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A shot in the dark: The current state of PCM hysteresis modelling in building energy simulation software

Dmitry Zhilyaev [a,*], Alejandro E. Albanesi [b], M. Cecilia Demarchi [b], Víctor D. Fachinotti [b], Hans L.M. Bakker [a], Henk M. Jonkers [a]

[a] Faculty of Civil Engineering and Geosciences, Delft University of Technology, Delft, 2628CN, the Netherlands
[b] CIMEC Centro de Investigación de Métodos Computacionales, CONICET-UNL, Col. Ruta 168 s/n, Predio CONICET, Santa Fe, 3000, Argentina

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ABSTRACT

Phase change materials (PCM) are receiving ever-growing attention as a promising construction material for improving building energy performance through thermal storage and peak load shifting. The analysis of PCM performance and decision-making related to PCM implementation in building envelopes often relies on building energy simulation software such as EnergyPlus – a de facto standard in the academic world and the industry. For a precise modelling of the dynamic PCM behaviour, it is essential to correctly account for PCM hysteresis. This work introduces two new implementations of PCM hysteresis models in EnergyPlus. Further, it provides an in-depth analysis of four publicly available EnergyPlus-based hysteresis models, including the two newly introduced ones, and identifies the existing limitations for each of them. Finally, it explores the effects of PCM model selection on decision-making using the example of novel PCM-embedded material development. The results of this study show that the current built-in hysteresis model in EnergyPlus is not implemented correctly, and none of the other analysed models is completely free of limitations. Moreover, this work draws attention to the existing contradictions between different PCM modelling approaches, highlighting the critical impact the selection of a PCM model has on PCM-related decision-making. We conclude that while the existing hysteresis models in EnergyPlus are operable – albeit with great caution – they are not yet at the stage where they could be used as a reliable decision-making support tool. Practical real-world integration of PCM in building envelopes is hardly possible without having dependable modelling tools to back it up, and the development of such tools requires far more attention than it is given at the moment.

1. Introduction

Phase change materials (PCM) as construction materials are attracting growing attention in the literature as a way to reduce heating, ventilation, and air conditioning (HVAC) energy demand in buildings, with the number of related publications increasing steadily over the last decade [1–4]. Due to time and budget constraints, full-scale real-world testing of PCM and PCM-embedded materials is limited, and most research relies on computational simulations. In these cases, the effect of PCM is evaluated based on full-building energy simulation results, which are then used to assess material performance and support design decisions at the material, component, and building levels.

Several tools have been developed for full-building energy simulation with EnergyPlus [5] developed and maintained by the National Renewable Energy Laboratory (NREL) being by far the most widely used one. It is open source and free, making it accessible to researchers and practitioners worldwide. Beyond academic research, it is also widely adopted in industry, with tools such as DesignBuilder [6], OpenStudio [7], Revit [8], Ladybug Tools [9], TRACE 3D [10], and others relying on the EnergyPlus engine for energy simulations. It can also be used in regulatory contexts, as several countries are setting energy performance requirements for buildings, and simulation tools like EnergyPlus could be used for compliance verification [11,12]. In addition, EnergyPlus and other simulation tools play a key role in building assessments such as Life Cycle Assessment (LCA) and Life Cycle Costing (LCC), where they are commonly used to estimate impacts during the use stage – often the most significant phase in the building lifecycle [13–16]. EnergyPlus is therefore essential in all areas where building energy simulations are required.

Compared to conventional construction materials, PCM require a different modelling approach due to their dynamic and nonlinear nature, which should also be reflected in full-building energy

* Corresponding author.
E-mail address: D.Zhilyaev@tudelft.nl (D. Zhilyaev).

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simulations [17,18]. In the literature, PCM and PCM-embedded materials are often modelled in a simplified way, where melting and solidification follow the same enthalpy curve [17,19,20]. In reality, however, PCM exhibit more complex behaviour, including hysteresis [21–23] and supercooling [24–26] effects. In some specific situations, those effects might not have a major impact on the results of simulations. The amount of hysteresis depends on multiple parameters, including material type, physical conditions, the rate of temperature change, the mass of the material, the presence of a nucleating agent, etc. [23] Thus, in some cases, the degree of hysteresis may be low, and simplified models that do not take hysteresis into account could provide a reasonable estimate of their performance. Furthermore, even when the degree of hysteresis is significant, if a PCM only undergoes full melting-solidification cycles, the effects of hysteresis on the results of simulations will be limited as well [22,23,27]. In such a case, advanced PCM models might not be required either. However, in the real-world application of PCM, and especially when it comes to the use of PCM in building envelopes, the effects of hysteresis cannot be ignored. First of all, in real-world cases, it is not possible to ensure that PCM always undergoes full melting-solidification cycles [23,28]. In case of incomplete cycles, as multiple studies showed, if the effects of hysteresis are not taken into account or are not modelled correctly, it could result in significant deviations between modelled and measured hourly temperatures and heat fluxes, as well as a greatly overestimated heat storage capacity of PCM [23,27,29]. This is especially important in the case of materials with a high degree of hysteresis, such as inorganic PCM [23]. Furthermore, microencapsulation of PCM [30,31] might significantly increase the observed hysteresis compared to pure PCM [32]. Consequently, construction materials with embedded microencapsulated phase change material (MPCM) particles will also exhibit high degrees of hysteresis. The effects of hysteresis should therefore be properly included in building energy modelling tools to improve the accuracy of simulations for buildings containing such materials.

In the context of PCM and their integration in the building envelope, EnergyPlus includes built-in models that allow to simulate energy performance of buildings taking into account the nonlinear nature of PCM. In its early development, EnergyPlus featured only a simplified PCM model, but in 2017, a hysteresis model was introduced and later in 2018 fully integrated into full-building energy simulations. Since then, it has been actively used in both academia and industry for assessment and decision-making related to PCM integration in buildings. As the model has been reportedly validated [22], the practitioners were provided with confidence in the results of their simulations. Consequently, the results of building energy simulations involving PCM are often taken at face value without a thorough check of the consistency of the outputs. However, although the current hysteresis model in EnergyPlus has been validated, the results of the validation showed inconsistencies in the case of partial melting and solidification cycles [22]. Those inconsistencies could potentially be explained by the fact that the hysteresis model in EnergyPlus is based on a simplified curve-switch theory and by the impossibility of taking supercooling effects into account [23,29]. However, some researchers have pointed out that the hysteresis model in EnergyPlus may not be implemented correctly [27,33,34]. To address these concerns, alternative hysteresis models have been proposed. While many of these are developed at the micro-level or for different software [29,35], some have also been implemented in EnergyPlus as replacements for the built-in model [27].

From the practitioner's perspective, the situation with PCM modelling and the validity of the models built into EnergyPlus is confusing and raises many questions. There is limited understanding of how the different models function, what are their inherent limitations, how they compare, and what consequences may arise from choosing one model over another. This study aims to close those gaps and has three main objectives:

1. To present two new implementations of hysteresis models in EnergyPlus: an improved version of the default EnergyPlus hysteresis model with corrected curve-switch behaviour, and the integration of the two-phase PCM model by Feng et al. [27] originally based on EnergyPlus v9.3 into a newer version of EnergyPlus v24.1.
2. To provide an in-depth analysis of four EnergyPlus-based hysteresis models and identify their inherent limitations. Those models include the default hysteresis model in EnergyPlus v24.1, the original two-phase model by Feng et al. [27], as well as the two models introduced as a part of this work.
3. To illustrate the practical significance of the findings and demonstrate how the selection of a hysteresis model can impact the decision-making process, using the example of a novel PCM-embedded material development.

This study is the first to provide such an in-depth analysis of different hysteresis models in EnergyPlus and aims to assist practitioners in making informed decisions regarding model selection. It also offers a set of guidelines on how to set up the models to obtain the most consistent results possible, along with an outlook for their future development.

2. Methodology

2.1. Overview of the approach

To demonstrate the effects of PCM model selection on decision-making, as well as to illustrate the limitations of the existing hysteresis models in EnergyPlus, we use an example case of novel thermal material development called NRG-Foam. The material has been developed as part of EU-funded "Integrated porous cementitious Nanocomposites in non-Residential building envelopes for Green active/passive energy STORAGE" (NRG-STORAGE) project [36]. NRG-Foam is a material based on cementitious foam with embedded MPCM particles that combines both insulating and energy storing properties. For the purposes of real-world testing and monitoring the performance of NRG-Foam, four demonstrator buildings have been constructed in Sofia, Bulgaria. All the tests and energy simulations performed as part of this work use the same demonstrator building configuration that represents the physical buildings in Sofia with the only difference between the cases being the configuration of NRG-Foam used. The following sections introduce the demonstrator building and NRG-Foam in more detail and provide information on how the parameters of NRG-Foam are linked to the building-level energy simulations.

2.2. Description of the demonstrator building

The building model used for all tests and illustrations in this work is a modified version of BESTEST 900 [38]. Fig. 1 shows the demonstrator building geometry and the main elements of the envelope, as well as a detail of the node locations in the PCM wall, and Table 1 provides a detailed list of properties for each component and material.

The walls of the building include NRG-Panels made of NRG-Foam, providing both insulation and energy storage. More detailed information on this material is given in the next section. The test building has an HVAC system with a dual setpoint: 20 °C for heating and 25 °C for cooling, selected as a setting providing a reasonable compromise between minimising energy consumption and maintaining thermal comfort in the building [39,40]. The temperature is assumed to be constantly maintained within this range throughout the year. In EnergyPlus, the HVAC system is modelled as an Ideal Loads Air System.

In this study, multiple configurations of the demonstrator building presented above are used in EnergyPlus simulations for hysteresis model testing. The only difference between the models is in the parameters of the NRG-Panels layer, while the rest of the building configuration remains the same. The EnergyPlus input .idf files for each simulated configuration used in this work are available in the repository.

While the physical demonstrator buildings were constructed and monitored in Sofia, in this study we model their energy performance under different climatic conditions. More specifically, Barcelona has been

Table 1
Overview of the constructions and material layers of the demonstrator building with their respective properties. Those values are further used in the input files of EnergyPlus. The final properties of NRG-Panels depend on the exact material configuration and thus are not provided in the table.

Construction	Material layer	Thickness	Thermal conductivity	Density	Specific heat	Roughness	Thermal absorptance	Solar absorptance	Visible absorptance
		m	W/mK	kg/m^3	J/kgK				
Walls	Plaster	0.01	0.47	1150	100	Rough	0.9	0.4	0.4
	NRG-Panels	Vary	Vary	Vary	Vary	Rough	0.9	0.6	0.6
	Hollow brick	0.25	0.31	500	900	Rough	0.9	0.6	0.6
	Gypsum - lime plaster	0.01	0.87	1750	1050	Rough	0.9	0.26	0.26
Roof	Bituminous sheet	0.002	0.17	600	1050	Rough	0.9	0.4	0.4
	Wooden board	0.015	0.17	550	2090	Rough	0.9	0.6	0.6
	Mineral wool	0.18	0.032	21	840	Rough	0.9	0.6	0.6
	Air buffer	Air gap with thermal resistance of 0.16 m^2 K/W							
	Plasterboard	0.016	0.21	900	840	Rough	0.9	0.26	0.26
Floor	Gravel	0.6	0.6	1550	900	Rough	0.9	0.6	0.6
	Bituminous sheet	0.005	0.17	1100	1050	Rough	0.98	0.98	0.98
	XPS insulation	0.1	0.033	32	1500	Rough	0.9	0.6	0.6
	Waterproof tarp	0.002	0.17	600	1050	Rough	0.9	0.6	0.6
	Reinforced concrete slab	0.2	1.63	2400	960	Rough	0.88	0.6	0.6
Windows	Triple glaze window	Simple Glazing System with U = 0.7 m^{2}K/W, solar heat gain of 0.34 and visible transmittance of 0.62							
Doors	Same as windows								

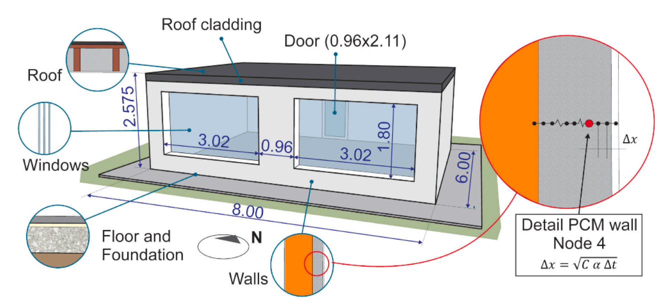

Fig. 1. Demonstrator building configuration, and a detail of the position of the nodes. In EnergyPlus, nodes are placed at material boundaries and within each layer. Interior nodes are full nodes, and their spacing is based on the square root of the product of a material's thermal diffusivity α, the timestep parameter Δt, and the space discretisation constant C: $\Delta x = \sqrt{C\alpha\Delta t}$ [37]. The number of nodes is obtained by dividing the layer thickness by Δx and rounding to the nearest integer; Δx is then adjusted to match the exact thickness. The enlarged detail of the wall in the figure shows the position of Node 4, which is mainly used for illustrative examples throughout this work. It is located inside the PCM layer close to the outside surface of the wall, but the exact position varies depending on the case.

