Numerical Study of Integrating the Phase Change Material with Building Envelop for Improved Indoor Thermal Comfort

Muwafaq Shyaa Alwan[*], **Humam Kareem Jalghaf** [**], **Endre Kovács**[***]

[*]College of Engineering, Al-Iraqia University, Baghdad, Iraq
Email: dr.muwafaqalwan@aliraqia.edu.iq
https://orcid.org/0000- 0002-5829-2929

[**] Department of Fluid and Heat Engineering, University of Miskolc, 3515 Miskolc, Hungary,
Department of Mechanical Engineering, University of Technology-Iraq, 10066 Baghdad, Iraq
Institute of Physics and Electrical Engineering, University of Miskolc, 3515 Miskolc, Hungary
Email: 20310@uotechnology.edu.iq
https://orcid.org/0000-0002-3901-3410

[***] Institute of Physics and Electrical Engineering, University of Miskolc, 3515 Miskolc, Hungary
Email: kendre01@gmail.com, endre.kovacs@uni-miskolc.hu
https://orcid.org/ 0000-0002-0439-3070

Abstract

This research simulates the temperature dynamics of the phase change material PCM using the new approach to calculate heat capacity, supported by advanced, efficient explicit numerical methods. The study examines many scenarios for building wall geometries and boundary conditions by controlling the heat loads and ensuring comfortable interior temperatures. Paraffin wax, selected for its distinct melting temperatures and latent heat capacities, is used as the PCM. The study consistently demonstrates the effectiveness of PCMs in decreasing the heat transfer indoors of the building, regardless of the wall material. This research helps to understand the PCMs' behaviour using the Effective Heat Capacity model, offering valuable insights for energy-efficient building design and highlighting the critical role of selecting suitable PCMs in construction.

Keywords- Phase Change Materials, Latent Heat, Sensible Heat, Numerical Methods, and Thermal Comfort.

I. INTRODUCTION

Nowadays, climate change has garnered significant attention from governments, organizers, scientists, researchers, engineers, and individuals alike, all of whom have embraced the responsibility of addressing this impending threat. The central concern of climate change revolves around planetary warming, leading to phenomena such as forest fires and hotspots in desert regions. However, by collectively assuming our responsibilities, we can effectively manage this peril and even transform its negative effects into opportunities. Jørgen Rose et al. [1] present an extensive numerical method to evaluate the latent storage performance of building components containing PCMs, aiming to understand their effects on heating and cooling demands. This method has been incorporated into the BSim hydrothermal simulation software. The study details comparisons between laboratory measurements of a specific PCM-integrated building component and the results generated by the developed simulation model. Additionally, the paper provides insights through simple calculations and an in-depth case study, providing a thorough synopsis of the research findings and their implications. A. D. Solomon [2] implements simplified relationships to approximate the dynamics behaviour of a phase change with constant initial and boundary temperatures. The investigation of N-Eicosene paraffin wax melting provides evidence for these correlations.

Miao Cui [3] investigates using the extended element differential method (EDM) and the effective heat capacity model in the numerical solution of phase change heat transfer issues. Applying the effective heat capacity method, the research builds the equations for governing the transient heat transfer involving phase changes throughout the entire domain. Analytical expressions of spatial derivatives are used to derive discrete equations for internal nodes, while flux equilibrium conditions are maintained for interface and outer boundary nodes. The accuracy and effectiveness of the approach are demonstrated with numerical examples. Xing Jin [4] compares the enthalpy technique and the effective heat capacity method, two popular computational heat transfer models for PCMs. The study identifies calculation errors inherent in the effective heat capacity method during phase transitions but notes its efficiency advantage over the enthalpy method. Y. Zhang [5] offers a range of adjusted computational methods designed to increase the 2D

http://doi.org/10.58564/IJSER.3.3.2024.235

effective heat capacity EHC model's predictive accuracy for transient heat transport in building walls containing PCMs. The improvements include considering the liquid percentage of PCMs during phase shift, accounting for various temperature turning points, and including unique melting and solidification temperature ranges. Validation experiments show that these modifications significantly reduce deviations compared to the original methods, with standard deviations and maximum deviations below 0.25°C and 0.55°C, respectively, and relative errors under 2.5% and 4.0%.

By literature, the present work highlights to numerical simulate the building wall consisting of Paraffin as a PCM to store the heat energy by using the recent explicit efficient methods while considering the change in heat capacity during and through the transition phase by using the *EHC* model in addition to using the gaussian function to represent the *EHC*, and applied the Dirichlet Boundary conditions.

