MATHEMATICAL MODELING OF THERMOCHEMICAL ENERGY STORAGE BY SALT HYDRATES

REVIEW 2

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1. INTRODUCTION

Fig 1 .

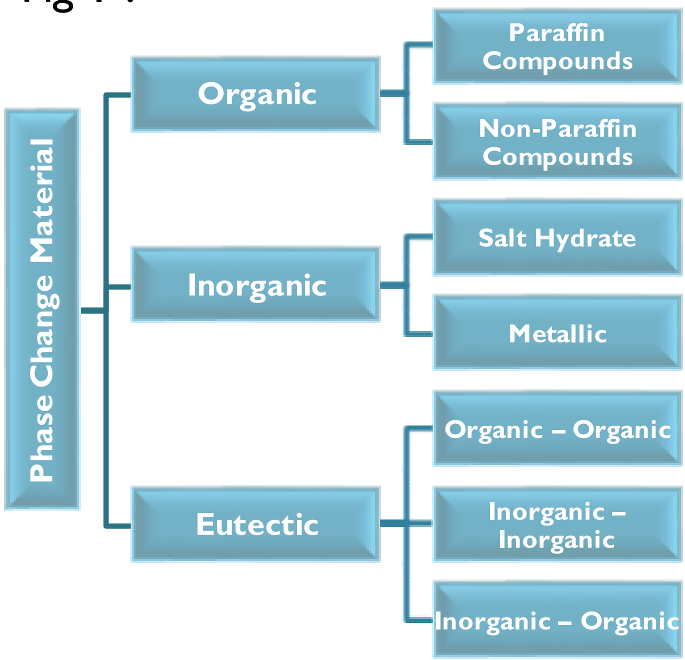


Fig 2.

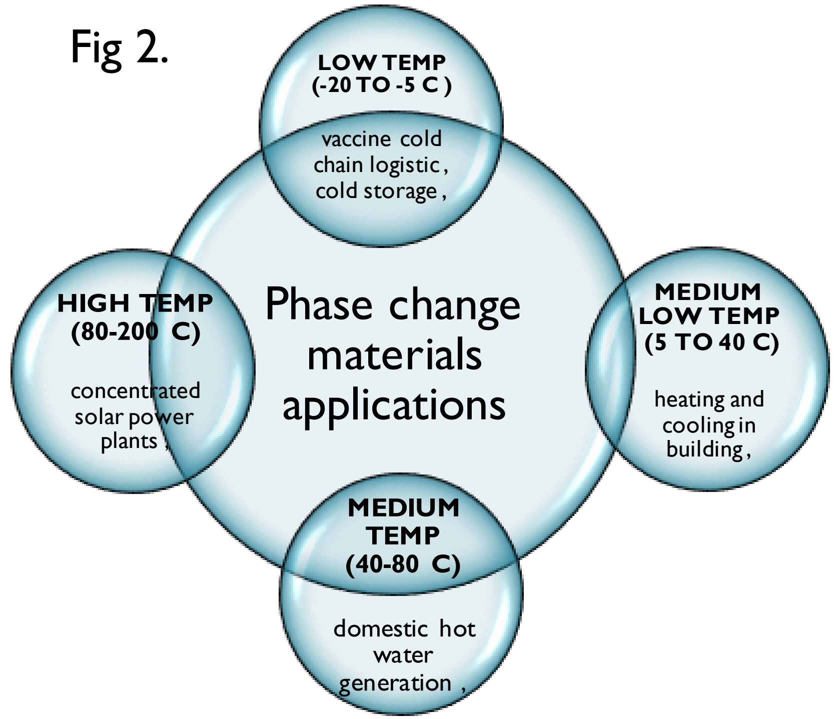


Fig 3 .

2. LITERATURE REVIEW

Our literature review includes works of various researchers like

- **M. Gaeini (2018)**, who studied thermochemical heat storage in salt hydrates.

