Thermal performance analysis of a thermocline thermal energy storage system with FLiNaK molten salt

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Abstract. A thermocline thermal storage unit with a heat transfer fluid (HTF) of high-temperature molten salt is considered as one of the most promising methods of thermal storage due to its lower cost and smaller size. The main objective of this work is to analyze the transient behavior of the available molten salt FLiNaK used as the HTF in heat transfer and heat storage in a thermocline thermal energy storage (TES) system. Thermal characteristics including temperature profiles influenced by different inlet velocities of HTF and different void fractions of porous heat storage medium are analyzed. The numerical investigation on the heat storage and heat transfer characteristics of FLiNaK has been carried out. A comparison between two different molten salts, FLiNaK and Hitec, has been explored in this paper with regards to their charging and discharging operations. The results indicate the system with FLiNaK has a greater energy storage capability, a shorter charging time and a higher output power. The numerical investigation reveals heat storage and heat transfer characteristics of the thermocline TES system with FLiNaK, and provide important references for molten salt selection of the TES system in the future.

1. Introduction
Thermal energy storage (TES) is very important in many engineering applications such as solar energy, space heating and waste heat recovery. Generally, in a TES system, the heat transfer fluid (HTF) used to carry heat from heat source to TES and the storage medium capable of retaining heat obtained from HTF for later discharge are required. The HTF, sometimes either used for direct fluid storage must have favourable properties for heat transfer include low freezing temperature and/or high maximum operational temperature, high heat capacity, high thermal conductivity, high density, good stability and low vapor pressure [1, 2]. And it is desirable for the storage medium to have high specific heat capacity, long term stability and compatibility with its containment [3]. Inorganic salt of a molten state has broad application prospects in TES of large-scale renewable energy due to its good performance of wide operation temperature range, low vapor pressure, low viscosity and relatively high density in heat storage and heat transfer [3, 4]. Thermal energy can be stored as sensible, latent, or a combination of both heats by the method of using molten salt as the HTF and storage material. Storage of the sensible heat is achieved by raising the temperature of the storage medium and the release of sensible heat is implemented by lowering the temperature of the storage medium [5]. The sensible heat storage has simpler heat transfer design, more flexible operation, more mature technology and cheaper cost than the latent heat storage [6].

In order to reduce the size and costs, a single tank system full filled with spherical particles which are made of some high thermal capacity material have been proposed [7-9], in which natural thermal...
stratification driven by buoyancy forces within single storage tank is taken into consideration to isolate hot and cold HTF. The single tank system uses porous medium to replace part of costly molten salt as a storage medium. There is a special region called thermocline characterized by a great temperature gradient between the coldest fluid and the hottest fluid in the storage tank, which separates the hot and cold fluids. The gradient of temperature in the thermocline mainly depends on the characteristics of the storage material and molten salt.

Currently the most widely used molten salt is nitrate-based, and different researches on the thermocline TES system with the nitrate salts have been conducted [10-13]. However, the maximum working temperature of nitrate salts is limited below 600°C because of its thermal stability, which restricts the improvement of power generation efficiency of the energy storage system. Thus, to find a suitable molten salt so as to raise the working temperature and extend operating temperature range will be of great significance.

The FLiNaK is one of the most common fluoride molten salts possessing a series of advantages include higher heat capacity, higher thermal conductivity, higher operational temperature and good heat transfer performance, which is widely used in the high-temperature hydrogen, nuclear fuel and other energy fields [14, 15].

The present work makes an analysis of the transient behavior and thermal characteristics during the charging and discharging modes of the single tank TES system with FLiNaK molten salt. Thermal characteristics including the temperature profiles influenced by different inlet velocities and different void fractions of the porous medium were analyzed. And Hitec molten salt is also considered as HTF to be compared with FLiNaK.

2. Mathematical model
As the previous studies on the single tank thermocline TES system, the mathematical model used is developed based on Schumann’s [16] original work. The geometry of a cylindrical thermocline single tank is illustrated in the figure 1, where the gray area is regarded as the analysis object. The packed bed is defined by the void fraction of $\varepsilon$ and the particles behave as continuous and isotropic porous medium. During the charging period, the hot molten salt flows into the storage tank from the upper inlet in the middle of the top of storage tank and transfer heat to the cold solid particles and molten salt, and then flows out of the tank through the outlet at the bottom of the tank with a lower temperature. In this process, a thermocline is formed between the hot molten salt and the cold one. When the thermocline has exited the storage tank completely and the filler materials have reached a uniform temperature as high as the temperature of inlet molten salt, it means the charging process has been completed. At last, the thermal energy is stored in the filler materials in the tank. During the discharging period, the cooled HTF enters the storage tank from the bottom of the tank, and the hot molten salt leaves the storage tank for applications. When the thermocline begins to get out from the tank, the effective discharging process is finished.