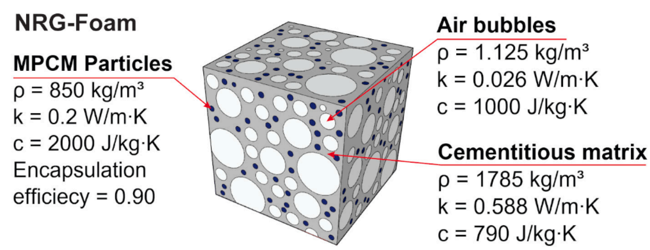

Fig. 2. Main components of NRG-Foam and their characteristics.

chosen as the test location. Compared to Sofia, it has a significantly warmer climate, making it more favourable for PCM utilisation. EnergyPlus simulations in this study rely on TMY weather data for Barcelona obtained from the EnergyPlus Weather Data portal [41] and can also be found in the repository.

2.3. NRG-foam and NRG-panels introduction

As it has already been introduced, NRG-Foam is a thermal material based on MPCM-embedded cementitious foam. Fig. 2 shows the composition of NRG-Foam as well as the key properties of its constituents that were used for calculations and simulations in this study. In order to apply NRG-Foam to the demonstrator buildings, it was cast into $0.4 \times 0.6 \times 0.1$ m panels and cured. These panels are referred to as NRG-Panels throughout the text.

Although physical demonstrator buildings were constructed in Sofia to test NRG-Panels in a real-world setting, these tests were limited in time and focused on a single panel configuration. The panels had a porosity of around 0.86, included 10 % MPCM by volume in the paste, and used NEXTEK 24D MPCM produced by Microtek with a melting temperature of 24 °C.

In this work, we assume that the configuration of NRG-Panels is not fixed but can be adjusted to minimise the heating and cooling demand of the demonstrator building. The following parameters are considered variable:

- Porosity
- Volumetric fraction of MPCM in the cement paste
- Panel thickness
- PCM melting temperature
- The degree of PCM hysteresis

Based on those parameters, it is possible to obtain the final properties of NRG-Panels that can be used in the input files for EnergyPlus simulations. The final thermal conductivity of NRG-Panels is obtained using Lewis-Nielsen theory which defines the effective thermal conductivity of the two-phase system using the following equations:

$$k = k_1 * (1 + AB\phi_2)/(1 - B\psi\phi_2) \quad (1)$$

$$B = (k_2/k_1 - 1)/(k_2/k_1 + A) \quad (2)$$

$$\psi = 1 + ((1 - \phi_m)/(\phi_m^2))\, \phi_2 \quad (3)$$

where k is the resulting conductivity of the two-phase system; k_1 and k_2 are conductivities of the matrix and dispersed material respectively; ϕ_2 is the volumetric fraction of the dispersed material; A is the shape constant for the filler particles; ϕ_m is the maximum packing fraction of filler particles. In order to calculate the effective thermal conductivity of NRG-Panels, the Lewis-Nielsen theory was applied twice. First, the effective thermal conductivity of cementitious paste is obtained using the properties of cement and MPCM particles as well as their fractions.

Then, the final thermal conductivity of NRG-Panels is obtained using the above calculated conductivity of the cementitious matrix, thermal conductivity of air bubbles and their corresponding fractions.

Density and effective specific heat of NRG-Panels are obtained using the mixture law based on the fractions of individual components and their fractions:

$$\rho_{eff} = \phi_a * \rho_a + \phi_c * \rho_c + \phi_p * \rho_p \tag{4}$$

$$c_{p,eff} = \frac{1}{\rho_{eff}}(\phi_a * \rho_a * \ c_{v,a} + \dots + \phi_c * \rho_c * \ c_{v,c} + \phi_p * \rho_p * \ c_{v,p}) \tag{5}$$

where ρ_{eff} and $c_{p,eff}$ are the effective density and specific heat of NRG-Panels; ϕ_a, ϕ_c and ϕ_p are volumetric fractions of air, cement paste and MPCM; ρ_a, ρ_c and ρ_p – densities of air, cement paste and MPCM; $c_{v,a}$, $c_{v,c}$ and $c_{v,p}$ – volumetric heat capacities of air, cement paste and MPCM.

The overall latent heat of fusion is calculated based on the mass fraction of MPCM in panels and the encapsulation efficiency:

$$L_{eff} = \rho_p/\rho_{eff} \quad * \phi_p * e_{MPCM} * L_{PCM} \tag{6}$$

where L_{eff} is the latent heat of fusion of NRG-Panels; ρ_p and ρ_{eff} are densities of MPCM and NRG-Panels; ϕ_p is the volumetric fraction of MPCM, e_{MPCM} is the encapsulation efficiency of MPCM (volume of the PCM core related to the total volume of MPCM particle); L_{PCM} is the latent heat of PCM material. Those calculations and the generation of the EnergyPlus input files were performed in MATLAB using a routine written for those purposes.

3. Numerial results

3.1. Description and examination of different EnergyPlus hysteresis models

Four different hysteresis models were analysed in this study:

- The current built-in hysteresis model in EnergyPlus.
- The modified version of the built-in EnergyPlus hysteresis model with corrected curve-switch transition behaviour developed as part of this work, in which we addressed discontinuities and physically unrealistic behaviour during the phase-change transitions. The source code for this version is provided in the repository.
- Two-phase PCM model based on EnergyPlus v9.3 developed by Feng et al. [27].
- Two-phase PCM model by Feng et al. [27] implemented in EnergyPlus v24.1 as part of this work. The source code for this version is provided in the repository.

The following sections provide an in-depth analysis of each model, including their working principles and identified limitations.

3.2. Current PCM model integrated in EnergyPlus

There are currently two ways of modelling PCM in EnergyPlus: using a single enthalpy curve without accounting for hysteresis, and a hysteresis model that uses separate curves for melting and solidification. Both approaches rely on the Conduction Finite Difference Solution Algorithm (CondFD). The hysteresis model was developed in cooperation between NREL and NRGSim and was first introduced in EnergyPlus version 8.8 (2017). Starting from version 8.9 (2018), it was fully integrated, allowing simulation of multi-layer components containing PCM layers.

The hysteresis model in EnergyPlus is reportedly based on a continuous enthalpy curve with a mushy region, as described in Egolf and Manz [42], and a constant heat capacity transition between melting and solidification curves in cases of incomplete phase change, as defined in Bony and Citherlet [43].

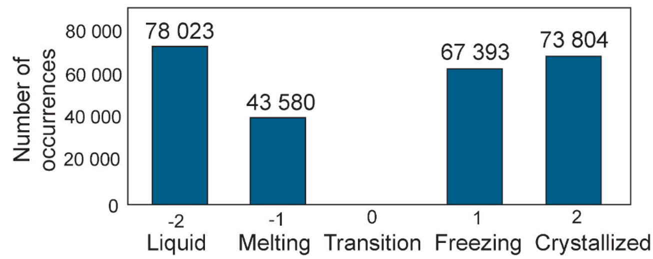

Fig. 3. Distribution of PCM states for Node 4 of the South wall over the whole simulation year for a selected configuration of the demonstrator building and using the current hysteresis model in EnergyPlus. The simulation has been performed using the time step of 2 min with a total of 262,800 time steps distributed across possible PCM states.

3.2.1. Identified limitations

While multiple sources (e.g., Feng et al. [27], Abdellatef et al. [29]) describe the built-in hysteresis model as based on the curve-switch method and specifically the work by Bony and Citherlet [43], it has been found that, in reality, it functions differently. Analysis of the model's source code shows that although the intention was indeed to follow the curve-switch method, the practical implementation has not been executed correctly. This can be demonstrated with a simple test: let us take an arbitrary configuration of the demonstrator building (file "model_test_1.idf" in the repository), run the energy simulation using the built-in hysteresis model, and analyse the parameters of the internal nodes of the PCM layer at each time step. In particular, let us focus on the "CondFD Phase Change State" and "CondFD Phase Change Node Specific Heat" variables for Node 4 in the south-facing wall, which output the PCM state and the modelled specific heat at that node. PCM states are encoded in EnergyPlus as follows:

- -2 - Liquid
- -1 - Melting
- 0 – Transition
- 1 - Freezing
- 2 – Crystallized

where the transition state is supposed to denote the switch between the curves during an incomplete melting or solidification cycle. Fig. 3 shows the distribution of the PCM states throughout the whole simulation year.

It can be observed from the model output that there is not a single time step where PCM is in the transition state. This would only be possible if the material underwent full melting–solidification cycles throughout the entire year, which is unrealistic. To explore this issue in more detail, Fig. 4 depicts the heat capacity, node temperature, and PCM state for two full days in January (27th and 28th). Multiple inconsistencies can be observed:

- PCM is not switching to Transition state during the incomplete melting cycle (frames #2 and #4).
- PCM is going from Melting into Liquid state even though the node temperature never reaches even the peak melting temperature of 20 degrees (frames #2 and #4).
- PCM is going from Liquid to Melting state (frame #3).
- PCM is going from Crystallized to Freezing state (frame #8).

All of these observations point to the fact that in its current form, the hysteresis model does not perform curve switching as intended (by PCM entering the Transition state) but instead jumps instantaneously between the melting and solidification curves. Fig. 5 shows the temperature–enthalpy curve for the same two days in January. It can be observed that, during the two analysed days, the PCM shifted isothermally between the melting and solidification curves eight times while never entering the transition state as required by the curve-switch theory. The red frames in Fig. 5 correspond to the same heat capacity discontinuities shown in Fig. 4.

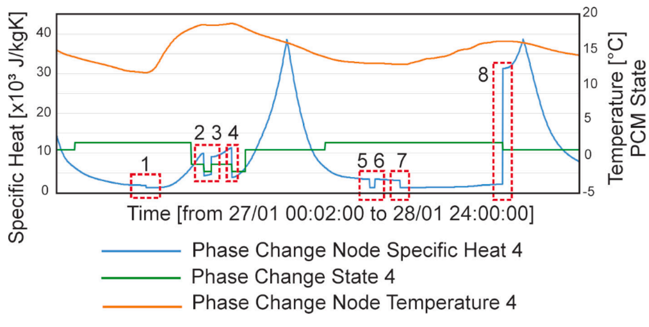

Fig. 4. Specific heat, Temperature and Phase change state for Node 4 in the South wall of the demonstrator building during the 27th and 28th of January. Red frame lines indicate the discontinuities in the specific heat function.

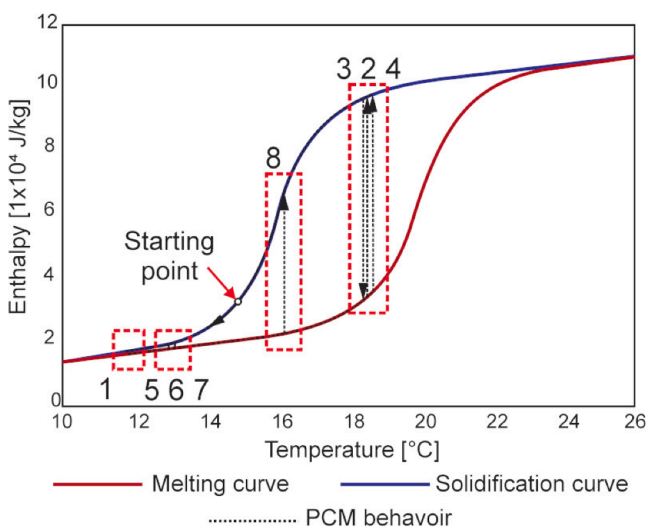

Fig. 5. Enthalpy curve for Node 4 in the South wall of the demonstrator building. The numbered frame lines correspond to the same specific heat discontinuities shown in Fig. 4.

According to [23], the approach with the isothermal transition between the curves is also used in TRNSYS model type399. However, this is not representative of the real-world behaviour of PCM and such a modelling approach might also lead to the overestimation of PCM latent heat [23].

3.3. Modified EnergyPlus PCM model with corrected curve switching

3.3.1. Model description

As illustrated in the previous section, the built-in EnergyPlus hysteresis model does not function as intended and is not realistically describing the real-world behaviour of PCM. To address this issue, a modified version of EnergyPlus has been developed, incorporating a functional curve-switch model along with other improvements. The following changes have been made:

- The code related to hysteresis modelling has been almost completely rewritten to follow the curve switching approach as outlined in Bony and Citherlet [43].
- The boundaries where PCM is considered to be fully frozen or fully melted have been extended to prevent large jumps in enthalpy when switching between melting and freezing curves in fully melted or fully frozen states.

The mathematical modelling of PCM properties during melting and solidification cycles in EnergyPlus relies on the work by Egolf and Manz [42], where specific enthalpy and other physical properties of PCM are defined using continuous functions. Between the frozen and liquid states, a so-called mushy region exists where PCM transitions from one state to another. In EnergyPlus, this region corresponds to the melting and freezing states. Its width is finite and defined by lower and upper limits. Outside the mushy region, PCM is considered either fully melted or fully frozen. The enthalpy curve is defined as a smooth exponential function that gradually decreases beyond the mushy region. As a result, the specific heat at the edges of the mushy region is higher than the sensible specific heat, which can cause significant discontinuities if the temperature reverses direction just outside this region, since a switch between curves will then occur.

- The part of the hysteresis algorithm that detects the reversal in PCM temperature change has been moved from the CondFD algorithm into the main hysteresis algorithm.

In the current version of EnergyPlus, this detection is handled in the CondFD code, but this causes an issue where the enthalpy and heat capacity calculations are based on data from the previous time step. In other words, not all variables are updated simultaneously, leading to synchronisation (timing) issues. In the updated version, all variables are calculated and updated at the same time.

- The transition between melting and freezing curves has been modified to happen at specific heat equal to the specific heat of fully frozen PCM.

As already mentioned, the curve-switch model implemented in this work is based on the approaches by Egolf and Manz [42] and Bony and Citherlet [43]. There is, however, a degree of incompatibility between these models. Egolf and Manz [42] describe a method for implementing a continuous enthalpy curve with a mushy region, capable of representing PCM with different specific heat in liquid and frozen states. Their work, however, does not address hysteresis and focuses only on a single enthalpy curve. In contrast, Bony and Citherlet [43] include hysteresis and implement a curve-switch mechanism for incomplete melting and solidification cycles, but assume that the specific heat of PCM is the same in solid and liquid states.

The analysis of the current hysteresis code in EnergyPlus showed that the intended way to resolve the incompatibility between the two underlying theories was to set the transition between melting and freezing curves at a heat capacity equal to the average of the fully frozen and fully melted values. However, depending on the PCM characteristics and the point where the transition begins, this can cause an issue where, instead of switching from the melting to the freezing curve, the PCM loops back to the melting curve. Fig. 6 illustrates this issue using an example where the liquid specific heat is three times the frozen specific heat (an exaggerated case chosen for the clarity of the illustration). To avoid this problem, the curve-switch model implemented in this study assumes that the transition occurs at a heat capacity equal to the fully frozen value.

- The Input Data Dictionary of EnergyPlus has been modified to allow peak melting and solidification temperatures of PCM to be negative.
- New variables have been added, allowing to also output enthalpy values for each node: CondFD Phase Change EnthNew (node enthalpy for the current time step), CondFD Phase Change EnthOld (node enthalpy for the previous time step).
- The initialisation temperature that EnergyPlus is using as the starting point for all the temperatures in the CondFD algorithm has been changed from 23.0 °C to −33.33 °C.

It has been observed that the modified version of EnergyPlus terminates with a fatal error if the initialisation temperature exactly matches the PCM's peak melting or solidification point. Since −33.33 °C is not representative of typical operating conditions or a PCM that could normally be utilised in construction, using such an uncommon and specific value makes this issue less likely to occur. We also note that while we

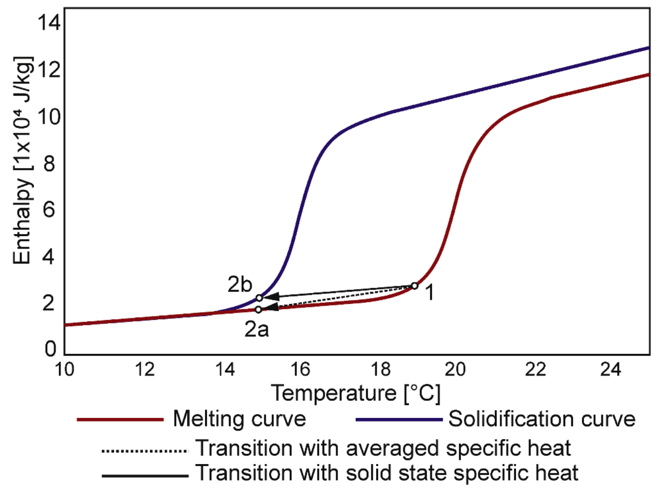

Fig. 6. Two cases of simulating the transition between the melting and solidification curves. Dotted line (1– > 2a) corresponds to the transition that happens at heat capacity equal to the average between fully melted and fully frozen heat capacities. Solid line (1– > 2b) is the transition at the fully frozen heat capacity.

did not notice significant deviations in our tests, the choice of the initialisation temperature could affect the simulation results, since the model needs time to warm up and stabilise. Therefore, we recommend a 15-day or longer warm-up period for the simulations.

3.3.2. Comparison with the original model

To illustrate the difference between the original and modified models, let us consider the same building example from the previous section describing the issues with the current EnergyPlus hysteresis model (file “model_test_1.idf” in the repository). Fig. 7(a) shows the temperature, phase change state, specific heat, and enthalpy curve for the same Node 4 in the south wall of the demonstrator building over the period of January 27th to 28th.

While discontinuities in specific heat can still be observed, they occur not due to instantaneous jumps between curves, but when PCM enters or exits the Transition state (see Fig. 7(b)). According to the curve-switch theory, and specifically the approach outlined by Bony and Citherlet [43], during the transition, the specific heat of PCM equals its sensible heat. As a result, depending on where the transition occurs, specific heat may show significant changes. This is thus an intrinsic feature of the curve-switch theory.

It is also possible to confirm that the modified model is stable and produces consistent results throughout the year. Fig. 8 presents the enthalpy curve over the full year for the same node used in the previous analysis. Fig. 8 shows that the resulting enthalpy curve follows the theoretical one, and all transitions between the curves align with a straight line having the same slope as in the fully crystallised or fully melted states.

3.3.3. Identified limitations

- Curve switching is a simplified model and may not be as precise as more comprehensive hysteresis approaches, such as curve scaling or the two-phase model.

According to comparison examples found in the literature, more advanced hysteresis models may produce results closer to experimentally obtained data for incomplete melting and solidification cycles [29]. Additionally, these models often show a lower degree of discontinuity in the PCM heat capacity function, making them more realistic than the curve-switch model, where heat capacity undergoes instantaneous and often significant changes not representative of real-world PCM behaviour.

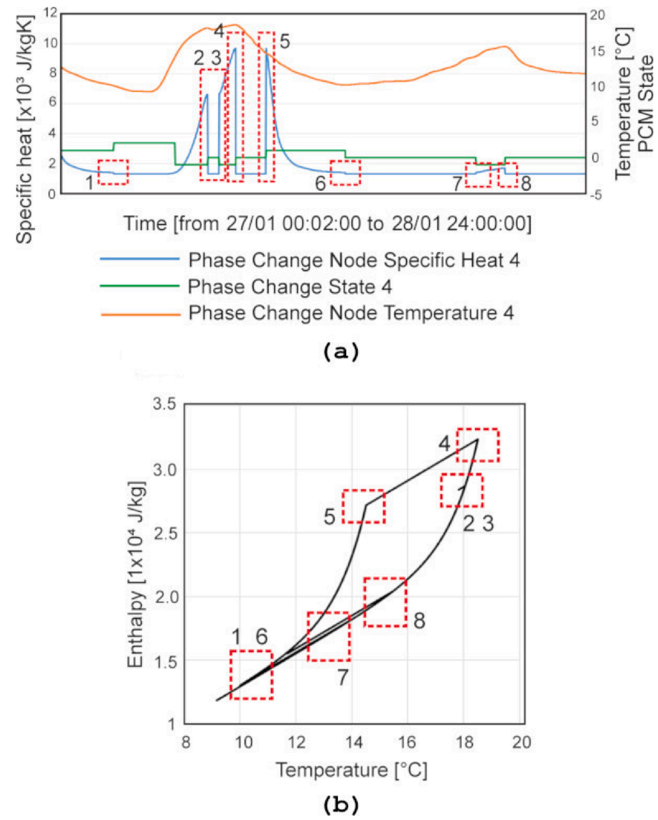

Fig. 7. Temperature, specific heat and phase change state for Node 4 in the South wall (a) and enthalpy curve for the same node (b) during the 27th and 28th of January. Red frame lines indicate the discontinuities in the specific heat function.

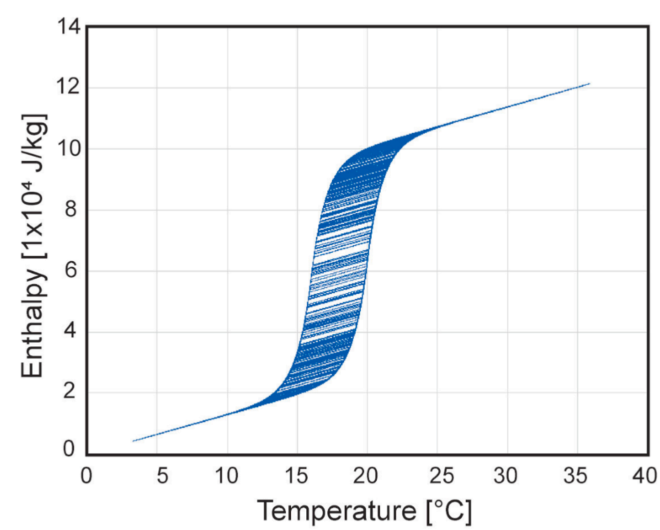

Fig. 8. Enthalpy curve for Node 4 in the South wall of the demonstrator building over the whole simulation year.

- Enthalpy jumps occur when switching between melting and freezing curves in PCM with different fully frozen and fully melted specific heat.

While the model allows simulating a PCM with different heat capacities in frozen and melted states, it experiences relatively large enthalpy jumps when switching between the curves. Fig. 9 illustrates this effect, showing the enthalpy curve over the full simulation year for a PCM with higher melted heat capacity than in the frozen state

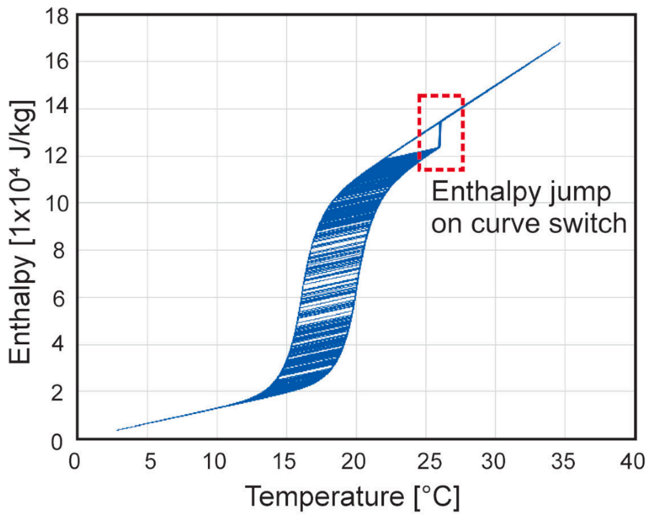

Fig. 9. Enthalpy curve for Node 4 in the South wall over the whole simulation year in the case of unequal specific heat capacity in frozen and melted states. The highlighted area shows point where the jump between the melting and solidification curves is occurring. Due to the difference in frozen and melted heat capacities, the enthalpy curve is experiencing a discontinuity and an enthalpy jump is unavoidable.

(file “model_test_2.idf” in the repository). It should be noted that the overall enthalpy across the fully frozen–fully melted–fully frozen cycle is preserved, and the enthalpy jump does not cause a major change in heat capacity. Consequently, it should not significantly affect simulation results, as those rely on heat capacity values rather than absolute enthalpy.

- The model has not been validated on a real case.

3.4. Two-phase PCM model based on EnergyPlus v9.3

To address the issues with the built-in EnergyPlus hysteresis model described in the previous sections, and to enable more realistic modelling of incomplete melting and solidification cycles compared to simple curve switching, Feng et al. [27] developed the EnhancedPCM model based on EnergyPlus v9.3. EnhancedPCM relies on the two-phase PCM transition theory, specifically the static hysteresis model presented by Barz and Sommer [35]. The EnhancedPCM model has also been validated using experimental data from [22].

Unlike the curve-switch EnergyPlus model described above where the state of PCM is described by five possible discrete values (frozen, melting, transition, freezing and melted), two-phase approach models PCM as consisting of two phases (liquid and solid) at any point in time. The proportion between these two phases is defined by the phase fraction parameter ξ:

$$\xi = \frac{m_l}{m_l + m_s} \tag{7}$$

where m_l is the mass of the liquid fraction and m_s of the solid fraction. The effective properties of PCM (specific heat and enthalpy) depend on the phase fraction and can be estimated using Eqs. (8) and (9).

$$c_{p,\xi} = \xi c_{p,l} + (1-\xi)c_{p,s} + \frac{\Delta\xi}{\Delta T}L \tag{8}$$

$$h_{j+1} = h_j + c_{p,\xi}(T_{j+1} - T_j) \tag{9}$$

where $c_{p,\xi}$ is the effective specific heat of PCM; $c_{p,l}$ and $c_{p,s}$ are specific heat capacities of liquid and solid fractions; L is the latent heat of PCM; $\Delta T = T_{j+1} - T_j$ is the temperature change between the current and previous time step; h_{j+1} and h_j are the current and previous enthalpies of PCM.

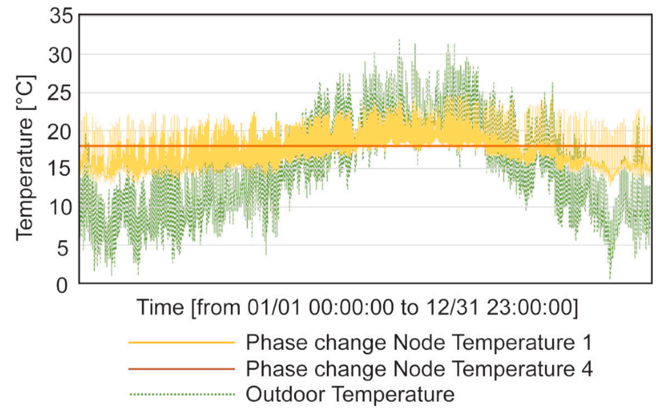

Fig. 10. Yearly temperature variation for Node 1 (outer node) and Node 4 (inner node) in the South wall of the demonstrator building.

Similarly to the curve-switch method, PCM properties are defined using a continuous function. However, while in the case of curve switching the exponential function is used to define PCM enthalpy, in the work of Feng et al. [27] it is used to define the phase fraction ξ:

$$\xi(T) = \frac{1}{2}\left(e^{\frac{-2|T-T_p|}{\tau_l}}\right), \text{ for } T \le T_p \tag{10}$$

$$\xi(T) = 1 - \frac{1}{2}\left(e^{\frac{-2|T-T_p|}{\tau_h}}\right), \text{ for } T > T_p \tag{11}$$

where T_p is the peak melting or solidification temperature of PCM, depending on which curve is modelled; τ_l is the lower width of the melting or solidification interval; τ_h is the upper width of the melting or solidification interval. The use of exponential functions allows for seamless integration of the new model into existing functions within the EnergyPlus code.

3.4.1. Identified limitations

- Intermittent issue where the model fails to initialise correctly, causing the temperature at all PCM nodes to remain constant throughout the entire simulation.

It has been observed that, depending on the building configuration, PCM layer properties, weather data, and CondFD algorithm parameters, the model may fail to initialise in some cases. Fig. 10 illustrates such a case, showing the temperature of two nodes in the south wall of the demonstrator building: one on the outside of the PCM layer (Node 1) and one on the inside (Node 4), along with the outdoor air temperature. The input EnergyPlus file “model_test_3_v93.idf” is provided in the repository.

From Fig. 10, it can be observed that while the temperature of the outside node (Node 1) changes, the temperature of Node 4, located inside the PCM layer, remains fixed at exactly 18 °C throughout the year. This value corresponds to the initialisation temperature set within the EnergyPlus code (specifically in the CondFD algorithm) and cannot be modified by the user through input parameters in .idf file. The only way to change it is by editing the source code and recompiling EnergyPlus. Interestingly, in the original EnergyPlus code, the initialisation temperature was set at 23 °C but was reduced to 18 °C by Feng et al [27]. This change was not explicitly explained by the authors, but it appears that they may also have encountered stability issues during the simulations.

Based on our experiments, we were not able to identify the logic behind these intermittent initialisation errors. In some cases, when comparing two nearly identical PCM configurations that differ only in peak melting temperature by one degree, one results in an initialisation error while the other does not. Similar behaviour was observed for other PCM layer parameters as well. However, the issue may not necessarily

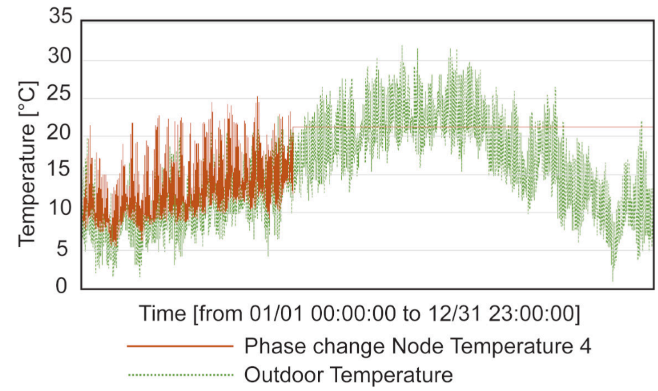

Fig. 11. An example of the model freeze issue. The graph shows the temperature profile of Node 4 in the South wall of the demonstrator building over the whole simulation period, together with the outdoor air temperature.

originate from the hysteresis model itself, but rather from the CondFD algorithm or the way the new two-phase hysteresis model interacts with it.

It is also important to note that the parameters of the CondFD algorithm play a significant role in this issue. In many cases, tweaking these parameters helped resolve the problem. Specifically, decreasing the space discretisation constant and relaxation factor, as well as increasing the number of time steps per hour, had a positive effect on reducing the likelihood of initialisation errors. However, due to the intermittent nature of the issue, there is no guarantee that it will not occur with certain combinations of the building, PCM and EnergyPlus parameters. Moreover, the parameter adjustments described above significantly increase simulation run times. Although manageable for a single case, this becomes a serious limitation for optimisation studies or situations where large numbers of configurations need to be evaluated simultaneously, and it is not feasible to manually check all EnergyPlus outputs. Even more concerning is that the error does not trigger any warnings or messages in the console or error file, making it very likely to go unnoticed, potentially leading users to incorrect conclusions.

- Intermittent issue where the model initialises correctly but freezes during the simulation run.

This issue is very similar to the previous one, but in this case, the simulation starts normally: node temperatures change, and all PCM parameters follow expected trends. However, at some point, the node temperatures freeze and remain unchanged for the rest of the simulation. Fig. 11 illustrates one such case (see the "model_test_4_v93.idf" file in the repository).

As shown in Fig. 11, the simulation appeared normal until one time step in May, after which no further changes occurred. Similarly to the initialisation issue, the model freeze is highly unpredictable and depends on the specific building case, PCM parameters, weather data, and EnergyPlus algorithm settings, especially CondFD parameters. In most cases, tweaking CondFD parameters helped resolve the issue. This issue, however, is even harder to spot since the outputs are partially correct in the beginning of the simulation run.

- Node heat capacity is taking unexpectedly high values outside of the peak melting and solidification.