- **Lin Liang (2017)**, who studied that a new cold storage phase change material eutectic hydrate salt ($K_2HPO_4 \cdot 3H_2O–NaH_2PO_4 \cdot 2H_2O–Na_2S_2O_3 \cdot 5H_2O$) was prepared, modified, and tested.

- **Luca Scapino (2017)** studied that sorption heat storage has the potential to store large amounts of thermal energy from renewables and other distributed energy sources.

- **Dongdong Li (2018)** studied the development of a multi-temperature thermodynamically consistent model for Salt Lake brine systems.

- **Christoph Rathgeber (2019)** worked on the modified BET equations that are extended to calculate solubility phase diagrams of concentrated salt solutions with relatively high-water activities within the range of under saturation.

And many more to add on.

2. Literature Review

Various Thermodynamic models are studied from literature.

- Debye-Huckel equation
- Davis Equation
- Pitzer Equation
- BET Model
- Pitzer Simonson Clegg

3. Research Gap and Novelty

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).

4. OBJECTIVE

1. Study of phase change of salt hydrates

2. Study of charging and discharging cycles

3. Study of capacity of batteries

4. Study of thermal management in batteries

5. METHODOLOGY

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.

$$\frac{F}{RT} = -(n_w + \nu n_s)\frac{4A_x I_x}{b} ln\left(1 + bI_x^{\frac{1}{2}}\right) + n_w ln\phi_w + \nu n_s ln\phi_s + \chi_{sw}\, n_w \phi_s$$

In which,

- F = Total Free energy
- n_w, n_s = no. of moles of water, salt respectively
- v_s, v_w = partial molar volume (m^3/mole) of salt, solvent respectively
- b = the closest approach parameter
- Total no. of ions per salt $\upsilon = \upsilon_M + \upsilon_X$
- Debye Huckel type constant
- χ_{sw} = salt-water interaction parameter

5. Methodology

The derivative of the total free energy equation w.r.t. moles of water and salt gives us chemical potential of water and salt hydrate respectively.

$$\frac{\mu_w - \mu_w^0}{RT} = \left(\frac{\delta \frac{F}{RT}}{\delta n_w}\right)_{n_s}$$

$$= \left(I_x ln\left(1 + bI_x^{\frac{1}{2}}\right)\right)\left[-\frac{\nu n_s}{n_w}\right] - \frac{(n_w + \nu n_s)}{2\left(1 + bI_x^{\frac{1}{2}}\right)}\frac{I_x^{-\frac{1}{2}}}{n_w} + ln\phi_w + \phi_s\left(1 - \frac{v_w}{v_s}\right)$$

$$- \chi_{sw}\phi_s^2 - \frac{\delta\chi_{sw}}{\delta\phi_s}\phi_s^2(1 - \phi_s)$$

- Finally, we can get the osmotic coefficient as,

$$\varphi = -\frac{1}{M_w \upsilon m} \times \left[\frac{\mu_w - \mu_w^0}{RT}\right]$$

6. RESULTS AND DISCUSSION

Parity plot for n=3

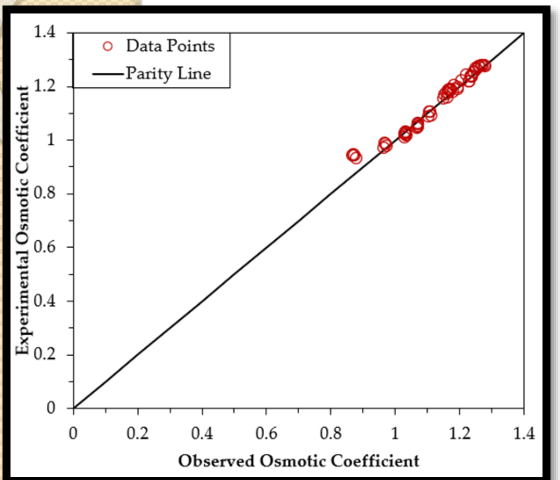


Fig 1: NaCl

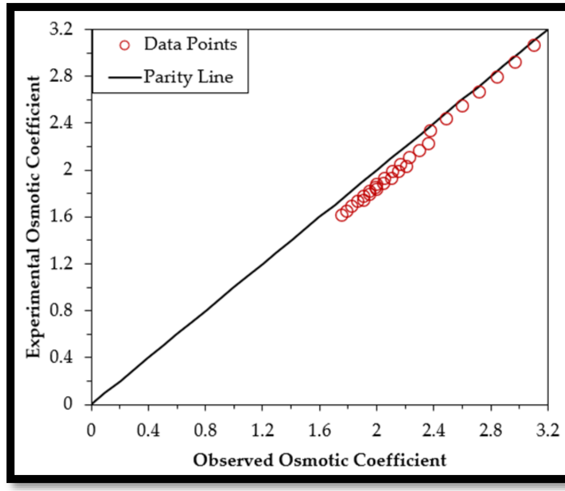


Fig 2: LiCl

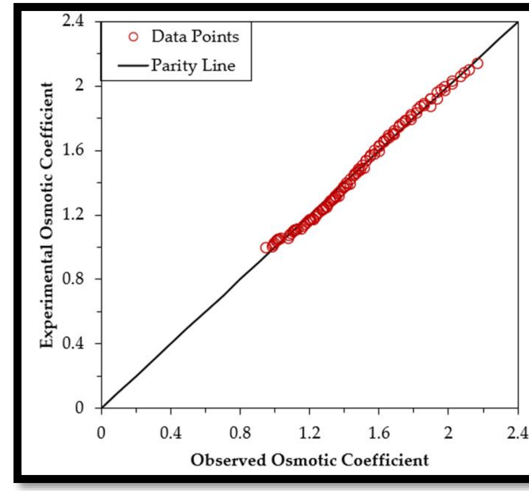


Fig 3: CaCl2

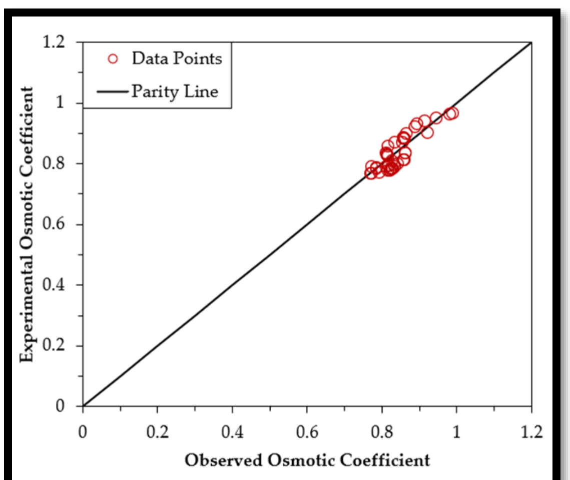


Fig 4: Li2SO4

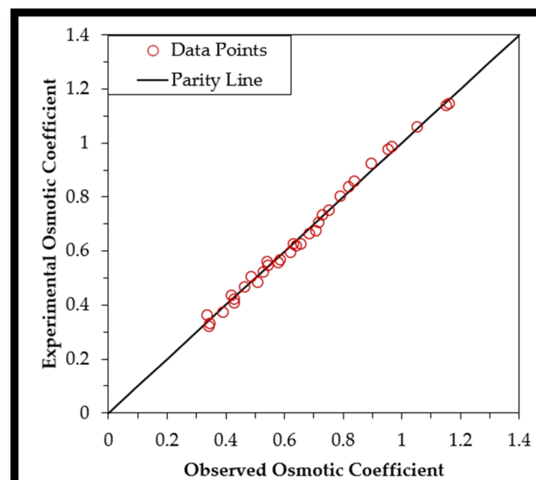
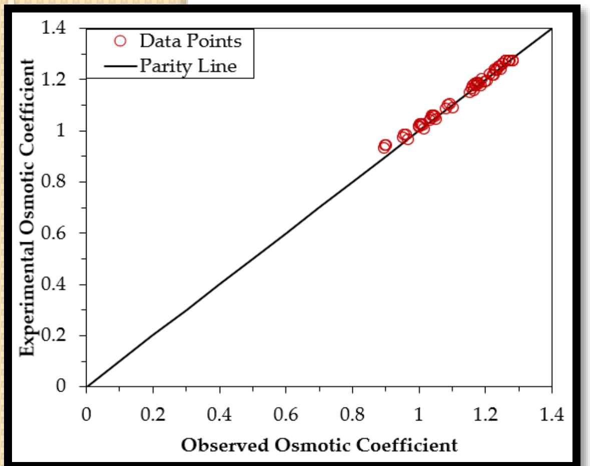


Fig 5 :MgSO4

Parity plot for n=4



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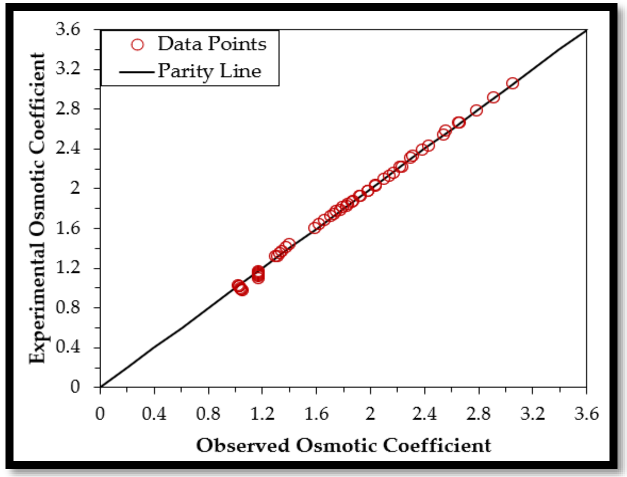
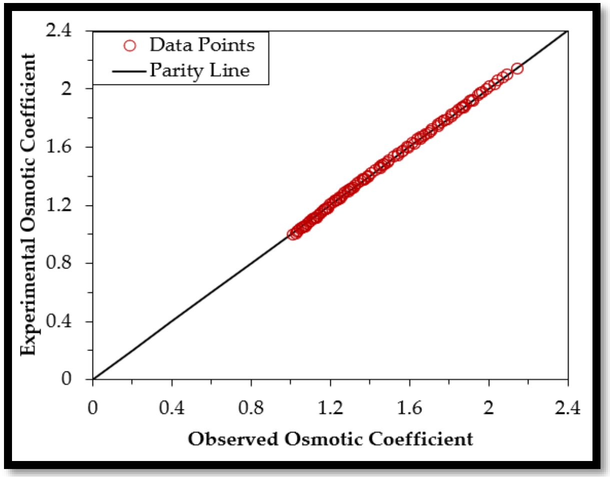


Fig 2: LiCl



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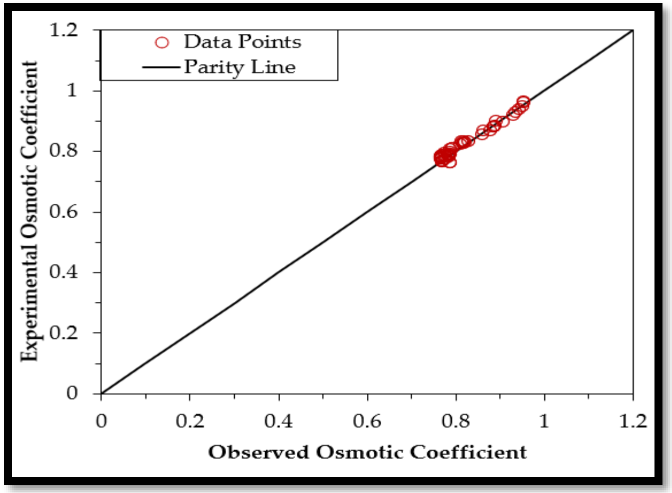