The main objective of this work is to analyze the thermal performance of the available FLiNaK molten salt in heat transfer and heat storage system. The mathematical model is developed with the multi-physics finite element analysis software COMSOL Multiphysics. The heat storage tank is an upstanding cylinder, 2 meter high and 1 meter in diameter. In the calculation and analysis, several reasonable assumptions employed for the simplification of the modeling and corresponding justifications are shown as follows:

(a) The packed-bed region is symmetrical along the axis direction. Distributors are assumed to ensure that the inlet HTF flow is uniformly distributed to create a well-formed thermocline. The characteristics of storage medium in the tank can be considered to be uniform in the radial direction, and the change only occurs in the axial direction;
(b) Physical properties of the porous media are kept constant;
(c) The Biot number of the filler particles is so small that the temperature distribution inside the sphere is regarded as uniform [17];
(d) The filler particles behave as continuous, homogeneous and isotropic porous medium;
(e) There is a complete thermal insulation between storage tank and environment.
Figure 1. Schematic diagram of the thermocline TES system during charging mode.

The temperatures of both solid and fluid phases are evaluated along the flow direction according to the energy equations (1) and (2) [18].

For the porous medium, the equation is:

\[
(1 - \varepsilon)\rho_s C_{p,s} \frac{\partial T_s}{\partial t} = (1 - \varepsilon)k_s \frac{\partial^2 T_s}{\partial z^2} - h_v (T_s - T_f)
\]

and for the HTF, the equation is:

\[
\varepsilon\rho_f C_{p,f} \frac{\partial T_f}{\partial t} + \rho_f C_{p,f} u \frac{\partial T_f}{\partial z} = \varepsilon k_f \frac{\partial^2 T_f}{\partial z^2} + h_v (T_s - T_f)
\]

where, \( h_v \) denotes the volumetric convective heat transfer coefficient between the solid particles and HTF, \( T_s, T_f, u, C_{p,s}, C_{p,f}, k_s \) and \( k_f \) respectively represent the temperature of solid material and fluid, the axial apparent velocity of HTF in the storage tank, the heat capacity of solid material and fluid, the thermal conductivities of solid material and fluid.

The \( h_v \) is linked to the convective heat transfer coefficient \( h_s \):

\[
h_v = \frac{6(1 - \varepsilon)}{d_s} h_s
\]

where \( d_s \) denotes the diameter of solid particles. The heat transfer coefficient \( h_s \) can be calculated from [17]:

\[
h_s = \frac{Nuk}{d_s}
\]

In the Eq.(4), the Nusselt number \( Nu \) is a function of Reynolds number and Prandtl number based on particle diameter.
\[ Nu_t = 2 + 1.1 \left( Re^{0.6} Pr^{0.33} \right) \]  

The FLiNaK (LiF-NaF-KF, 46.5-11.5-42.0 mol%) is an eutectic mixture of inorganic salts with melting temperature of 454 °C [15] and boiling point of 1570 °C. The Hitec® (KNO3-NaNO3-NaNO2, 44-7-49 mol%) is also an eutectic mixture of inorganic salts and in a stable liquid state ranging between 142 °C to 600 °C. The average thermo-physical properties such as specific heat capacity and thermal conductivity of FLiNaK (1882.8 J kg\(^{-1}\) K\(^{-1}\), 0.92 W m\(^{-1}\) K\(^{-1}\)) are respectively higher than them of Hitec (1560 J kg\(^{-1}\) K\(^{-1}\), 0.51 W m\(^{-1}\) K\(^{-1}\)).

