

Melting Process Investigation of KCl Salt as a PCM by Enthalpy-Porosity Simulation Model with Temperature-dependent Physical Properties

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Abstract: Salt as a phase change material (PCM) in thermal energy storage (TES) can store solar thermal energy in the form of latent heat by experiencing a process known as the melting process. Recently, the melting process can be observed and investigated using an enthalpy-porosity simulation model. However, the use of enthalpy-porosity simulation model is still focused on constant physical properties, i.e., density and viscosity, of the PCM, and thus, the changes in the physical properties with respect to temperature during the melting process are not included in the simulation process. Therefore, this study aims to use the enthalpy-porosity simulation model with temperature-dependent physical properties of the PCM to investigate the melting process. The salt in this study is Potassium Chloride (KCl), and the computational domain is a concentric tube based on the assumption that the salt is fully contained within the computational domain. The physical properties of the KCl salt (density and viscosity) are set as functions of temperature to include the changes in the physical properties with respect to temperature during the melting process. The simulation results show that the melting process period is 450 s. In addition, the tendency of the melting rate, which is defined as the change in liquid fraction per unit time, is observed to decrease during the melting process. Compared with the constant physical properties of the KCl salt, the melting period of the KCl salt with temperature-dependent physical properties is observed to be shorter, with a deviation of 28.57%.

Keywords: melting process, KCl salt, phase change material, physical properties, enthalpy-porosity simulation model



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1. Introduction

In practice, the availability of renewable energy in the form of thermal energy derived from the sun is fluctuating and thus, a thermal energy storage medium is highly necessary. In recent eras, the utilization of thermal energy storage (TES) represents a viable approach to storing the thermal energy derived from the sun by using a phase change material (PCM) as the storage medium [1]. One of the preferable PCM is salt, such as potassium chloride (KCl). By utilizing KCl salt as PCM, the thermal energy derived from

the sun can be stored in the form of latent heat [2]. The process of storing latent heat in KCl salt results in a phase transition of KCl salt from a solid to a liquid state, which is known as the melting process. The behaviors of the melting process, such as the melting process period and the melting rate, which is defined as the change in liquid fraction per unit of time, can be employed to evaluate KCl salt as PCM [3], [4]. Hence, the melting process investigation of KCl as PCM is highly needed.

Experimental methods were conducted in many studies to observe the melting process of a PCM. One of the experimental methods utilized a confocal optical microscope to observe transient changes in PCM microstructure within the mushy zone (a zone where solid and liquid phases coexist during the melting process) [5]. The results show that transient changes in PCM microstructure within the mushy zone are highly dependent on the changes in liquid fraction and PCM temperature. Despite the effectiveness of the experimental method, the operation of it is costly.

Another method to observe the melting process with relatively low operational costs is numerical simulation by utilizing the enthalpy-porosity simulation model [6]. In the enthalpy-porosity simulation model, the melting process of a PCM is modeled because of the addition of enthalpy and the melting rate, which represents the porosity within the mushy zone [7]. One of the studies that utilized the enthalpy-porosity simulation model showed that the melting process occurred within a computational domain of concentric double pipes with constant PCM density [8]. By utilizing the enthalpy-porosity simulation model, the changes in the melting rate during the melting process and the melting period of a PCM with constant physical properties, *i.e.*, constant density and viscosity, can be observed [9], [10]. Despite the advantages of the enthalpy-porosity simulation model, its use is still focused on the constant physical properties of the PCM, and thus, the changes in the physical properties with respect to temperature during the melting process are not included in the simulation process. In fact, the density and viscosity of a material change simultaneously due to temperature changes during the melting process [11], [12].

Therefore, this study aims to use the enthalpy-porosity simulation model with temperature-dependent physical properties of the PCM to investigate the melting process of KCl salt. The physical properties of the KCl salt, *i.e.*, density and viscosity, are set as functions of temperature to include the changes in the physical properties during the melting process. Thus, the objectives of this study are to simulate the melting rate during the melting process by using the enthalpy-porosity simulation model with temperature-dependent physical properties; to investigate the melting process of KCl as PCM by obtaining the melting period and the melting rate, and to compare the melting period between temperature-dependent physical properties and constant physical properties.

