_L X_S #\n");
```

$$x_{Si}^L = 1 - x_{Ge}^L$$
$$x_{Si}^{Dia} = 1 - x_{Ge}^{Dia}$$

```
double **data
```

- Data Matrix

X_{liq}	X_{dia}	T	$Count$
\vdots	\vdots	\vdots	\vdots
\vdots	\vdots	\vdots	\vdots

```
while (1) {  
    data_mat[i][0] = *Newton(x_L_ini, x_S_ini, temp, max_count);  
    data_mat[i][1] = *(Newton(x_L_ini, x_S_ini, temp, max_count)+1);  
    data_mat[i][2] = temp;  
    data_mat[i][3] = *(Newton(x_L_ini, x_S_ini, temp, max_count) + 2);  
    i++;  
    temp = temp - interval;  
    if (temp < temp_min) {  
        data_mat[i][0] = 0;  
        data_mat[i][1] = 0;  
        data_mat[i][2] = temp_min;  
        data_mat[i][3] = 0;  
        i++;  
        break;  
    }  
}
```

```
double *Newton
```

- Newton's Method

Solution at certain T

```
double **inverse_matrix
```

```
double **Jacobian
```

Homework #4

1500	0.473711	0.740143	6	1340	0.162728	0.411171	9	1532	0.551140	0.791672	7
1496	0.464396	0.733441	6	1336	0.156535	0.400898	7	1536	0.561183	0.797865	7
1492	0.455160	0.726677	5	1332	0.150418	0.390496	10	1540	0.571307	0.804007	7
1488	0.446006	0.719850	5	1328	0.144375	0.379962	11	1544	0.581512	0.810098	7
1484	0.436931	0.712960	5	1324	0.138407	0.369293	10	1548	0.591799	0.816138	7
1480	0.427937	0.706006	5	1320	0.132513	0.358488	13	1552	0.602166	0.822128	7
1476	0.419022	0.698985	5	1316	0.126693	0.347542	9	1556	0.612616	0.828070	7
1472	0.410188	0.691898	5	1312	0.120947	0.336454	10	1560	0.623146	0.833964	7
1468	0.401433	0.684742	5	1308	0.115275	0.325219	10	1564	0.633758	0.839811	8
1464	0.392759	0.677517	5	1304	0.109675	0.313835	8	1568	0.644451	0.845611	8
1460	0.384163	0.670222	5	1300	0.104149	0.302300	12	1572	0.655226	0.851365	8
1456	0.375648	0.662855	5	1296	0.098696	0.290608	11	1576	0.666083	0.857075	9
1452	0.367212	0.655414	4	1292	0.093316	0.278758	8	1580	0.677021	0.862740	9
1448	0.358855	0.647900	4	1288	0.088008	0.266746	7	1584	0.688041	0.868361	17
1444	0.350578	0.640309	4	1284	0.082772	0.254568	12	1588	0.699143	0.873940	42