In this study, the thermo-physical properties (heat capacity, thermal conductivity, density and viscosity) of molten salt are functions of temperature [19-22]. The input parameters of porosity and thermal properties of porous medium are tabulated in Table 1.

| Parameters                                      | FLiNaK | Hitec |
|------------------------------------------------|--------|-------|
| Initial temperature of charging mode (K)       | 773    | 473   |
| Inlet fluid temperature of charging mode (K)   | 973    | 673   |
| Initial temperature of discharging mode (K)    | 973    | 673   |
| Inlet fluid temperature of discharging mode (K)| 773    | 473   |
| Diameter of storage tank (m)                   | 1      | 1     |
| Height of storage tank (m)                     | 2      | 2     |
| Diameter of spherical particles (m)            | 0.01   | 0.01  |
| Void fraction                                  | 0.2/0.3/0.4 | 0.4 |
| Thermal conductivity of porous medium (W m\(^{-1}\) K\(^{-1}\)) | 1      | 1     |
| Specific heat capacity of porous medium (J kg\(^{-1}\) K\(^{-1}\)) | 1500   | 1500  |
| Density of porous medium (kg m\(^{-3}\))       | 2000   | 2000  |
| Inlet velocity of charge and discharging mode (m s\(^{-1}\)) | 0.001/0.005/0.01 | 0.001 |
| Initial pressure (bar)                         | 1      | 1     |

Initial conditions:

\[ T_f(z,0) = T_{in} , \quad T_s(z,0) = T_{in} \quad (0 \leq z \leq H) \]  

Boundary conditions:

\[ T_f(2,t) = T_{in} , \quad T_s(2,t) = T_{in} \quad (t > 0) \]  

Where, \( T_{in} \) denotes the initial temperature of porous medium and molten salt, \( T_{in} \) represents the inlet temperature of the molten salt.

The reported experimental results of Yang et al. (2012) [13] are used here to validate the numerical model. The diameter and height of the thermal storage tank built for the reported TES system was 263 and 550 mm, respectively. The diameter of the filler particle was 30 mm, whereas the density of the filler material was 2100 kg/m\(^3\). Composite nitrate salt was used as HTF. The numerical results for the temperature profiles of molten salt at position \( x = 0.25 \) m and \( x = 0.5 \) m are compared with the experimental ones in figure 2. The simulation uses the same conditions as described in experiment. Within the experimental uncertainty, the results from the simulations appear to agree well with the experiments. Thus, the numerical method is reliable and the model is suitable for the thermal performance analysis of a TES with molten salts.
Figure 2. Comparison between the experimental and numerical results for the axial temperature profiles of molten salt at positions of \( x = 0.25 \) m and \( x = 0.5 \) m.

3. Results and discussion

3.1. Temperature profiles

The temperature distributions of the FLiNaK molten salt and porous medium during the charging mode are shown in figure 3 (a). The left side of the picture represents the fluid domain and the right side represents the porous medium domain. It is observed that the temperature of the fluid is higher than the porous medium at a same height.

Figure 3 (b) shows the temperature profiles along the HTF flow direction of the FLiNaK and porous medium at a given charging time of 920 sec (to facilitate observation, total charging time is 2230 sec). In this case, the inlet velocity of fluid is 0.001 m/s, the void fraction of porous material is 0.4, and the diameter of filler particle is 0.01 m. This figure indicates that the thickness of thermocline accounts for about 62.5% of the entire height of storage tank at this moment. A same conclusion with figure 3 (a) can be easily obtained from figure 3 (b) that the temperature of fluid is slightly higher than the temperature of porous medium when compared at a same position, and the temperature difference is mainly occurs in the transition region and peaks in the middle of the thermocline.

3.2. Influence of HTF inlet velocity

The influence of HTF velocity on the thermal performance of the storage system is investigated in this section. figure 4 shows the temperature difference distribution for FLiNaK molten salt along the axial flow direction under various HTF inlet velocities. To facilitate observation, the curves were selected when the flowing distance along axial direction of HTF thermal front reached the half of the tank height. The charging times of each curve are respectively 920, 185, 97 sec, and three inlet velocities 0.001, 0.005, 0.01 m/s are considered respectively. With the increase in the value of inlet velocity, the Reynolds number increases. It is clear that the temperature difference between HTF and porous solid particles occurs in transition region of thermocline becomes larger and the local thermal non-equilibrium becomes more obvious with the rise in the Reynolds number. As a matter of fact, the increase of Reynolds number enhances the effect of heat transfer between HTF and porous medium.

3.3. Influence of void fraction

The temperature distributions at the outlet of storage tank with FLiNaK molten salt during the charging mode for the various void fractions are presented in figure 5. In this case, the inlet velocity of HTF is 0.001 m/s and filler particle diameter is 0.01 m. With the decrease of void fraction, the overall time of charging process becomes shorter. That is because the thermal conductivity of the porous
material is larger than the thermal conductivity of FLiNaK molten salt [22]. Reducing the void fraction of porous material results in an increase of the volume fraction of porous medium to the whole storage tank, so that it will enhance the effect of heat transfer between HTF and porous medium and speed up the charging process.