2. Methods

2.1. Mathematical Model

The melting process of KCl salt as PCM in this study is modeled by utilizing the enthalpy-porosity simulation model with temperature-dependent physical properties. In general, the enthalpy-porosity simulation model consists of three governing equations: continuity, momentum, and energy equations. The continuity and momentum equations can be expressed as equation (1) and (2) [13].

$$\frac{\partial \rho(T)}{\partial t} + \nabla \cdot [\rho(T)\mathbf{U}] = 0 \quad (1)$$

$$\frac{\partial [\rho(T)\mathbf{U}]}{\partial t} + \nabla \cdot [\rho(T)\mathbf{U}\mathbf{U}] = -\nabla p + \nabla \cdot \mu(T)(\nabla\mathbf{U} + \nabla\mathbf{U}^T) + \rho(T)\mathbf{g} - \frac{(1 - L\varphi)^2}{(L\varphi^3 + \epsilon)} A_{\text{Mush}}\mathbf{U} \quad (2)$$

where $\rho(T)$ and $\mu(T)$ are temperature-dependent density and viscosity of KCl salt, \mathbf{U} is velocity vector, \mathbf{g} is the gravitational acceleration, $L\varphi$ is liquid fraction, and A_{Mush} is mushy zone number. The liquid fraction in equation (2) represents the porosity of the mushy zone, because the interaction between the liquid and the solid phase within the mushy zone is analogous to the interaction between liquid and solid phase within a porous medium. It is recommended to set the mushy zone number in the range of 10^3 to 10^7 , because the last term in the right-hand side of equation (2) must be able to dampen the momentum in the solid phase [14]. In addition, ϵ in equation (2) is a small number to prevent errors in calculations in the case of $L\varphi = 0$.

The last governing equation in the enthalpy-porosity simulation model is the energy equation which is expressed as equation (3) and (4).

$$\frac{\partial}{\partial t}(\rho(T)h) + \nabla \cdot (\rho(T)\mathbf{U}h) = k\nabla^2 T \quad (3)$$

$$h = h_{\text{ref}} - c_p T + c_p T_{\text{ref}} + L\varphi L \quad (4)$$

where h is specific enthalpy of KCl salt, k is thermal conductivity of KCl salt, T is temperature, T_{ref} is reference temperature, h_{ref} is specific enthalpy at the T_{ref} , c_p is specific heat of KCl salt, and L is latent heat of KCl salt. During the melting process, $L\varphi$ will change from 0 to 1, resulting in the increment of h as shown in equation (4).

In addition, the t_{Melt} can be determined by calculating the total time needed for KCl salt to fully melt, which can be expressed as equation (5).

$$t_{\text{Melt}} = t|_{L\varphi=1} - t|_{L\varphi=0} \quad (5)$$

where $t|_{L\varphi=1}$ is the time when the melting process is ended and $t|_{L\varphi=0}$ is the time when the melting process is started. Furthermore, the $L\dot{\varphi}$ can be calculated using equation (6).

$$L\dot{\varphi} = \frac{L\varphi^{t+\Delta t} - L\varphi^t}{\Delta t} \quad (6)$$

where t is timestep, and Δt is timestep size.