Fig 4: Li2SO4

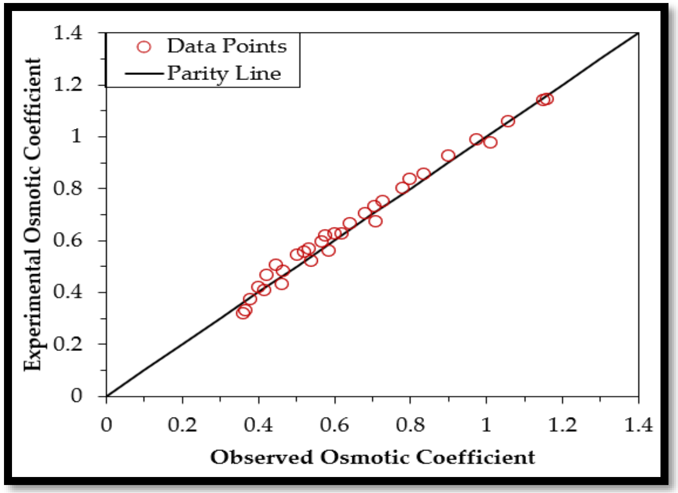


Fig 5 :MgSO4

Phase diagram graphs for n=3 and n=4

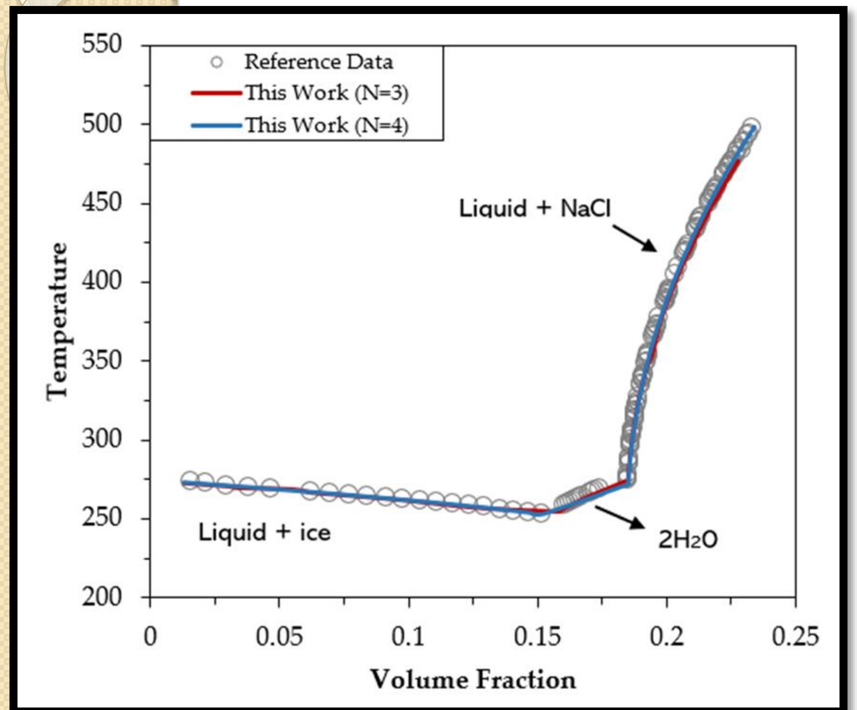
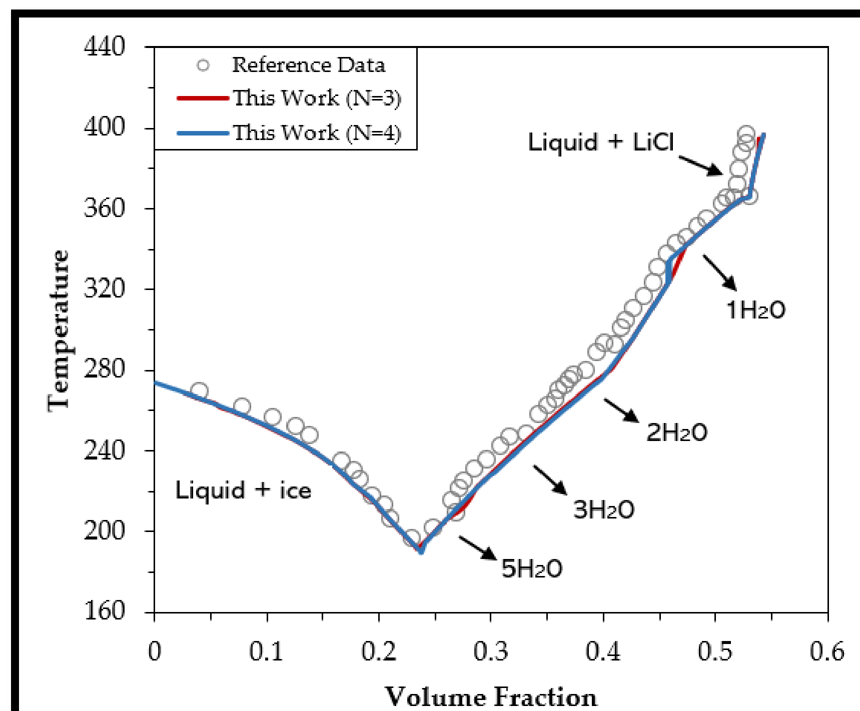


Fig 1: NaCl

Fig 2: LiCl



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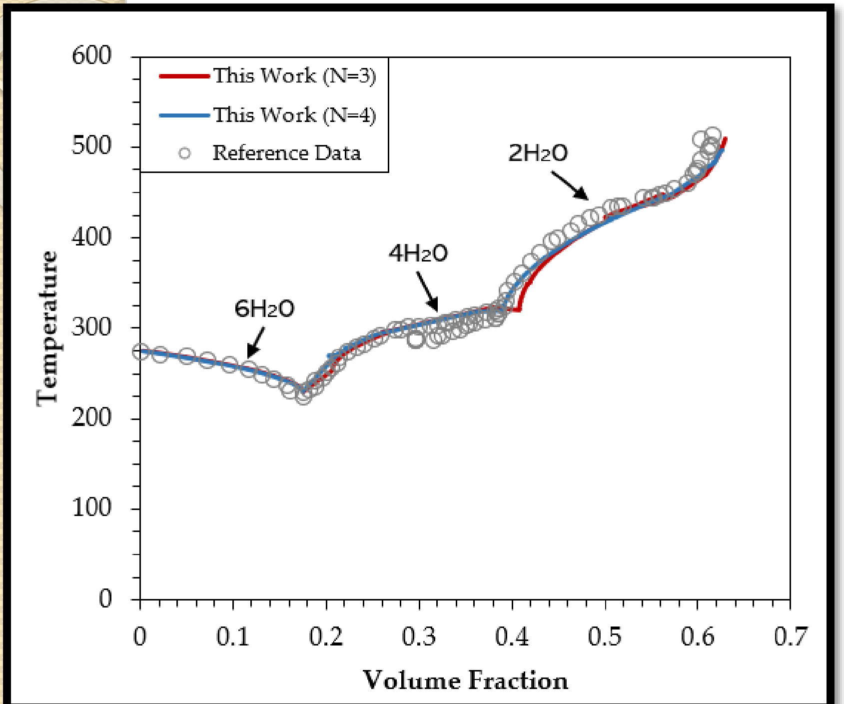
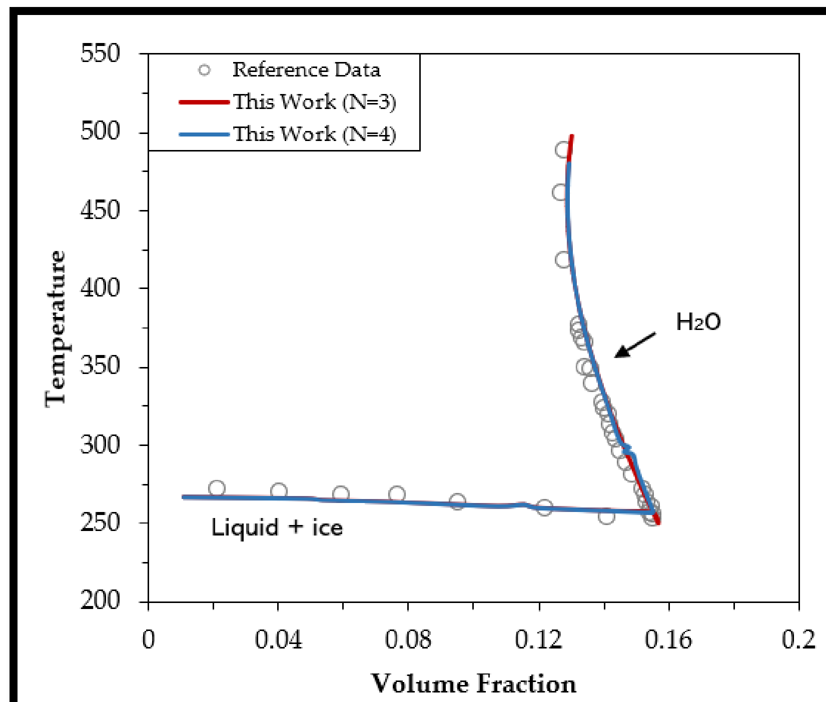