1440	0.342379	0.632642	4	1280	0.077608	0.242221	10	1592	0.710326	0.879476	10
1436	0.334260	0.624896	5	1276	0.072516	0.229700	12	1596	0.721591	0.884971	20
1432	0.326219	0.617070	5	1272	0.067496	0.217003	12	1600	0.732938	0.890424	12
1428	0.318257	0.609163	5	1268	0.062547	0.204125	13	1604	0.744367	0.895837	14
1424	0.310374	0.601173	5	1264	0.057668	0.191062	14	1608	0.755877	0.901210	8
1420	0.302569	0.593098	5	1260	0.052861	0.177811	19	1612	0.767470	0.906545	11
1416	0.294843	0.584937	5	1256	0.048124	0.164366	11	1616	0.779144	0.911840	9
1412	0.287195	0.576689	5	1252	0.043457	0.150724	29	1620	0.790900	0.917098	8
1408	0.279625	0.568352	5	1248	0.038860	0.136880	12	1624	0.802738	0.922318	10
1404	0.272133	0.559924	5	1244	0.034333	0.122830	10	1628	0.814658	0.927501	11
1400	0.264718	0.551403	6	1240	0.029875	0.108568	13	1632	0.826660	0.932648	17
1396	0.257381	0.542787	6	1236	0.025486	0.094091	7	1636	0.838744	0.937759	10
1392	0.250122	0.534076	6	1232	0.021166	0.079392	13	1640	0.850910	0.942834	9
1388	0.242940	0.525266	6	1228	0.016915	0.064467	10	1644	0.863158	0.947875	9
1384	0.235835	0.516357	6	1224	0.012732	0.049311	17	1648	0.875488	0.952882	10
1380	0.228807	0.507345	6	1220	0.008617	0.033917	15	1652	0.887899	0.957855	8
1376	0.221856	0.498230	6	1216	0.004570	0.018282	13	1656	0.900393	0.962795	13
1372	0.214982	0.489009	7	1212	0.000590	0.002398	181	1660	0.912969	0.967701	41
1368	0.208184	0.479681	7	1211	0.000000	0.000000	0	1664	0.925627	0.972576	11
1364	0.201463	0.470242	7	1210	0.000000	0.000000	0	1668	0.938366	0.977418	11
1360	0.194818	0.460690	7	1508	0.492584	0.753368	6	1672	0.951188	0.982230	11
1356	0.188249	0.451025	7	1512	0.502141	0.759893	6	1676	0.964091	0.987010	29
1352	0.181755	0.441242	7	1516	0.511779	0.766359	6	1680	0.977077	0.991760	17
1348	0.175337	0.431341	8	1520	0.521498	0.772770	6	1684	0.990144	0.996479	11
1344	0.168995	0.421318	8	1524	0.531298	0.779125	6	1687	1.000000	1.000000	0
1340	0.162728	0.411171	9	1528	0.541179	0.785425	6				
				1532	0.551140	0.791672	7				

- Initial Temp : 1500K
- Initial X_L, X_S : 0.4 0.6
- Interval of Temp. : 4K
- Number of loop : 1000

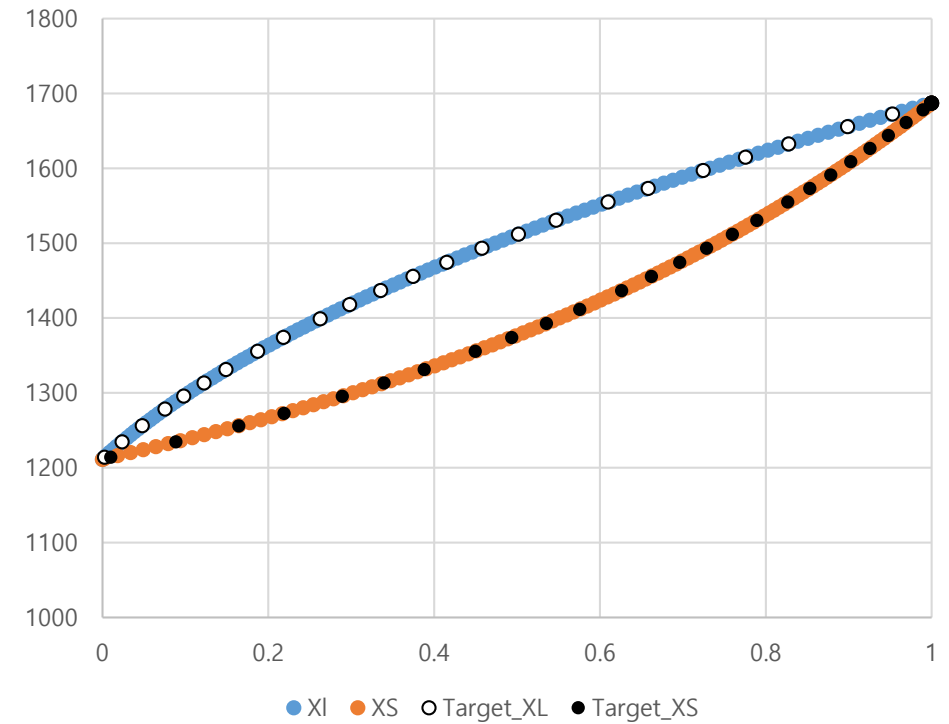
계속하려면 아무 키나 누르십시오 . . .

Homework #4

파일(F)	편집(E)	서식(O)	보기(V)	도움말(H)
Temp	X_L	X_S		#
1500	0.473711	0.740143		6
1496	0.464396	0.733441		6
1492	0.455160	0.726677		5
1488	0.446006	0.719850		5
1484	0.436931	0.712960		5
1480	0.427937	0.706006		5
1476	0.419022	0.698985		5
1472	0.410188	0.691898		5
1468	0.401433	0.684742		5
1464	0.392759	0.677517		5
1460	0.384163	0.670222		5
1456	0.375648	0.662855		5
1452	0.367212	0.655414		4
1448	0.358855	0.647900		4
1444	0.350578	0.640309		4
1440	0.342379	0.632642		4
1436	0.334260	0.624896		5
1432	0.326219	0.617070		5
1428	0.318257	0.609163		5
1424	0.310374	0.601173		5
1420	0.302569	0.593098		5
1416	0.294843	0.584937		5
1412	0.287195	0.576689		5
1408	0.279625	0.568352		5
1404	0.272133	0.559924		5
1400	0.264718	0.551403		6
1396	0.257381	0.542787		6
1392	0.250122	0.534076		6
1388	0.242940	0.525266		6
1384	0.235835	0.516357		6
1380	0.228807	0.507345		6
1376	0.221856	0.498230		6
1372	0.214982	0.489009		7

파일(F)	편집(E)	서식(O)	보기(V)	도움말(H)
Temp	X_L	X_S		#
1500	0.473711	0.740143		6
1496	0.464396	0.733441		6
1492	0.455160	0.726677		5
1488	0.446006	0.719850		5
1484	0.436931	0.712960		5
1480	0.427937	0.706006		5
1476	0.419022	0.698985		5
1472	0.410188	0.691898		5
1468	0.401433	0.684742		5
1464	0.392759	0.677517		5
1460	0.384163	0.670222		5
1456	0.375648	0.662855		5
1452	0.367212	0.655414		4
1448	0.358855	0.647900		4
1444	0.350578	0.640309		4
1440	0.342379	0.632642		4
1436	0.334260	0.624896		5
1432	0.326219	0.617070		5
1428	0.318257	0.609163		5
1424	0.310374	0.601173		5
1420	0.302569	0.593098		5
1416	0.294843	0.584937		5
1412	0.287195	0.576689		5
1408	0.279625	0.568352		5
1404	0.272133	0.559924		5
1400	0.264718	0.551403		6
1396	0.257381	0.542787		6
1392	0.250122	0.534076		6
1388	0.242940	0.525266		6
1384	0.235835	0.516357		6
1380	0.228807	0.507345		6
1376	0.221856	0.498230		6
1372	0.214982	0.489009		7