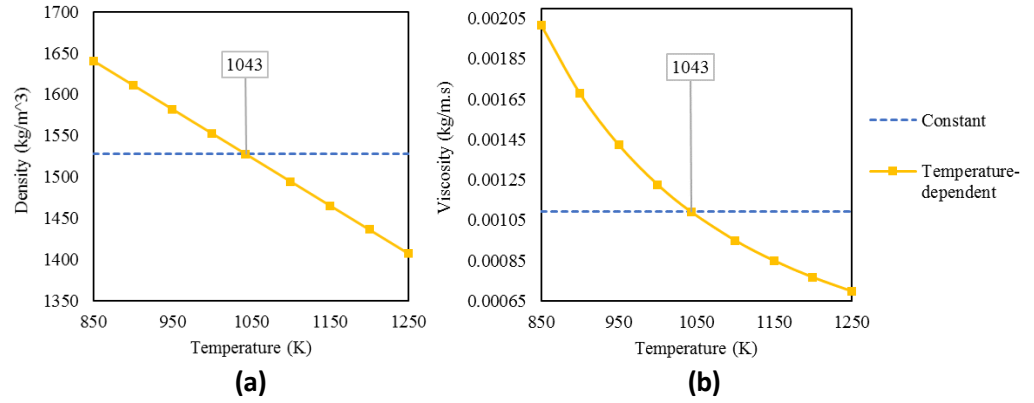
As shown in equation (1) and (2), the density and viscosity of the KCl salt are expressed as functions of temperature. The expressions are based on the theory that the density of a material is linearly decreased and the viscosity is exponentially decreased as the temperature increases [11], [12]. The density and viscosity of KCl salt are expressed as equation (7) and (8) [15].

$$\rho(T) = 2.1359 - 5.831 \times 10^{-4}T \quad (7)$$

$$\mu(T) = 7.32 \cdot 10^{-2} \exp(5601.7/RT) \quad (8)$$

The visualization of the temperature-dependent density and viscosity is shown in Figure 1.

Figure 1. Comparison between temperature-dependent: **(a)** density; and **(b)** viscosity; both with their respective constant values.



As mentioned earlier in the introduction section, one of the objectives of this study is to compare the melting period between temperature-dependent physical properties and constant physical properties. A minor discrepancy exists in the mathematical model for constant physical properties case, specifically in the body force (third term on the right-hand side) in equation (2). In the case of constant physical properties, the body force is approximated by using the Boussinesq approximation [16]. Table 1 shows the constant physical and thermal properties in this study for both the temperature-dependent physical properties case and the constant physical properties case.

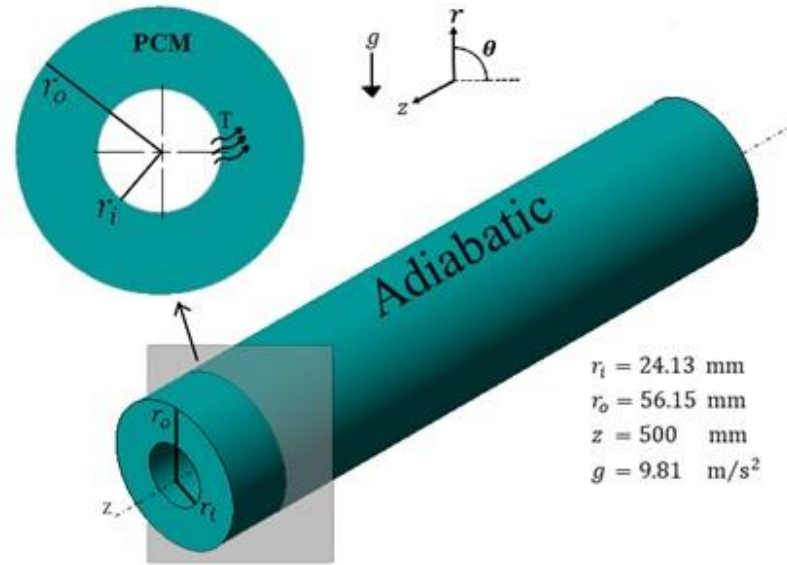
Table 1. Physical and thermal properties of KCl salt.

Properties	Value	Unit	Reference
Density (ρ)	1,527	$\text{kg}\cdot\text{m}^{-3}$	[17]
Specific heat (C_p)	987	$\text{J}\cdot\text{kg}^{-1}\cdot\text{K}^{-1}$	[17]
Thermal conductivity (k)	1.3757	$\text{W}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$	[17]
Viscosity (μ)	0.001092	$\text{kg}\cdot\text{m}^{-1}\cdot\text{s}^{-1}$	[17]
Thermal expansion coefficient	0.000194	K^{-1}	[18]
Latent heat (L)	356,054	$\text{J}\cdot\text{kg}^{-1}$	[17]
Melting temperature (T_{melt})	1,043	K	[17]

2.2. Physical Model

The physical model in this study consists of the computational domain and its respective boundary conditions. The computational domain in this study is defined as a concentric tube, which represents the PCM in a shell and tube TES. The KCl salt is assumed to have fully filled the annulus with heat transfer fluid (HTF) flowing along the inner radius of the concentric tube. Figure 2 shows the computational domain and its respective boundary conditions. As shown in Fig 2, the HTF region is not part of the computational domain, and thus, only the temperature of the HTF is needed to define the boundary condition at $r = r_i$.

Figure 2. Computational domain and its respective boundary conditions.



According to Figure 2, the dimensions of the computational domain are based on the design which is described in reference [19]. The boundary conditions shown in Figure 2 can be grouped into:

- No-slip boundary condition:

$$\mathbf{U}|_{r=r_o=r_i} = 0 \quad (9)$$

$$\mathbf{U}|_{z=0=500 \text{ mm}} = 0 \quad (10)$$

- Temperature boundary condition:

$$T|_{r=r_i} = T_{\text{melt}} + 0.2T_{\text{melt}} \quad (11)$$

- Adiabatic boundary condition:

$$\left. \frac{dT}{dr} \right|_{r=r_o} = 0 \quad (12)$$

Additionally, the enthalpy-porosity simulation model was solved in transient conditions with a total time of 1000 s with a timestep size Δt of 1 s. The initial condition as shown in Figure 2 is:

$$T|_{t=0} = T_{\text{melt}} - 0.025T_{\text{melt}} \quad (13)$$

To solve the enthalpy-porosity model, the computational domain shown in Figure 2 was discretized as depicted in Figure 3. According to Figure 3, the discretization scheme resulting in structured mesh with final characteristics are presented in Table 2.

Figure 3. Discretized computational domain.

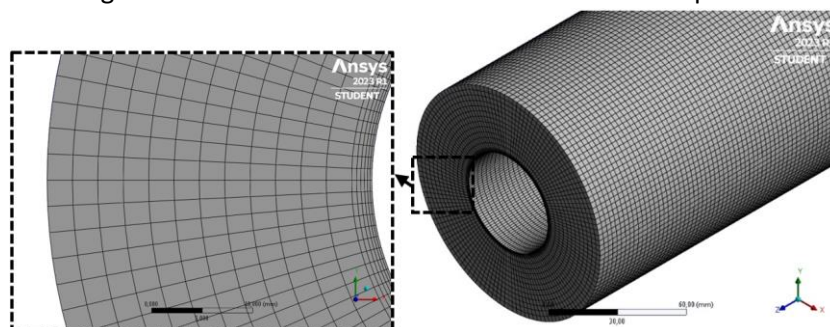


Table 2. Discretization characteristics.

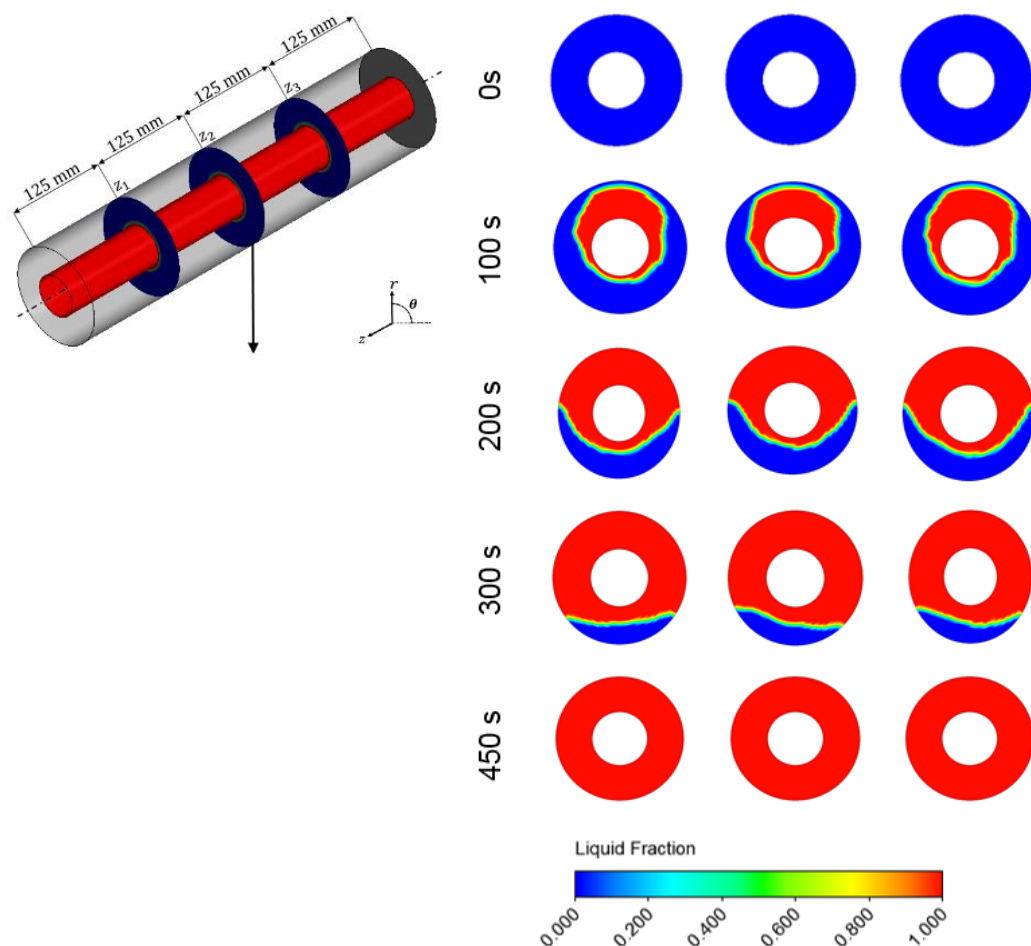
Characteristics	Value
Number of elements	467,568
Maximum skewness	0.028691
Minimum skewness	0.01441
Average skewness	0.017416

3. Results and Discussion

3.1. Liquid Fraction of KCl Salt as PCM During Melting Process

In this study, the melting process of KCl salt as PCM was simulated by an enthalpy-porosity simulation model with temperature-dependent physical properties: density and viscosity. Figure 4 shows the melting process at three designated planes.

Figure 4. Melting process of KCl salt as PCM.



As shown in Figure 4, at the beginning of the melting process, the KCl salt is in solid phase which can be indicated by the blue color observed at the three designated planes. In this case, the liquid fraction $L\varphi$ is equal to 0. Due to the elevated temperature at the inner radius relative to the initial temperature of KCl salt, a heat transfer from the HTF to the KCl salt occurs and initiates the melting process in the KCl salt.

Furthermore, the liquid phase which is represented by the $L\varphi$ indicated by the red color in Figure 4, emerges from the inner radius of the computational domain. After the $L\varphi$ emerges, the solid phase is pushed downwards in the direction of gravity because the solid phase has higher density compared to the liquid phase, as shown in Figure 1.

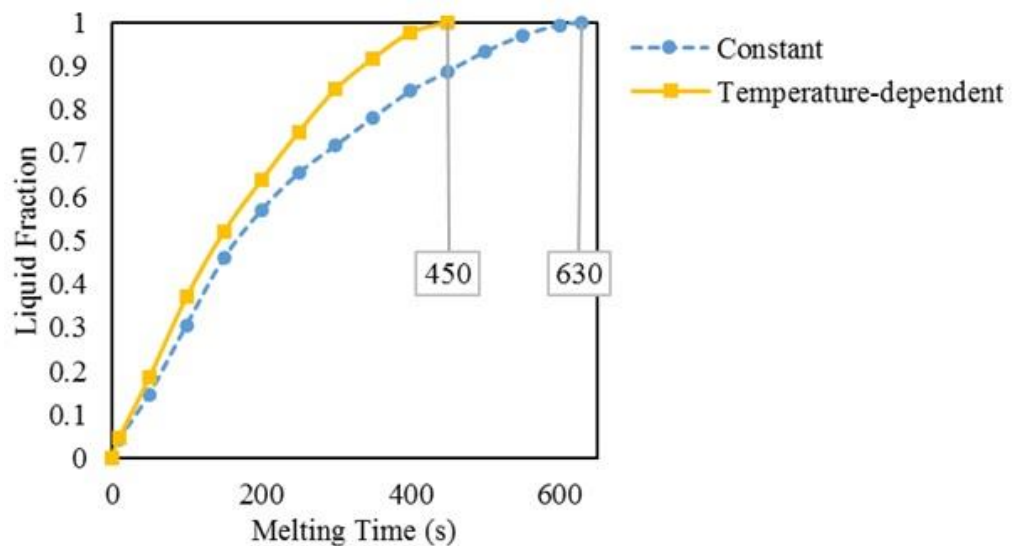
Therefore, the body force of the solid phase is higher than that of the liquid phase. Additionally, during the melting process, the viscosity of the KCl salt decreases, as shown in Figure 1, resulting in a reduction in the shear stress of the KCl salt [20]. The shear stress reduction causes the KCl salt particles to move with greater freedom, thereby creating an inhomogeneous distribution, as depicted in Figure 4. These results are similar to that in references [21], [22].

Furthermore, Figure 4 illustrates that the mushy zone, indicated by the other color between blue and red, is a mere thin layer. This is because in pure materials, the melting process occurs under conditions that are close to isothermal.

3.2. Investigation of Melting Process Period and Melting Rate

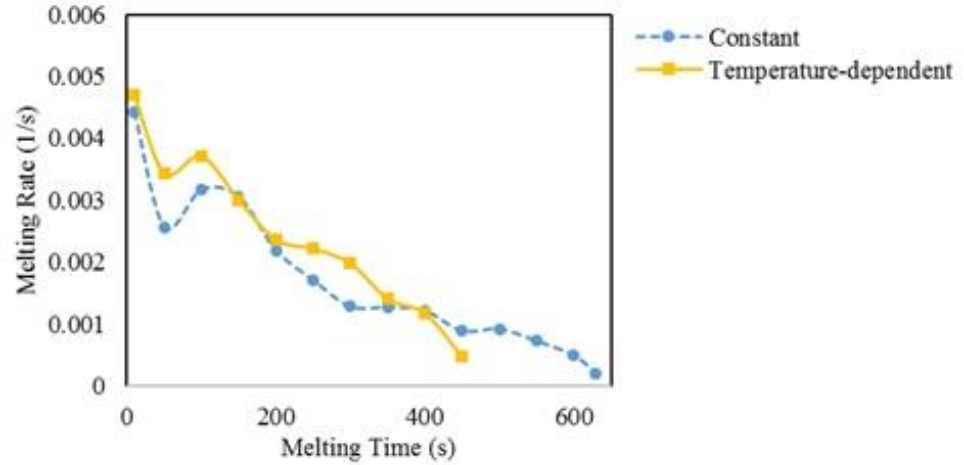
Figure 5 shows the $L\phi$ changes during the melting process. As shown in Figure 5, the $L\phi$ changes from 0 to 1 in 450 s which means the melting process of KCl salt with temperature-dependent physical properties takes 450 s until the entire KCl salt within the computational domain is completely melted. On the other hand, the $L\phi$ of KCl salt with constant physical properties changes from 0 to 1 in 630 s. Hence, the melting process period of the KCl salt with temperature-dependent physical properties is shorter than with constant physical properties.

Figure 5. Changes in liquid fraction $L\phi$ during melting process.



Furthermore, Figure 6 shows the melting rate $L\dot{\phi}$ of KCl salt during the melting process which is calculated by equation (6). According to Figure 6, the tendency of the $L\dot{\phi}$ during the melting process is observed to decline. The observed decline in the $L\dot{\phi}$ shows that the phase transition from the solid phase to liquid phase becomes slower over time. In other words, the increase in the $L\phi$ over time is observed to become smaller.

Figure 6. Melting rate $L\dot{\phi}$ of KCl salt during melting process.



The $L\dot{\phi}$ of KCl salt with constant physical properties also shows the same tendency, but the values are relatively smaller than that with temperature-dependent physical properties. This means that the increase in the $L\dot{\phi}$ with constant physical properties is less than that with temperature-dependent physical properties.

3.3. Comparison of Melting Process Period

Figure 7 shows the melting process period t_{Melt} of KCl salt with temperature-dependent physical properties and with constant physical properties. A deviation δ between the two values is observed since the t_{Melt} of the KCl salt with temperature-dependent physical properties is shorter compared to the other one. The δ can be calculated by equation (14).

$$\delta = \left| \frac{Temp t_{Melt} - Const t_{Melt}}{Const t_{Melt}} \right| 100\% \quad (14)$$

where $Temp t_{Melt}$ is the t_{Melt} of KCl salt with temperature-dependent physical properties and $Const t_{Melt}$ is the t_{Melt} of KCl salt with constant physical properties.

Figure 6. Melting rate $L\dot{\phi}$ of KCl salt during melting process.

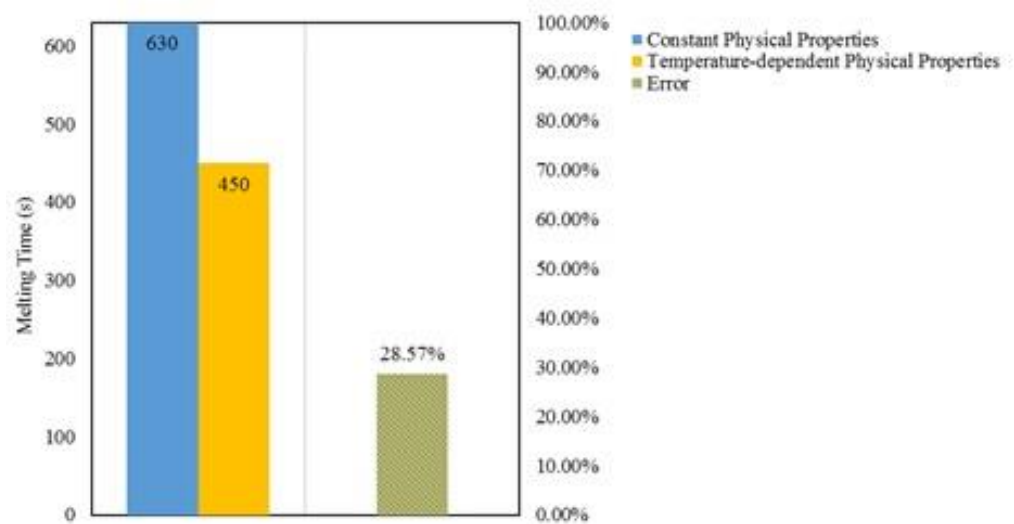


Figure 7 also shows the value of the δ which is 28.57%. The alteration of the physical properties from constant to temperature-dependent resulted in a notable change in the t_{Melt} . This observation highlights the necessity of considering changes in physical properties with temperature in the simulation model of the melting process.

4. Conclusion

The process of melting KCl salt as a PCM has been successfully simulated by the enthalpy-porosity simulation model with temperature-dependent physical properties (density and viscosity). During the melting process, the liquid fraction $L\phi$ pushes the solid phase downwards since the density of the solid phase is higher than that of the liquid phase. Additionally, the distribution of the $L\phi$ is inhomogeneous due to the reduction in the shear stress during the melting process.

Furthermore, the investigation of the melting process period t_{Melt} and the melting rate $L\dot{\phi}$ shows that the t_{Melt} of KCl salt with temperature-dependent physical properties is shorter than that with constant physical properties and the $L\dot{\phi}$ of both physical properties are observed to decline during the melting process. The comparison of the t_{Melt} between temperature-dependent physical properties and constant properties shows that the deviation between the two is 28.57% which suggests that considering changes in physical properties with temperature in the simulation model of the melting process is necessary.

This study shows the importance of considering temperature-dependent physical properties in the simulation model of the melting process without a validation technique. Therefore, it is recommended to provide a validation technique in the next studies to evaluate the results of this study.

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