II. PROBLEM STUDY AND NUMERICAL METHODS

We used MATLAB to code the recent numerical methods and algorithms to simulate the PCM materials by applying the effective heat capacity (EHC) model. It suggests that because of material inhomogeneities, the thermal conductivity k, specific heat c, and density ρ depend on the temperature and the space.

We utilized MATLAB to implement recent numerical algorithms for simulating PCMs using the EHC model. This method accounts for variations in specific heat *c*, thermal conductivity *k*, and density *ρ*, which are influenced by space and temperature changes. In one dimension, the behaviour of temperature can be predicted using the following partial differential equation, known as the heat conduction equation:

$$\frac{\partial u}{\partial t}=\frac{1}{\rho\left(x,u\right)c\left(x,u\right)}\nabla(k\left(x,u\right)\nabla u)+q\,. \qquad (1)$$

In terms of cell variables, which means that $u_i\ k_i\ \rho_i\ and\ c_i$ are the temperature, thermal conductivity, density, and specific heat of cell *i*, respectively. Since the same material boundaries are as the cell borders, we write the average $\left(\frac{k_i+k_{i+1}}{2}\right)$ instead of $k\left(x_i+\frac{\Delta x}{2}\right)$ then the discretization be:

$$\frac{du_i}{dt}=\frac{1}{c_i\rho_i\Delta x}\left(k_{i,i+1}\frac{u_{i+1}-u_i}{\Delta x}+k_{i,i-1}\frac{u_{i-1}-u_i}{\Delta x}\right)+\frac{1}{c_i\rho_i\Delta z}\left(k_{i,i+N_x}\frac{u_{i+N_x}-u_i}{\Delta z}+k_{i,i-N_x}\frac{u_{i-N_x}-u_i}{\Delta z}\right) \qquad (2)$$

The cell volume can calculate as $V=\Delta x\Delta y\Delta z$, the horizontal and vertical thermal resistances calculated between the neighbouring cells, as below:

$$R_{i,i+1}\approx\frac{\Delta x}{2k_i\Delta z}+\frac{\Delta x}{2k_{i+1}\Delta z}\text{, and } R_{i,i+N_x}\approx\frac{\Delta z}{2k_i\Delta x}+\frac{\Delta z}{2k_{i+N_x}\Delta x}$$

Latent heat capacity LHC and Sensible heat capacity SHC are the two forms of heat capacity that we consider when calculating the cell's heat capacity. Common materials with a sensible heat capacity are brick and concrete, which are incapable of changing phases under typical circumstances. The EHC for phase change materials (PCMs) is calculated as the product of LHC and SHC at each phase, accounting for phase transitions, as follows:

$$C_i^{So}=c_i^{So}\rho_i^{So}V_i\,,and\quad C_i^{Li}=c_i^{Li}\rho_i^{Li}V_i \qquad (3)$$

The sensible heat capacity (SHC) for PCM in both liquid and solid states is represented here. The Gaussian function centred is defined as g at the critical temperature u_{cr} of material with the standard deviation σ to calculate the EHC of the PCM as follows:

$$g(i)=\frac{1}{\sigma\sqrt{2\pi}}\exp\left(\frac{-\left(u_i-u_{cr}\right)^2}{2\,\sigma^2}\right)\,. \qquad (4)$$

At the phase transition region, the following formulas are used to calculate the thermal properties:

$$k_i=\frac{\left(\left(k_i^{Li}-k_i^{So}\right)\left(u_i-u_{cr}\right)+\sigma\left(k_i^{Li}+k_i^{So}\right)\right)}{2\,\sigma}\,. \qquad (5)$$

$$\rho_i=\frac{\left(\left(\rho_i^{Li}-\rho_i^{So}\right)\left(u_i-u_{cr}\right)+\sigma\left(\rho_i^{Li}+\rho_i^{So}\right)\right)}{2\,\sigma}\,. \qquad (6)$$

$$c_i=\frac{\left(\left(c_i^{Li}-c_i^{So}\right)\left(u_i-u_{cr}\right)+\sigma\left(c_i^{Li}+c_i^{So}\right)\right)}{2\sigma}\,. \qquad (7)$$

At the phase transition, EHC is used as follows:

$$EHC_i=SHC_i+LHC_i\,. \qquad (8)$$

$$SHC_i=c_i\rho_iV_i\,. \qquad (9)$$

$$LHC_i = H_i g_i \rho_i V_i \ . \qquad (10)$$

III. NUMERICAL METHODS MODELING AND SETUP

In the current study the new Numerical methods used to calculate the heat transfer equation, we used the following expression

$$r_i = \Delta t \sum_{j \neq i} \frac{1}{C_i R_{ij}} \text{ and } A_i = \Delta t \sum_{j \neq i} \frac{u_j^n}{C_i R_{ij}} + \Delta t \cdot q_i$$

The following numerical method details:

1.1. The Explicit Euler Method[3]

$$u_i^{n+1} = \left(1 - r_i\right) u_i^n + A_i \ . \qquad (11)$$

1.2. Shifted-Hopscotch SH method[4]

For the first half-time step:

$$u_i^{n+1/2} = \frac{u_i^n + A_i^{\text{half}}}{1 + r_i / 2} \ . \qquad (12)$$

For the full-time steps:

$$u_i^{\mu+1} = \frac{\left(1 - r_i / 2\right) u_i^{\mu} + A_i^{\mu+1/2}}{1 + r_i / 2} \ . \qquad (13)$$

For the last half-time step:

$$u_i^{n+2} = \left(1 - r_i\right) u_i^{n+1} + \frac{A_i^{n+3/2}}{2} \ . \qquad (14)$$

where μ is set to n where even nodes and $n+1$ where odd nodes.

1.3. The asymmetric Hopscotch ASH Method [3] is a variation of the standard SH method, which involves only three stages instead of five. It applies equation (12) for the initial half-time step, equation (13) for the full-time step, and equation (14) for the final half-time step.

1.4. Leapfrog-Hopscotch LH method[5] incorporates two half-time steps, one at the beginning and one at the end, along with several full-time steps. It uses equation (12) for the half-time steps and equation (13) for the full-time steps.

After we calculated the heat capacities and *EHC*, we calculated sensible heat Q_S, total latent heat Q_L, and the total heat Q_T of thermal systems as follows:

$$Q_T^t = Q_T^{t-1} + \sum_{i=1}^{N} EHC\left(u_i^t - u_i^{t-1}\right) \ , \qquad (15)$$

$$Q_{Se}^t = Q_{Se}^{t-1} + \sum_{i=1}^{N} SHC\left(u_i^t - u_i^{t-1}\right) \ , \qquad (16)$$

$$Q_{La}^t = Q_{La}^{t-1} + \sum_{i=1}^{N} LHC\left(u_i^t - u_i^{t-1}\right) \ . \qquad (17)$$

IV. GEOMETRY, MATERIALS PROPERTIES AND BOUNDARY CONDITIONS

In the current work, we have many cases of study for thermal analysis; the building's main components are brick walls and concrete; the figure shows the geometry, and Tables 1 and 2 lists the materials' properties.

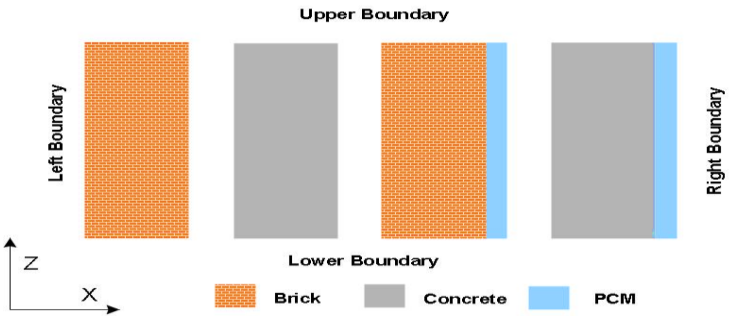

Figure 1. section geometries of cases study

TABLE 1. THE PROPERTIES OF STRUCTURAL MATERIALS.

Material	$\rho\left(\mathrm{kg\cdot m^{-3}}\right)$	$k\ \left(\mathrm{W\cdot m^{-1}\cdot K^{-1}}\right)$	$c\ \left(\mathrm{J\cdot kg^{-1}\cdot K^{-1}}\right)$
Brick	1600	0.73	800
Concrete	2300	1.70	840

TABLE 2. THE PCM PROPERTIES [2].

