**CHAPTER 3**

**METHODOLOGY**

**3.1) MODEL 1**

The osmotic coefficient (φ) of an aqueous electrolyte is related to the chemical potential of water, (µw), as follow:

In the given equation for the osmotic coefficient (φ), the terms have specific meanings:

µ0w is the chemical potential of water in its standard state.

Mw is the molecular mass of water.

is the number of ions produced on dissociation of one molecule of the electrolyte.

m is the molality of the electrolyte solution, R is the gas constant and T, the absolute temperature.

These variables collectively determine the extent of deviation from ideal behaviour in solutions, providing insights into the behaviour of solutes and solvents in solution dynamics.

In this work, Gibbs free energy term is given by long range (Lr) electrostatic contributions b/w ions and short range (Sr) interaction b/w all species.

Using Pitzer`s form of the Debye- Huckle (PDH) function as the electrostatic contribution to the free energy. So,

were,

nw, ns = no. of moles of water, salt respectively

vs, vw = partial molar volume (m3/mole) of salt, solvent respectively

b = the closest approach parameter

Total no. of ions per salt

Debye Huckel type constant

Where Mw = molecular weight of solvent i.e., water in gram/mol,

NA = Avogadro number,

K = Boltzmann constant, ε = permittivity of vacuum, e = electronic charge,

DS = dielectric constant of water, VS = the molar volume of water

I = the ionic strength or

The expression for the short-range interaction contribution of aqueous salt solution is obtained from Flory- Huggins theory as given below,

Where χsw = salt-water interaction parameter, which dependent on the salt concentration and temperature

and represent the moles of salt hydrate and water in salt hydrate solution, respectively. is the number of Kuhn segments in Salt hydrate chain.

The term is the generalized Flory-Huggins parameter and considered as the function of the volume fraction of the salt hydrate, , and temperature, .

is temperature dependent coefficient and as expressed as:

and are constants.

is temperature dependent coefficient are calculated using nonlinear regression method.

Derivative of Equation (4) w.r.t. moles of water and salt gives us chemical potential of water and salt hydrate respectively.

Combining equation 1 and 5 we get,

The condition for the phase equilibrium between two separate phases (Phase-1 and Phase-2) are given by,

And

By solving equation simultaneously, phase diagram can be obtained.

The critical point is given by the following conditions:

