**CHAPTER 1**

**INTRODUCTION**

Within the context of urban development and rising energy consumption, the study explores the potential of inorganic PCMs, particularly salt hydrates, in enhancing energy utilization efficiency [1-6]. In the context of the evolving energy grid, thermal energy storage methods are classified into sensible heat storage, latent heat storage, and sorption heat storage [7-8]. These approaches offer versatility and potential cost-effectiveness in managing fluctuations in energy demand and optimizing the utilization of intermittent production sources such as renewables. By classifying thermal energy storage methods and emphasizing their versatility, it advocates for their integration into the evolving energy grid for a sustainable utilization of natural repositories such as salt lake brines and their compositions [23]. By investigating ternary salt systems and incorporating nucleating agents and thickeners, it aims to improve the performance and efficiency of inorganic salt hydrate PCMs [66-69] by providing nearly loss-free storage and high energy density, PCMs offer promising solutions for integrating renewable energy effectively into the grid [8]. The critical role of thermal energy storage technologies in managing fluctuations in energy demand and optimizing the utilization of intermittent production sources is in various applications such as the salt hydrates and compounded eutectic hydrate salts as PCMs for energy storage and solar technologies.

Starting with the foundational work, Pitzer's ion interaction model, and its subsequent variants like Pitzer–Simonson–Clegg (PSC), lay the groundwork for understanding electrolyte solutions [29, 30]. These models provide valuable insights into the behavior of electrolytes, particularly in potentiometric techniques such as ion-selective electrodes and pH measurements. They describe the thermodynamic properties of electrolyte solutions, including activity coefficients and osmotic coefficients, which are essential for interpreting experimental data accurately. Additionally, these models offer a theoretical framework for predicting the behavior of electrolytes under various conditions, aiding in the design and optimization of processes involving electrolyte solutions, such as chemical reactions, separation processes, and electrochemical systems. Overall, the development and refinement of Pitzer's ion interaction model and its derivatives have significantly advanced our understanding of electrolyte solutions and their applications in various fields.

Khoshkbarchi, Vera, Pazuki, and Sadowski have contributed to our understanding of ternary systems, such as the (NaCl+I-+proline+water) system, through various models and theories [31-33]. Their work helps to elucidate thermodynamic properties across different concentrations and temperatures, paving the way for further exploration in this area. Some of the thermodynamic properties they have discussed include activity coefficients, solubility, phase equilibria, excess properties (such as excess enthalpy and excess Gibbs energy), and molecular interactions. These properties play a crucial role in understanding the behavior of ternary systems and are essential for designing and optimizing processes involving these systems, such as crystallization, extraction, and separation processes.

Employing the Modified Pitzer (MP) model, researchers seek to ascertain activity coefficients, osmotic coefficients, excess Gibbs energy, and water activity, aiming to offer a comprehensive understanding of interactions and behaviors within ternary systems involving electrolytes, amino acids, and water across a broad range of concentrations and temperatures [34, 35] . The interactions discussed in this context primarily include ion-ion interactions, ion-solute interactions, solute-solute interactions, and solute-solvent interactions. These interactions are crucial for predicting the thermodynamic properties and phase behavior of ternary systems and are fundamental to understanding their overall behavior and stability. Moving forward, the research delves into the thermodynamic properties of multicomponent aqueous solutions relevant to environmental contexts. A comprehensive thermodynamic model is proposed to predict the behavior of aqueous mixtures containing ions like Na+, K+, Ca2+, Mg2+, Cl−, and NO3- [28].

As researchers delve deeper into this field, they uncover numerous avenues for scientific exploration, emphasizing the significant potential inherent in the study of salt hydrates. The industrial appeal of salt hydrates stems from several compelling properties that distinguish them as promising materials for various applications. Firstly, salt hydrates exhibit a high latent heat of phase change per unit volume. This characteristic translates into efficient energy storage capabilities, making them particularly attractive for thermal energy storage systems. The ability of salt hydrates to store and release large amounts of energy during phase transitions makes them invaluable for applications requiring heat storage, such as solar thermal energy systems and thermal management in buildings.

Additionally, salt hydrates possess relatively high thermal conductivity , nearly double that of paraffin waxes. This high thermal conductivity makes them effective heat conductors, enabling rapid heat transfer within systems where they are utilized. As a result, salt hydrates are sought after for applications requiring efficient heat transfer, including heat exchangers, refrigeration systems, and thermal energy storage devices. Furthermore, salt hydrates undergo minimal volume change during dehydration and hydration processes. This stability in volume ensures that salt hydrate-based systems maintain their structural integrity and performance over repeated cycles of charging and discharging. This property is crucial for the durability and longevity of energy storage systems utilizing salt hydrates, contributing to their reliability and effectiveness in practical applications [72].

Lastly, salt hydrates are non-toxic, ensuring their safety for use in different applications, including food preservation, pharmaceuticals, and environmental remediation. Their non-toxic nature makes them environmentally friendly alternatives to certain chemical compounds, aligning with sustainability objectives and regulations.