```
FILE *file;  
file = fopen("result.txt", "w");  
  
fprintf(file, "Temp X_L      X_S      #\n");
```



Homework #4

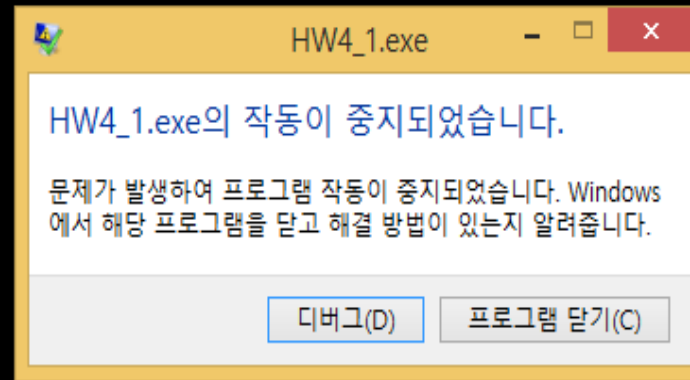
<Homework #4> Multicomponent Phase Equilibria

```
Input initial temperature <1211 < T < 1687> : 1400
Input initial X_L, X_S : 0.9 0.1
Input interval of temp. : 4
Input max. loop number : 1000
```

1400	0.264718	0.551403	6
1396	0.257381	0.542787	6
1392	0.250122	0.534076	6
1388	0.242940	0.525266	6
1384	0.235835	0.516357	6
1380	0.228807	0.507345	6
1376	0.221856	0.498230	6
1372	0.214982	0.489009	6
1368	0.208184	0.479681	6
1364	0.201463	0.470242	6
1360	0.194818	0.460690	6
1356	0.188249	0.451025	6
1352	0.181755	0.441242	6
1348	0.175337	0.431341	6
1344	0.168995	0.421318	6
1340	0.162728	0.411171	6
1336	0.156535	0.400898	6

<Homework #4> Multicomponent Phase Equilibria

```
Input initial temperature <1211 < T < 1687> : 1500
Input initial X_L, X_S : 0.4 0.6
Input interval of temp. : 3
Input max. loop number : 1000
```



<Homework #4> Multicomponent Phase Equilibria

```
Input initial temperature <1211 < T < 1687> : 1500
Input initial X_L, X_S : 0.5 0.5
Input interval of temp. : 4
Input max. loop number : 1000
```

```
Not independent. Inv. Matrix cannot exist.
계속하려면 아무 키나 누르십시오 . . .
```

<Homework #4> Multicomponent Phase Equilibria