Material	$\rho\left(\mathrm{kg\cdot m^{-3}}\right)$	$k\ \left(\mathrm{W\cdot m^{-1}\cdot K^{-1}}\right)$	$c\ \left(\mathrm{J\cdot kg^{-1}\cdot K^{-1}}\right)$	$Latent\ Heat\left(\mathrm{J\cdot kg^{-1}}\right)$
PCM_{Solid}	856	0.15	2210	247000
PCM_{Liquid}	778	0.15	2010	

The mesh spacing value will be $\Delta x = 3.334\times 10^{-4}$ consistent across all scenarios, chosen based on a mesh dependency analysis. To determine the initial temperature, we employed a linear relationship using temperature data recorded every hour from a weather forecasting website for Baghdad, Iraq, on July 28.

$$u\left(x,z,t=0\right)=Matrix\ values$$

In all cases, Neumann boundary conditions were applied to the upper and lower sides. Dirichlet boundary conditions were used on the left side, with a constant temperature representing the interior comfort level, set to 298 K.

$$u_z(x,z=0,t)=u_z(x,z=L_z,t)=0$$

Dirichlet BC was applied on the right side.

$$u_x(x=L_x,z,t)=Array\ values$$

Where the array represents the temperature during 24 hours interpolated at each one hour.

V. RESULTS AND DISCUSSIONS

The study's findings of overall heat, heat savings, and heat leaking inside are covered in depth in this section. Plotting values along the x-axis, Figure 2 presents a comparative examination of EHC, LHC, and SHC. Phase change materials (PCM)-infused brick and concrete walls are included in this comparison.

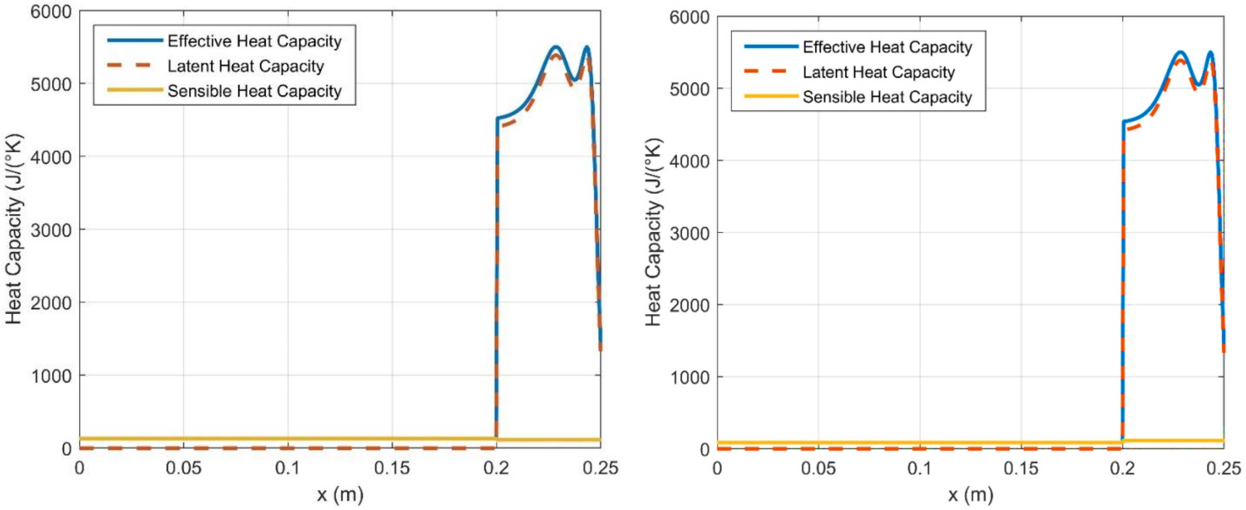

Figure 2. The heat capacities in the case of Brick+PCM on the Left, Concrete +PCM on the Right

Figure 3 shows the instant total heat transfer plotted during the time study. The figure shows that the heat transfer in concrete is much higher than in brick, and almost all of this energy goes to the inside. While it is clear the effect of using PCM to store the energy during the melting process. A detailed analysis of the values presented in Table 3 indicates that employing PCM in conjunction with brick and concrete amplifies the overall heat transfer. The cooling load, or heat transmission via the wall structure from the outer environment to the interior space, is plotted in Figure 4.

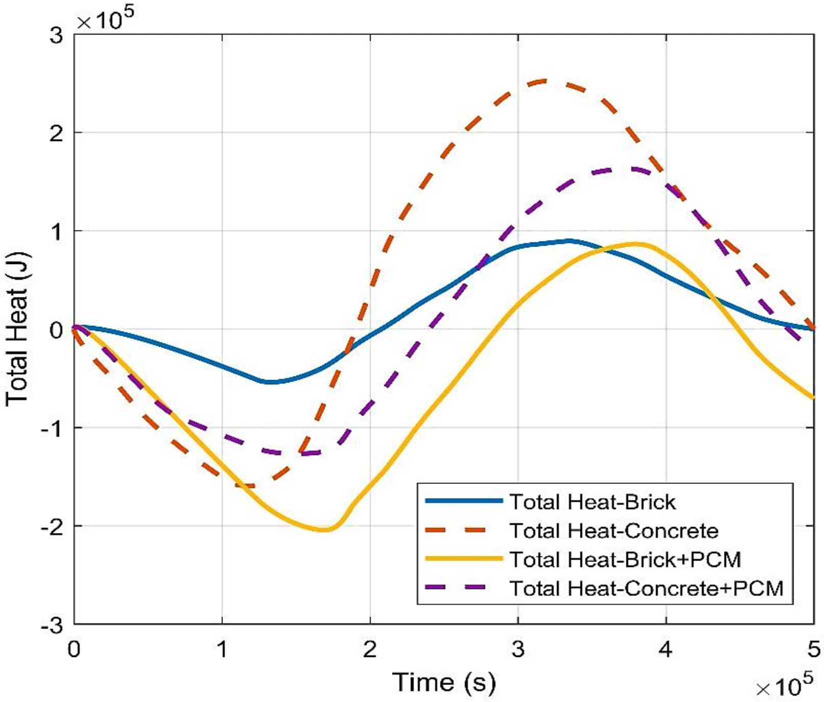

Figure 3. The total heat contents

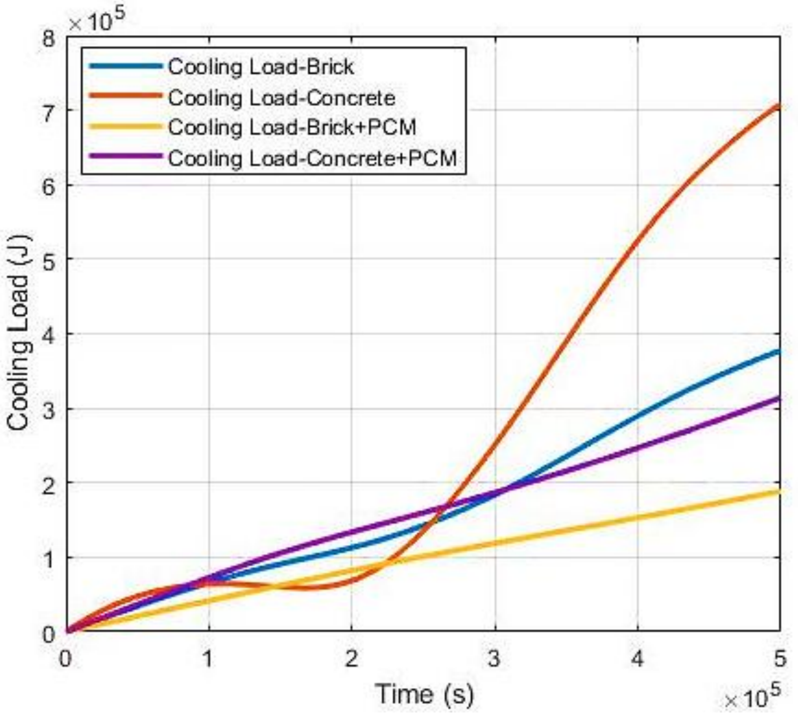

Figure 4. The Cooling loads

Figure 5 plots the history of EHC at selected points within the PCM (x = 0.246, 0.233, and 0.2166 m), illustrating the heat-saving mechanism during the phase transition, which involves the storage and release of latent heat.