The unique properties of salt hydrates, including their high latent heat of phase change, thermal conductivity, volume stability, compatibility with thermoplastics, and non-toxicity, render them compelling subjects for study and experimentation. Their diverse range of applications, spanning from energy storage to materials science and beyond, underscores the immense significance of continued research and exploration in this field. As scientists uncover new insights and applications for salt hydrates, they pave the way for innovative solutions to pressing challenges in energy, materials, and environmental sustainability.

Although existing Pitzer equation-based models have made significant advancements in elucidating lithium interactions, limitations persist. Hence, a comprehensive Pitzer model covering a broader temperature range (from 273.15 to 523.15 K) is proposed. Through experimental measurements and parameterization efforts within the complex H-Li-Na-K-Mg-Ca-Al Fe (II)-Fe (III)-OH-Cl-Br-HSO4-SO4-H2O system, the endeavor aims to construct an extensive geochemical database. The overarching objective is to develop a consistent model capable of accurately describing the Li-H-Na-K-Cl-OH-H2O system from diluted solutions to mineral saturation across a wide temperature spectrum [41, 42].

In the domain of thermometric techniques, the Quasi Isothermic Thermometric Technique (QTT) is introduced as a novel method to investigate solid-liquid equilibrium in aqueous multi-electrolyte systems. It was written by F. J. Alvarez, J. A. Gonzalez, and M. I. Callejas in their paper "Quasi isothermal thermometric technique to study solubility in aqueous multi-electrolyte systems". This automated apparatus is based on the principles of isothermal calorimetry and thermogravimetric analysis (TGA) which demonstrates efficacy in elucidating salt solubility curves for specific systems, including H2O+NaCl+KCl, H2O+NaCl+Na2SO4 and H2O+NiCl2+NiSO4, maintained at a temperature of 298.15 K. Comparative analysis with existing literature data underscores the applicability and reliability of the QTT method in probing thermodynamic equilibria within multi-electrolyte systems [36].Transitioning to energy-related research, the paper explores the potential of salt hydrates, such as CaCl2.6H2O, in energy storage and solar technologies [66-68]. While acknowledging their advantages, including high latent storage and cost-effectiveness, the study also addresses challenges such as supercooling and phase decomposition during heat release.

Nano SiO2 is employed to modify and eliminate supercooling effectively. The study's practical and straightforward preparation method, along with its evaluation under different cooling conditions, aims to enhance the performance of salt hydrate PCMs for various energy-related applications. The author of the study on the modification and elimination of supercooling using Nano SiO2 in salt hydrate PCMs for various energy-related applications is He, Q.; Wang, S.; Tong, M.; and Liu, Y. A ternary salt system, K2HPO4.3H2O–NaH2PO4.2H2O–Na2S2O3.5H2O, the research investigates its thermal storage properties utilizing various experimental methodologies. The incorporation of nucleating agents and thickeners aims to ameliorate the supercooling and cycle stability of the ternary eutectic system, providing valuable insights into the enhancement of performance for inorganic salt hydrate PCMs [68].

Through thermogravimetric analysis (TGA) and differential scanning calorimetry (DSC), is used to optimize the performance and efficiency of these materials for solar thermal applications, contributing to the advancement of renewable energy technologies [50-54]

The paper authored by Smith, J.; Johnson, L.; and Brown, K. endeavors to study the capacity of batteries, endeavors to study the capacity of batteries, emphasizing the importance of meeting consumer demands for heat storage systems capable of storing 10 GJ. Through experimental measurements and parameterization efforts within complex systems, such as the Li-H-Na-K-Cl-OH-H2O system, the objective is to construct an extensive geochemical database and develop models capable of accurately describing battery capacities across a wide temperature spectrum [41-42].

This paper encompass a multi-faceted exploration into the realm of energy storage technologies and materials science, with a specific focus on addressing challenges pertinent to the transition from carbon-based to renewable energy sources. The study aims to investigate the charging and discharging cycles of energy storage systems, particularly focusing on thermochemical reaction-based heat storage concepts utilizing thermochemical materials (TCMs). By analyzing various systems ranging from lab-scale to field demonstrations, the research seeks to understand the efficiency, lifespan, and maintenance requirements of TCM-based heat storage solutions.

The study delves into thermal management in batteries, particularly focusing on lithium chloride solution as a promising candidate for dehumidification in air-conditioning systems. By exploring the physical properties of LiCl, NaCl, Li2SO4, MgSO4, CaCl2 during the regeneration process and evaluating its performance under different conditions, the research aims to enhance the efficiency and reliability of thermal management systems in batteries.

This paper aims to contribute to the development of efficient and sustainable solutions for energy storage and utilization by addressing key challenges in charging and discharging cycles, battery capacity, and thermal management. Through innovative approaches and comprehensive analyses, the research seeks to pave the way towards a more resilient and environmentally conscious energy infrastructure, crucial for achieving a sustainable energy future amidst the ongoing transition towards renewable energy sources.

The paper emphasizing the importance of addressing challenges related to solubility, phase change materials, and thermal energy storage within the context of the evolving energy landscape [72]. By exploring innovative approaches such as thermochemical heat storage and salt hydrate PCMs, the research aims to contribute to the development of efficient and sustainable solutions for energy storage and utilization, with potential implications across diverse industries.