![Figure 3](image1.png)

**Figure 3.** Temperature distributions of the FLiNaK molten salt and porous medium in storage tank during charging mode: (a) 2D temperature distributions, (b) 1D temperature profiles along the axial direction.

![Figure 4](image2.png)

**Figure 4.** Temperature differences between FLiNaK and porous medium along the axial distance during charging mode at different inlet velocities.

![Figure 5](image3.png)

**Figure 5.** Temperature profiles with time of HTF for various void fractions at the outlet of the storage tank during charging mode.

### 3.4. Comparison between FLiNaK and Hitec

#### 3.4.1. Influence on the temperature difference

Figure 6 shows the temperature differences between the HTF of various salts and the porous medium. In this case, the inlet velocity is 0.001 m/s, the void fraction is 0.4, the diameter of spherical particle is 0.01 m, and the flowing distance along the axial direction was a half of the tank height. It can be clearly demonstrated in the figure 6 that the temperature difference between FLiNaK and porous medium is smaller than that between Hitec and porous medium. The thickness of thermocline in the TES system with FLiNaK is slightly thicker than
in the TES system with Hitec. These results are attributed to a fact that the thermal conductivity of FLiNaK is higher than the thermal conductivity of Hitec. Namely, the higher the thermal conductivity of HTF is, the more for the HTF contributes to the temperature uniformity of filler material and the thickness increase of thermocline.

![Temperature differences between the HTF of various salts and the porous medium.](image)

**Figure 6.** Temperature differences between the HTF of various salts and the porous medium.

### 3.4.2. Analysis on charging and discharging processes

Figure 7 and 8 give the outlet temperature changes during charging and discharging processes for different HTFs. For this case, the void fraction, the inlet velocity, filler particle’s diameter and the temperature difference from initial state to the completion status of heat storage are respectively set as 0.4, 0.001 m/s, 0.01 m, and 200 K.

According to the figure 7 (a) and (b), when the storage tank is fully loaded, it can be achieved by calculation that the energy stored in the FLiNaK-TES system is 1.14 times of the Hitec-TES system, and the charging period of the system with FLiNaK is just 95.3% of the system with Hitec. The results calculated indicate that the TES system with FLiNaK has a greater energy storage capability than the TES system with Hitec. This is because the thermal capacity and thermal conductivity of FLiNaK are higher than Hitec.

![Temperature profiles at the outlet of the storage tank.](image)

**Figure 7.** Temperature profiles at the outlet of the storage tank (a) of FLiNaK system during charging mode, (b) of Hitec system during charging mode.

During the discharging process, based on the requirement of a stable thermal output, it is considered that the heat released from the beginning of discharging mode until the moment that the thermocline start to leave the tank as the effective heat storage capacity, and the period of heat releasing as the effective discharging time.
Figure 8 (a) and (b) also indicate that the effective discharging time of the system with FLiNaK is obviously shorter than the system with Hitec. After deduction, the output power for the system with FLiNaK is 1.5 times of the system with Hitec.

![Figure 8](image)

**Figure 8.** Temperature profiles at the outlet of the storage tank (a) of FLiNaK system during discharging mode, (b) of Hitec system during discharging mode.

### 4. Conclusion

In this study, a molten salt with higher heat capacity and lower viscosity was brought into the thermocline TES system. Thermal characteristics of the heat transfer and heat storage of the energy storage system with FLiNaK are systematically explored.

During charging process, there is a small temperature difference mainly occurring in the transition region between FLiNaK and porous medium. With the increase of void fraction, the overall time of charging process will become longer. When working in the same condition, the temperature difference between FLiNaK and porous medium will be smaller than that between Hitec and porous medium, and the thickness of thermocline in the system of FLiNaK will be slightly thicker than that in the system with Hitec. Due to the higher heat capacity and thermal conductivity of FLiNaK compared with Hitec, the thermal energy stored by the FLiNaK-TES system is larger and the time spent by the system with FLiNaK is shorter when the storage systems are both fully loaded and the changed temperature from initial state to completion status is set at a constant value.

During the discharging process, the effective discharge time of the system with FLiNaK is obviously shorter than the system with Hitec and the output power for the system with FLiNaK is 1.5 times of the system with Hitec according to numerical results.

The TES system with FLiNaK is a high performance thermal storage system and can be applied to different industries. This study provides important guidelines for designing a storage tank with filler particles for a TES system.

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