**CHAPTER 4**

**RESULTS AND DISCUSSION**

**4.1) REGARDING PARAMETERS**

**Table 1 –** Unknown Parameters for N = 3

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **NaCl** | **LiCl** | **Li2SO4** | **MgSO4** | **CaCl2** |
| **a** | 79.25810001 | -13416.83325 | 1805.607702 | 41812.72232 | 6917.205725 |
| **b** | 0.392577746 | -13655.82569 | -1.52985731 | -1710403.759 | -2045.137046 |
| **c** | 406.7499327 | 1438.11892 | -162.818885 | -124710.7606 | -40191.75976 |
| **d** | 79.25813745 | -17830.20198 | 1804.459355 | 25437.18659 | 8303.19844 |
| **e** | 0.393322704 | 1813.197152 | -1.53831223 | -1693135.758 | -6.0165132628 |
| **f** | 406.7499327 | 1840.796406 | -314.8768451 | 114649.0606 | 38116.51935 |
| **g** | -461.7558628 | 216895.324 | -16834.84598 | -49205.42678 | -55686.377 |
| **h** | -1.299947942 | 15369.79572 | -5.859168109 | 3900142.407 | 1578.732542 |
| **i** | -2712.455354 | -25218.75124 | -5264.96013 | 5674.916688 | 7106.784597 |
| **j** | -286.6609284 | -200587.7443 | -73341.05538 | -57730.37146 | 109013.936 |
| **k** | -0.825744651 | -92.36609842 | -3.144404132 | 75602.14676 | -3999.432868 |
| **l** | -1677.795905 | 6619.358175 | 4942.140603 | 4823.346649 | -22960.88857 |

**Table 2 –** Unknown Parameters for N = 4

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | **NaCl** | **LiCl** | **Li2SO4** | **MgSO4** | **CaCl2** |
| **a** | -0.212294839 | -8475.14118 | 1583.531513 | 735.2502247 | 8261.720861 |
| **b** | -335.4371663 | 1.951984408 | -1.523361753 | -0.791706136 | 0.574569962 |
| **c** | 10342.4994 | 11063.71503 | 335.0484774 | -175.5402835 | -2205.145069 |
| **d** | -0.207433846 | -8762.679933 | 1586.790475 | 735.2499917 | 8514.638057 |
| **e** | -323.2401916 | 1.945589229 | -1.521177232 | -0791302324 | 0.57414814 |
| **f** | -35421.30669 | -5249.227446 | 309.9047436 | -175.5427682 | 637.5750879 |
| **g** | -4.150170132 | 139528.488 | -21459.34288 | 6263.204201 | -64139.42738 |
| **h** | 357.187306 | -2.140533011 | -5.649620842 | -1.789600289 | -1.661789026 |
| **i** | 3024.992372 | -42267.20539 | -16192.5649 | -3417.892075 | 1822.071307 |
| **j** | -1.176700102 | -28829.39158 | -51230.10337 | -10121.37875 | 119035.627 |
| **k** | 9279.052789 | -3.087335404 | -3.048952414 | -1.185368643 | -1.257998805 |
| **l** | 0 | 49056.73421 | 52595.85194 | 2229.518494 | -1687.598625 |
| **m** | 102073.3323 | -139583.3918 | -4265.223202 | -1750.261638 | 5734.631344 |
| **n** | -0.353976317 | -2.475147526 | -1.159889792 | -0.569492703 | -0.617783764 |
| **o** | -33101.67039 | -35949.50214 | -78519.87037 | -6399.459638 | -28747.96172 |

**RESULT GRAPHS**

**4.2) FOR N = 3**

1. **NaCl**
2. **LiCl**
3. **CaCl2**
4. **Li2SO4**
5. **MgSO4**

**4.3) FOR N = 4**

1. **NaCl**

1. **LiCl**
2. **CaCl2**
3. **Li2SO4**
4. **MgSO4**

The model calculated phase diagrams of the Li2SO4+H2O, NaCl+ H2O, LiCl+ H2O, MgSO4+ H2O and CaCl2+ H2O systems compared with solubility data reported in literature are plotted in the above graphs. The unknown parameters of the equation 5, which helped us achieve this were tabulated in the table 1. There were 12 and 15 unknown parameters were there for n=3 and n=4 respectively. As shown in above graphs, most of the solid-liquid equilibria data, i.e. the points on the solubility curve, can be reproduced well using the present comprehensive thermodynamic models. Ice solubility data for all these systems can be accurately predicted even though they were not used in model parameterization.

For NaCl, we were able to exactly map the data against the literature work. We can able to observed minor changes in the temperature with an increase in the volume fraction from 0.02 to 0.15, above with there is a sudden increase in the temperature from 250K till 550K. This shift indicates the reduction in the water molecules attached with NaCl from ice, NaCl.2H2O to NaCl.H2O. Similarly, our model well performed in tracing the graphs for Li2SO4 as shown in the above graphs. There was a slight deviation for CaCl2 between the volume fraction of 0.42 to 0.53, which is a region of 2 H2O molecules attached with it.

The available solubility data of MgSO4 between the volume fraction of salt hydrate from 0.10 to 0.12 and 0.16 till 0.18 are kind of scattered and hard to give a critical evaluation on their reliability. Nevertheless, the model result was not affected by the scattered experimental data significantly in those volume fraction of salt hydrate but gave a regular variation. In the system of MgSO4+ H2O, the solubilities of metastable solid phases MgSO4·4 H2O (cr) and MgSO4·5 H2O (cr) were also tried to simulate except for those stable solid phases. MgSO4·11 H2O (cr) was recognized as stable phase at low temperature, although the solid phase corresponding to its solubilities in early literature were determined as MgSO4·12 H2O.

The difference of eutectic temperature of Li2SO4· H2O +ice between the present model predicted value and that recommended by Linke [76] and Sohr et al. [75] is about 2 K. According to the critical evaluation of Sohr et al. [75], the uncertainty of the eutectic temperature is 2 K. So, in such an uncertainty range, the present model result agrees with the recent recommendation of Sohr et al. [75] well. The eutectic composition of this invariant point predicted from the present model agree with those reported by Linke [76] and Sohr et al. [75] in absolute error 0.6% weight percentage, which is in accordance with the uncertainty reported by Sohr et al. [75] recently.

The parity plot for each salt hydrates explains how well this model has predicted its output compared to the Literature data. Our model almost traced its value with the literature value and gave us the error deviation of less than 4%.