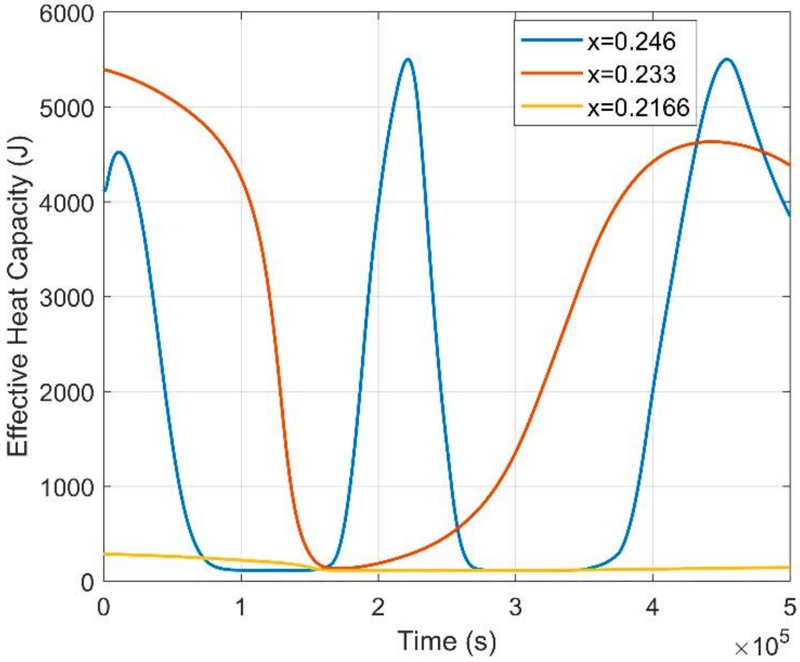

Figure 5. The EHC history through PCM in the case of Brick+ PCM

The temperature history profiles taken at the brick section of the wall's core are shown in Figures 6 and 7. It is clear that, in the absence of PCM, the temperature profile for the wall substantially resembles the applied boundary (outside temperature profile), albeit with a little temporal lag that represents the delay in heat transmission. With starting temperatures of 308 K and 302 K, adding PCM significantly improves the interior temperature's ability to remain within the intended comfort range [9]. This implies that a significant quantity of heat energy from the environment is efficiently saved as latent heat in PCM1.

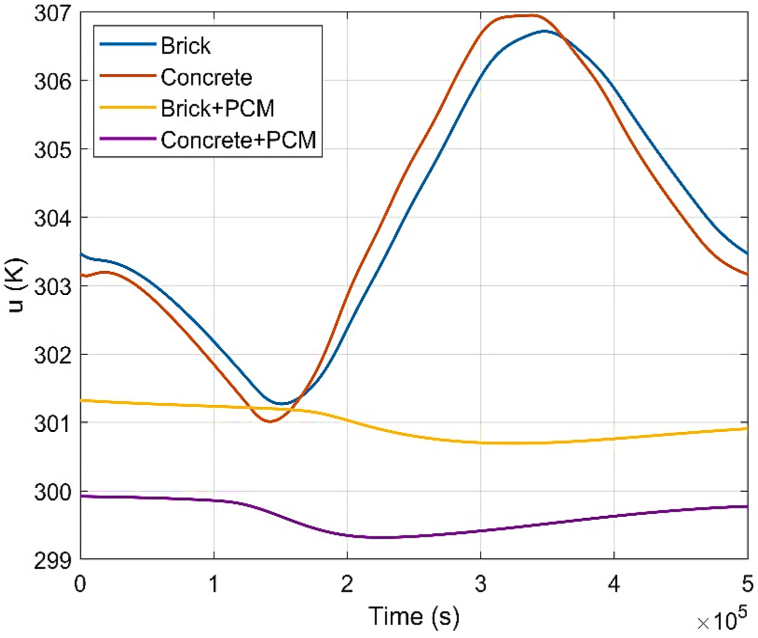

Figure 6. The temperature history in the brick portion's midsection

TABLE 3. THE RESULTS IN WITH DIRICHLET BOUNDARIES FOR PCM

Parameters	Brick	Concrete	Brick+PCM	Concrete+PCM
$\max(Q_{Total})\ KJ/m^2$	89.509×10^3	150.07×10^3	204.41×10^3	163×10^3
$mean(Q_{Total})\ KJ/m^2$	39.245×10^3	64.070×10^3	84.962×10^3	87.487×10^3
$\max(Q_{Sensible})\ KJ/m^2$	89.509×10^3	251.80×10^3	24.668×10^3	58.265×10^3
$mean(Q_{Sensible})\ KJ/m^2$	39.245×10^3	131.98×10^3	14.752×10^3	23.885×10^3
$\max(Q_{Latent})\ KJ/m^2$	0	0	182.59×10^3	172.10×10^3
$mean(Q_{Latent})\ KJ/m^2$	0	0	80.930×10^3	79.302×10^3
$\max(Q_{Cooling})\ J/m^2$	377.78×10^3	879.75×10^3	188.70×10^3	314.30×10^3
$mean(Q_{Cooling})\ J/m^2$	168.26×10^3	391.83×10^3	98.121×10^3	159.58×10^3

VI. Conclusions

The research concludes with the following key observations:

1. Effectiveness of Numerical Algorithms: All the novel numerical algorithms examined effectively address the challenges associated with phase change simulations.

2. Effective Heat Capacity Model Reliability: The study confirms that the model is a trustworthy computational tool for phase change material (PCM) simulation.

3. Interior Temperature Regulation: The efficient heat storage of PCMs is demonstrated by their ability to keep interior temperatures near to original values when combined with brick or concrete.

4. Consistent Performance Across Wall Materials: PCMs consistently exhibit the ability to store a substantial amount of heat energy as latent heat, regardless of the wall material used, highlighting their effectiveness in reducing heat infiltration.

In summary, this study emphasizes the essential role of PCMs in lowering cooling loads, maintaining stable indoor temperatures, and minimizing external heat intrusion. Optimal energy efficiency and thermal comfort in buildings rely on the careful selection of PCMs based on their latent heat properties and melting temperatures. For colder climates, PCMs with lower melting points are particularly beneficial, especially when combined with solar panels to capture and store daytime solar energy for use during colder nights. These findings have significant implications for designing.

REFERENCES

[1] [1] J. L. A. C. N. U. et al. Rose, "NUMERICAL METHOD FOR CALCULATING LATENT HEAT STORAGE IN CONSTRUCTIONS CONTAINING PHASE CHANGE MATERIAL," Build. Simul., no. Eleventh International IBPSA Conference Glasgow, Scotland July 27-30, 2009, pp. 400–407, 2009.

[2] [2] A. D. Solomon, "An easily computable solution to a two-phase Stefan problem," Sol. Energy, vol. 23, no. 6, pp. 525–528, Jan. 1979, doi: 10.1016/0038-092X(79)90077-X.

[3] [3] M. Cui, C. Zhang, B. Zhang, B. Xu, H. Peng, and X. wei Gao, "Numerical solution of phase change heat transfer problems by effective heat capacity model and element differential method," J. Comput. Sci., vol. 60, p. 101593, Apr. 2022, doi: 10.1016/J.JOCS.2022.101593.

[4] [4] X. Jin, H. Hu, X. Shi, X. Zhou, and X. Zhang, "Comparison of two numerical heat transfer models for phase change material board," Appl. Therm. Eng., vol. 128, pp. 1331–1339, Jan. 2018, doi: 10.1016/J.APPLTHERMALENG.2017.09.015.

[5] [5] Y. Zhang, "Modified computational methods using effective heat capacity model for the thermal evaluation of PCM outfitted walls," Int. Commun. Heat Mass Transf., vol. 108, p. 104278, Nov. 2019, doi: 10.1016/J.ICHEATMASSTRANSFER.2019.104278.

[6] [6] H. K. Jalghaf, E. Kovács, and B. Bolló, "Comparison of Old and New Stable Explicit Methods for Heat Conduction, Convection, and Radiation in an Insulated Wall with Thermal Bridging," Buildings, vol. 12, no. 9, pp. 1–26, 2022, doi: 10.3390/buildings12091365.

[7] [7] Á. Nagy, M. Saleh, I. Omle, H. Kareem, and E. Kovács, "New Stable, Explicit, Shifted-Hopscotch Algorithms for the Heat Equation," Math. Comput. Appl., vol. 26, no. 3, p. 61, 2021, doi: 10.3390/mca26030061.

[8] [8] Á. Nagy, I. Omle, H. Kareem, E. Kovács, I. F. Barna, and G. Bognar, "Stable, Explicit, Leapfrog-Hopscotch Algorithms for the Diffusion Equation," Computation, vol. 9, no. 8, p. 92, 2021.

[9] [9] K. Kant, A. Shukla, and A. Sharma, "Numerical simulation of building wall incorporating phase change material for cooling load reduction," Energy Clim. Chang., vol. 1, p. 100008, 2020, doi: https://doi.org/10.1016/j.egycc.2020.100008.