```
Input initial temperature <1211 < T < 1687> : 1700
Input initial X_L, X_S : 0.4 0.6
Input interval of temp. : 4
Input max. loop number : 1000
```

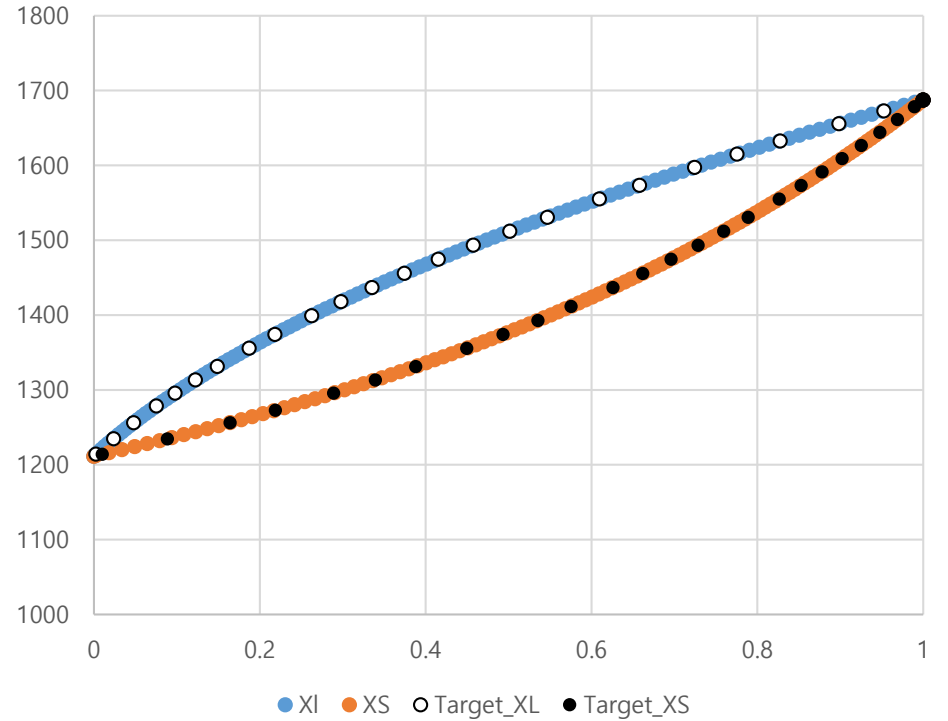
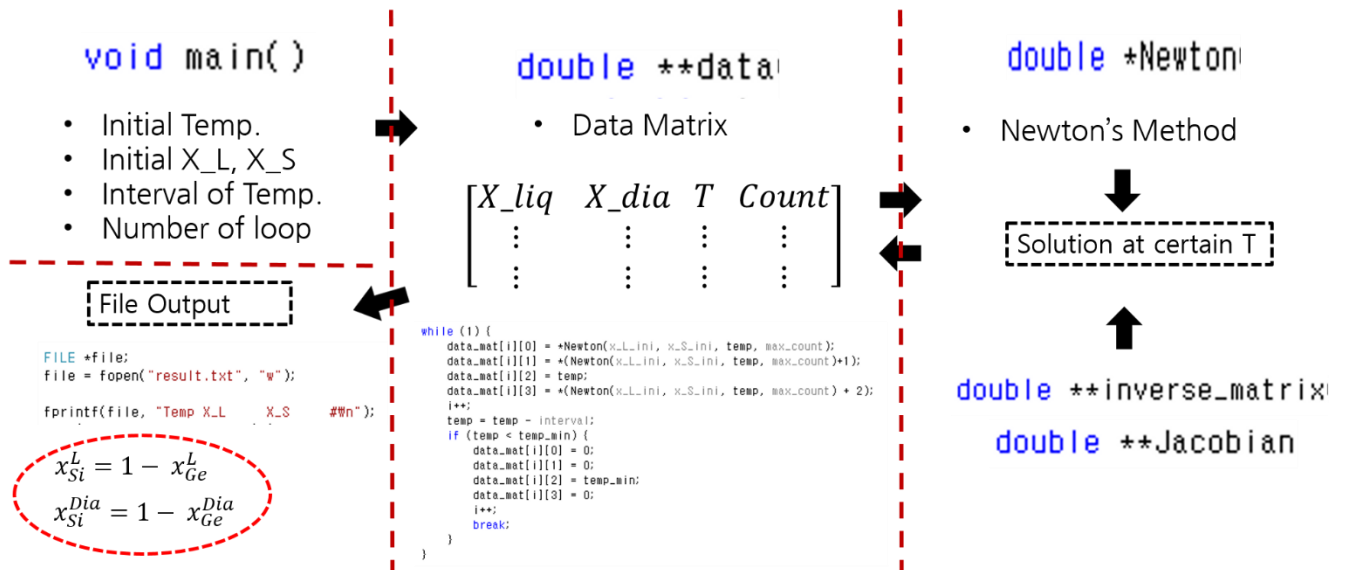
```
Not independent. Inv. Matrix cannot exist.
계속하려면 아무 키나 누르십시오 . . .
```

<Homework #4> Multicomponent Phase Equilibria

```
Input initial temperature <1211 < T < 1687> : 1200
Input initial X_L, X_S : 0.4 0.6
Input interval of temp. : 4
Input max. loop number : 1000
```

```
Not independent. Inv. Matrix cannot exist.
계속하려면 아무 키나 누르십시오 . . .
```

Question & Answer



```

<Homework #4> Multicomponent Phase Equilibria
Input initial temperature (1211 < T < 1687) : 1500
Input initial X_L, X_S : 0.5 0.5
Input interval of temp : 4
Input max. loop number : 1000

Not independent. Inv. Matrix cannot exist.
계속하려면 아무 키나 누르십시오 . . .
    
```