Fig 3: CaCl2

Fig 4: Li2SO4



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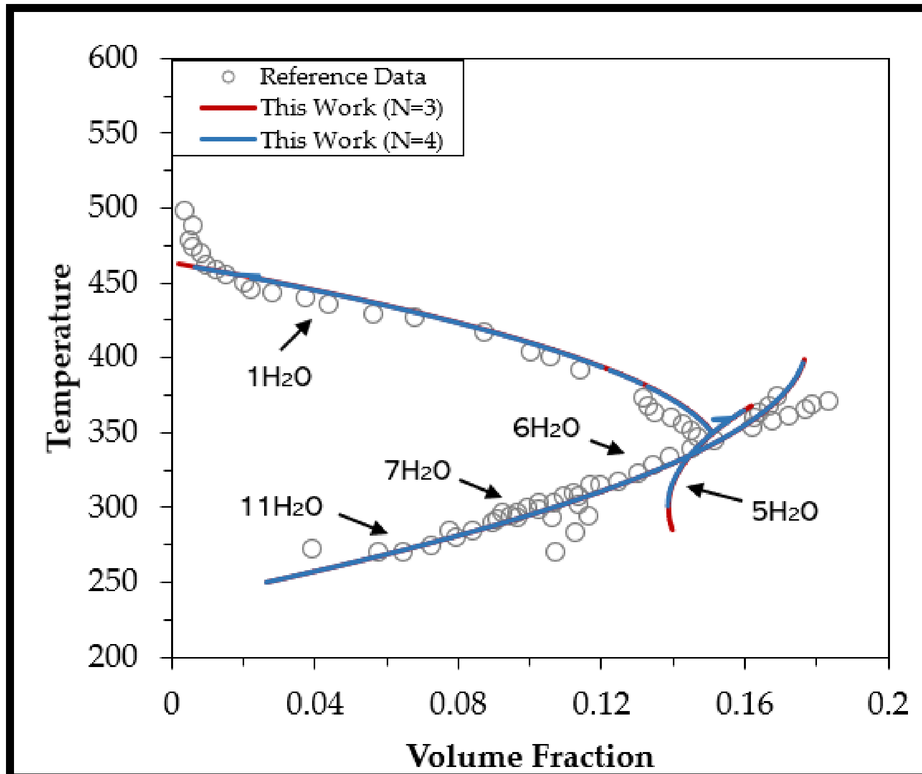

Fig 5 :MgSO4

7. WORK PLAN

Work done till now :

1. Literature reviews
2. Developed a mathematical model for various salt hydrates
3. Solve the model for various salt hydrates
4. Draft of our work is ready in form of research article

Work plan for future :

5. Extend our model for mixer of salt hydrates and eutectic salts
6. Submit our work in renowned journal

! THANK YOU !