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Analysis of equivalent heat capacity forms and their influence on energy storage in PCMs

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INTRODUCTION & AIM

Phase Change Materials (PCMs) are widely used for thermal energy storage because of their high latent heat capacity. However, accurately modeling energy storage in PCMs remains challenging, particularly when using the equivalent heat capacity method.

Several equivalent Cp formulations have been proposed in the literature, but significant discrepancies may occur in predicting heat capacity and enthalpy.

Therefore, the main objective of this work is:

• To evaluate different equivalent heat capacity formulations used for PCM modeling

.• To improve the conventional D(T)-based formulation

.• To identify the most accurate model through comparison with experimental DSC measurements.

METHOD

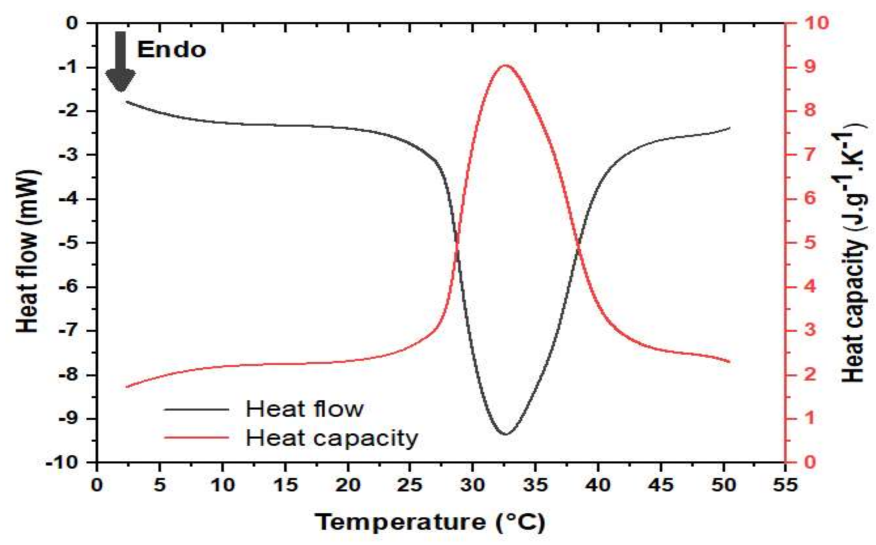
1. Bio-Based PCM Characterization

A sustainable bio-based PCM synthesized from local vegetable oils and beeswax was experimentally characterized using Differential Scanning Calorimetry (DSC).Main thermal properties:

• Melting range: 27–38.3 °C

• Latent heat of fusion: 64 kJ/kg

• Approximately 9000 experimental DSC data points were collected.



DSC curves of various bio-based sample at a scanning rate of 2 °C/min

❖ **Energy equation:**

$$\begin{cases} \rho Cp_{eq}\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial x}+v\frac{\partial T}{\partial y}\right)=k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right) & \textit{dans le MCP} \\ \rho Cp\frac{\partial T}{\partial t}+\nabla.(-k\nabla T)=0 & \textit{dans les matériaux de construction} \end{cases}$$

2. Numerical Model

Numerical simulations were performed using COMSOL Multiphysics under realistic summer conditions in Constantine, Algeria.

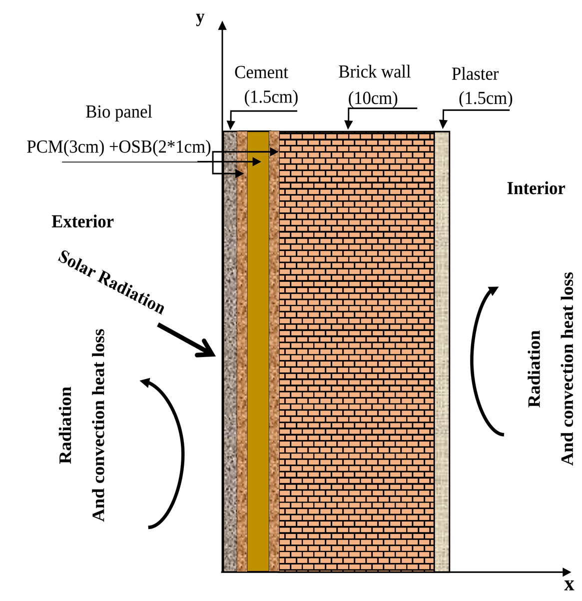
The investigated wall configuration consists of a 1.5 cm cement mortar layer, a 15 cm brick layer, a 1 cm OSB layer, a 3 cm PCM layer, another 1 cm OSB layer, and a 1.5 cm interior plaster layer.

Boundary conditions include:

• Solar radiation

• Convective heat transfer

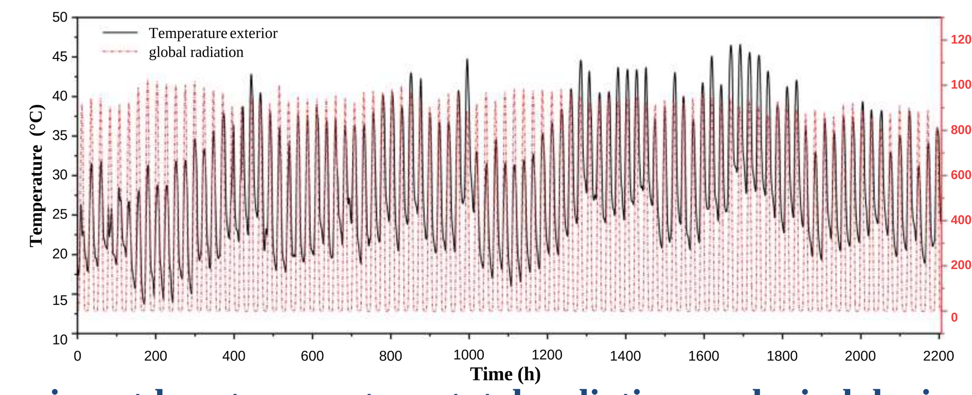
• Radiative heat exchange



Simulated wall configuration

On exterior surface: $-k_{cement}\frac{\partial T}{\partial x}=h_e(T_e-T_{cement})+\varepsilon_{cement}\sigma\left(T_e^{\,4}-T_{cement}^{\,4}\right)+\alpha_{cement}I(t)$

On interior surface: $-k_{plaster}\frac{\partial T}{\partial x}=h_i(T_i-T_{plaster})+\varepsilon_{plaster}\sigma\left(T_i^{\,4}-T_{plaster}^{\,4}\right)$



Temporal variations in outdoor temperature, total radiation, and wind during the summer in Constantine

❖ **Continuity Equation :** $\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0$

❖**Equation of momentum in PCM:**

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right)=-\frac{\partial P}{\partial x}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)+A(T)\times u$$

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)-=-\frac{\partial P}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+A(T)\times v+F_b$$

The density of the MCP: $\rho(T)=\rho_s+(\rho_l-\rho_s)\times B(T)$

The function B(T) exhibits a linear behavior in the phase transition region:

$$B(T)=\begin{cases} 0 & T<(T_{pic}-\Delta T) \\ \frac{(T-T_{pic}+\Delta T)}{2\,\Delta T} & T_{pic}-\Delta T\le T\le T_{pic}+\Delta T \\ 1 & T>T_{pic}+\Delta T \end{cases}$$

3. Equivalent Heat Capacity Models

Four equivalent heat capacity formulations were investigated:

1- A $C_p$formulation based on the $D(T)$function, combining the heat capacity of the PCM in its different states, was adopted from previous studies ([K. Kant et al., 2017, 2018, 2020; M. Nouira et al., 2018; T. Bouzennada et al., 2020])

$$Cp_{eq}(T)=Cp_s+(Cp_l-Cp_s)\times B(T)+D(T)\times L$$

2- Cp as a function of D(T) divided by (T_{endset}-T_{onset}) " was proposed (Model 2).

$$Cp_{eq}(T)=Cp_s+(Cp_l-Cp_s)\times B(T)+D(T)\times\frac{L}{T_{endset}-T_{onset}}$$

3- Experimental data (DSC experimental data)

4- The correlation-based thermal capacity model based on experimental data (Model 1):

$$Cp_{eq}=\begin{cases} Cp_s(T)=1.4327+0.1643T-1.16\times10^{-2}T^2+2.8\times10^{-4}T^3 \\ Cp_{in}(T)=-146.966+9.25078T-0.13690T^2 \\ Cp_l(T)=40.017-1.908T+3.198\times10^{-2}T^2-1.78\times10^{-4}T^3 \end{cases}$$

5- A widely used model for phase transition modeling (Model 3) was adopted based on the works of M. Ahmad et al. (2006), E. M. Alawadhi et al. (2008), and P. Lamberg et al. (2004).

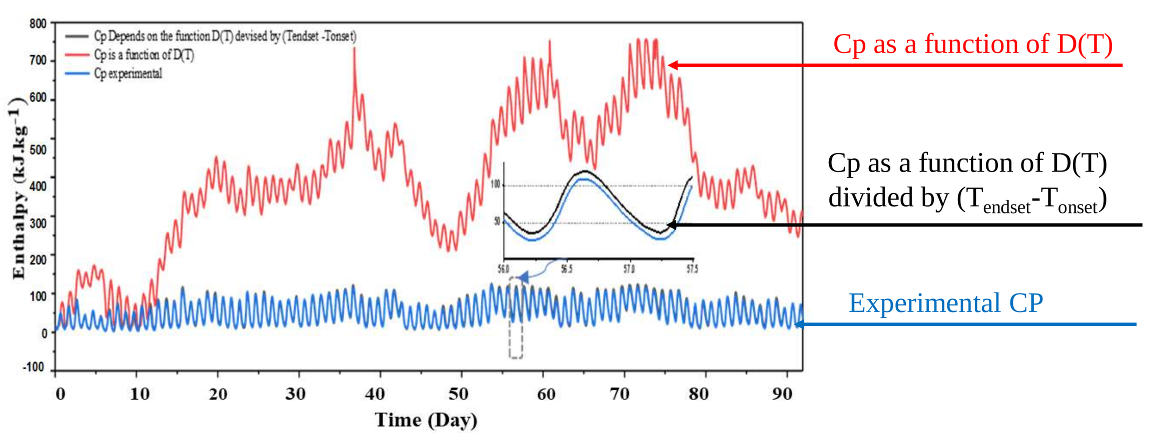
$$Cp_{eq}=\begin{cases} Cp_s & T<T_{onset} \\ \frac{Cp_s+Cp_l}{2}+\frac{L}{T_{endset}-T_{onset}} & T_{onset}<T<T_{endset} \\ Cp_l & T_l<T \end{cases}$$

6- Model 4 corresponds to the phase change model implemented in COMSOL Multiphysics, which has been widely used in previous studies [M. H. Baghban et al. (2010), M. I. Hasan et al. (2018), M. Li et al. (2019), and Y. Hamidi et al. (2012)].

$$Cp_{eq}(T)=\frac{1}{\theta_s\rho_s+\theta_l\rho_l}(\theta_s\rho_s Cp_s+\theta_l\rho_l Cp_l)+L\frac{\partial\alpha_m}{\partial T}$$

RESULTS & DISCUSSION

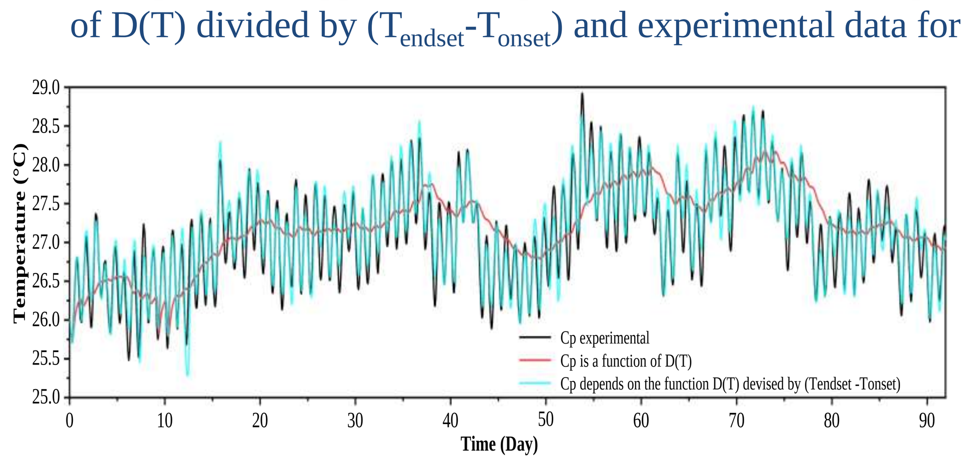
1- Verification of the Conventional D(T) Formulation



Enthalpy variation at the center of the PCM layer during the summer equivalent Cp various approaches: Cp as a function of D(T), Cp as a function of D(T) divided by (T_{endset}-T_{onset}) and experimental data for Cp.

✓ The conventional $D(T)\times L$ formulation generates unrealistic heat capacity peaks and significant enthalpy errors.

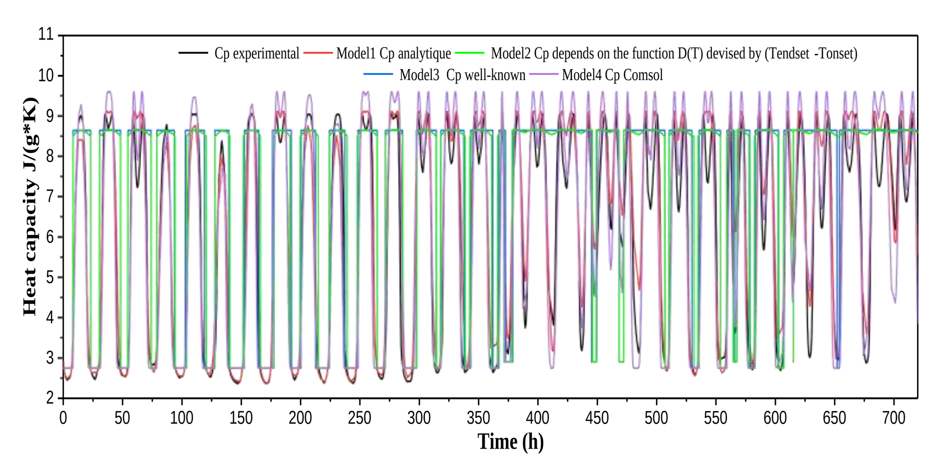
✓ Introducing the scaling factor 1/(Tendset−Tonset) substantially improves the agreement with experimental DSC data, ensures a stable and realistic heat capacity baseline (~9 J/(g·K)), and maintains physically consistent enthalpy variations within the range of 8–120 kJ/kg.

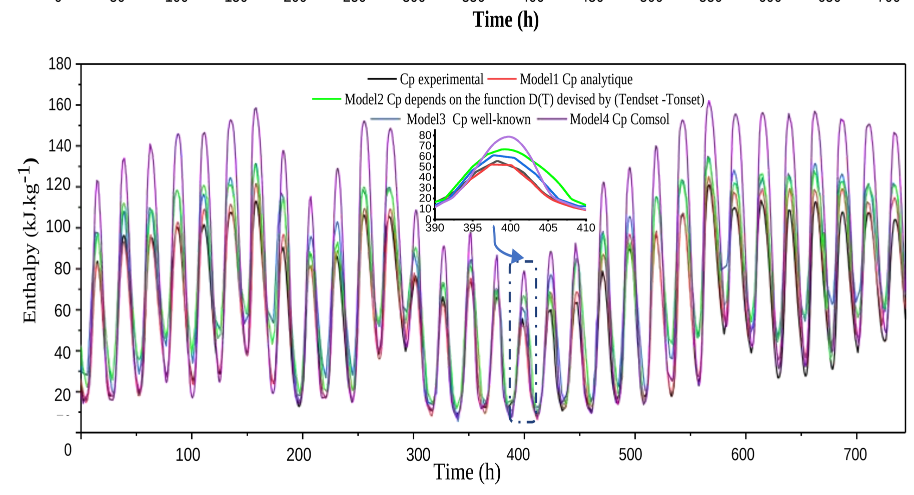


Variation in indoor wall temperature in summer with different approaches to equivalent Cp.

The optimized $C_p$model, obtained by dividing $D(T)\times L$ by the phase change interval $(T_{endset}-T_{onset})$,predicts indoor surface temperatures that closely match those obtained from experimental C_p data, demonstrating a more realistic representation of the thermal storage behavior of the bio-based PCM.

2- Evaluate equivalent Cp approaches for modeling energy storage in PCMs





Heat Capacity and Enthalpy Variations at the Center of the PCM Layer in July Using Different Equivalent Heat Capacity Models

✓ Model 1 (The correlation-based thermal capacity model derived from experimental data C_p) provides the most accurate fit to the experimental results.

✓ These models reproduce the phase transition satisfactorily, although they exhibit simplified rectangular heat capacity profiles in the transition region (~8.6 J/(g·K)).

✓ Models 2 and 3 show only minor deviations, with maximum discrepancies remaining below **20 kJ/kg**.

✓ Limitations of COMSOL Standard Formulation (Model 4): The standard formulation overestimates the heat capacity peak (up to **9.6 J/(g·K)**), resulting in significant enthalpy errors that may reach **45 kJ/kg**.

CONCLUSIONS

In conclusion:

• A sustainable bio-based PCM exhibiting a melting range of 27–38 °C and a latent heat of 64 kJ/kg was successfully developed.

• The conventional D(T)×L formulation is unsuitable for PCMs exhibiting phase transition intervals greater than 1 °C.

• Dividing the term D(T)×L by the interval (Tendset − Tonset) considerably improves modeling accuracy.

• The correlation-based model derived from experimental Cp data provides the highest accuracy.

• The COMSOL built-in phase change model requires validation for each specific PCM.

• The optimal Cp formulation significantly improves the prediction of thermal energy storage and building thermal performance.

FUTURE WORK

• Experimental validation under real climatic conditions.

• Long-term thermal cycling analysis.

• Integration of nanoparticles to enhance thermal conductivity.