

example, BET parameters of NaCl are determined and applied to calculate solubility phase diagrams of NaCl + H<sub>2</sub>O, NaCl + LiCl + H<sub>2</sub>O, and NaCl + CaCl<sub>2</sub> + H<sub>2</sub>O within the temperature range of around 250–500 K. In the ternary systems, the best agreement with solubility data from literature is obtained using constant BET parameters of NaCl and an additional temperature-dependent regular solution parameter to account for salt-salt interaction.

## **2.2 Various Models Available**

Various Thermodynamic models are studied from literature.

### **1-Debye–Hückel equation**

The Debye Hückel equation is a mathematical expression developed to explain certain properties of electrolyte solutions, or substances found in solutions in the form of charged particles (ions). The Debye Hückel equation accounts for the interactions between the different ions, which are the primary cause of differences between the properties of dilute electrolyte solutions and those of so-called ideal solutions.

The Debye-Hückel theory is based on three assumptions of how ions act in solution:

1. Electrolytes completely dissociate into ions in solution
2. Solutions of Electrolytes are very dilute, on the order of 0.01 M
3. Each ion is surrounded by ions of the opposite charge, on average

### **2- Davies equation**

Davies equation is useful at ionic strengths up to 0.5M, making it a better choice than the Debye-Huckel Model. It makes better calculation in concentrated solutions than Debye-Huckel Model. This equation was originally published in 1938. The calculation gets deviated from experiment for electrolytes that dissociate into ions with higher charges

### **3 -Pitzer**

Pitzer equations were first introduced by physical chemist Kenneth Pitzer. The parameters of Pitzer equations are linear combination of a parameters which differentiate amongst ions and solvent. The parameters are derived from various experimental data such as activity data and salt solubility. The equations are made of an extended Debye-Huckel limiting law and a virial expansion. Pitzer equations are based on an ion interaction approach, where strong interactions are treated as ion pair formation but weaker interactions are treated as ion-ion interactions that contribute to the respective ions activity coefficients. The Pitzer equations are based on an extension of the Debye-Hückel equation using a virial equation approach, where the interactions between pairs and triplets of ions and molecules are described by empirical parameters. A Pitzer model is therefore dependent on a wealth of experimental data that underlie the database of Pitzer parameters. Pitzer modelling of the major components of seawater (seawater electrolyte) is well established, and is being applied to trace metals as the relevant experimental data become available.

### **4- B-E-T Method**

BET method is also used for predicting phase change across a range of temperature and concentration. The main parameter used in BET modelling is  $r$  and  $\varepsilon$ . These parameters are temperature dependent. The number of binding sites on salt is represented by  $r$  and  $\varepsilon$  represents the difference between the molar enthalpy of adsorption of water on the salt and the molar enthalpy of liquefaction of water.

### **5- Pitzer Simonson Clegg**

It is one of the most popular model for predicting behavior of mixed electrolytes. In the PSC model, the excess Gibbs energy is represented by summation of short-range and long-range interactions. The long-range forces contribution is represented by the extended DH expression and short-range interaction term is represented by Margules expansion which includes the parameters for the interaction of solvent -anion, solvent-cation, and the disassociation of all electrolyte.

### **2.3 Research gap**

There is wide research gap in the Salt hydrates such as

1. Lack of experimental data at high temperature and pressure and validation,
2. Model accounting for salt hydrates at elevated temperature, pressure, and concentration
3. Accounting of unstable chemical reactions
4. Accounting of complex phase equilibria (vapor: liquid: solid).