Specific heat can reach very high values during peak melting and solidification. However, it has been observed that this model sometimes produces extremely high specific heat values at the far edges of the melting and solidification curves. Fig. 12 illustrates this issue (EnergyPlus input file "model_test_1_v93.idf" provided in the repository). Since EnergyPlus 9.3 cannot directly output node-specific heat, the "CondFD Surface Heat Capacitance Inner Half Node" variable has been used instead for this illustration.

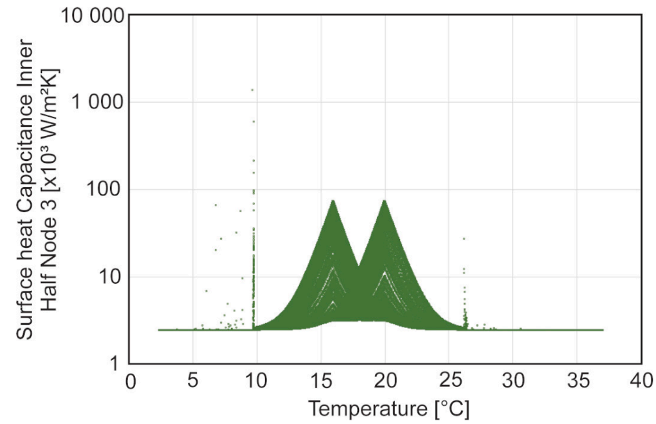

Fig. 12. Surface Heat Capacitance (Inner Half Node) for Node 3 in the South wall of the demonstrator building over the whole simulation period. Note the logarithmic scale of the vertical axis.

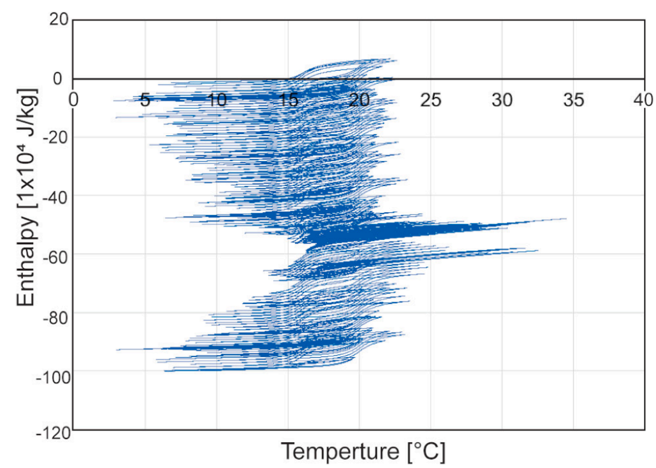

Fig. 13. Enthalpy drift in the case of PCM with different specific heat capacities in liquid and solid states.

Fig. 12 clearly shows the expected melting and solidification peaks in the middle, but also two narrow abnormal spikes in heat capacity far outside the melting and solidification intervals. The heat capacitance values at those spikes are often much higher than even during peak melting and solidification.

While the outliers are significant, they are unlikely to have a major impact on overall building performance, as they occur during only a small number of time steps. However, it is possible that this issue is related to the model freeze problem described above. For example, depending on the magnitude of the heat capacity spike, the simulation may either recover or become stuck at this abnormally high value.

- If PCM has different heat capacities in frozen and melted states, enthalpy is not preserved over the full melting–solidification cycle.

As discussed earlier, EnergyPlus allows users to define different specific heat values for the liquid and solid states of PCM. However, in the hysteresis model by Feng et al. [27], assigning different heat capacities to the solid and liquid phases causes enthalpy to break the closed loop and drift away. Fig. 13 illustrates this effect. The input file "model_test_2_v93.idf" used for this simulation is provided in the repository. The impact of the enthalpy drift on the overall results of the simulation is, however, unclear.

- The model is implemented in EnergyPlus v9.3, which is an old and possibly outdated version.

3.5. Two-phase PCM model based on EnergyPlus v24.1

This model is an adaptation of the one by Feng et al. [27], integrated into a newer version of EnergyPlus (24.1). Additional changes that have been made:

- The initialisation temperature has been changed to −33.33 °C.

Due to the observation that initialisation and model freeze issues (see Section 3.4) often occur when the PCM melting temperature is significantly lower than the initialisation temperature, the initialisation has been changed to −33.33 °C. However, since this parameter is not properly documented, it is unclear whether its modification affects other parts of the CondFD algorithm. Based on the tests performed in this work, changing the initialisation temperature did not have a major effect on the results of the building energy simulations.

- Modifications have been made to the EnergyPlus Input Data Dictionary to allow simulation of PCM with negative melting and freezing temperatures.

3.5.1. Identified limitations

Since this version uses Feng et al. [27] hysteresis model without modifications, it exhibits similar issues:

- There are still heat capacity outliers, albeit the frequency of their occurrence is lower than in the version 9.3.
- Simulation stability might still be an issue sometimes, but the change in the initialisation temperature reduces the number of cases where the model is not initialising properly or freezing during the simulation.
- Unlike the original model of Feng et al. [27] this version has not been validated using a real-world case.

3.6. The impacts of hysteresis model selection on decision-making

To understand the impact that the choice of hysteresis model might have on practitioners and decision-makers, let us illustrate it with an example of material design optimisation. A novel thermal material, NRG-Panels, has already been introduced in the Methodology section. For a material designer developing such a product, it is essential to identify the optimal material configuration that minimises heating and cooling loads. Because many material parameters can be adjusted, the number of possible combinations is virtually unlimited, making it physically impossible to test all of them in the lab or under real-world conditions. As a result, design decisions are highly dependent on the outcomes of full-building energy simulations.

Let us take the demonstrator building described in the Methodology section and try to find the best-performing NRG-Panels configuration for this particular case. In theory, one could define an optimisation problem to minimise building energy demand and solve it to find the optimal panel configuration. However, due to the intermittent issues described before, the optimisation algorithm may be misled and converge to a sub-optimal solution. As discussed previously, tweaking the CondFD parameters, such as reducing the time step, space discretisation constant, and temperature relaxation coefficient, can improve simulation stability, but these adjustments result in extremely long simulation times, making optimisation impractical.

Due to these limitations, a batch simulation approach was used in this study instead of optimisation. First, for each variable material parameter, a set of possible values was preselected. In our case, the parameters and their values were as follows:

- Material porosity: 0.05, 0.2, 0.4, 0.6, 0.8, 0.95.
- MPCM fraction: 0.01, 0.2, 0.4, 0.6.
- Panel thickness: 0.1 m, 0.2 m, 0.3 m.
- PCM peak melting temperature: 18 °C, 19 °C, 20 °C, 21 °C, 22 °C, 23 °C, 24 °C, 25 °C, 26 °C, 27 °C, 28 °C, 29 °C, 30 °C.

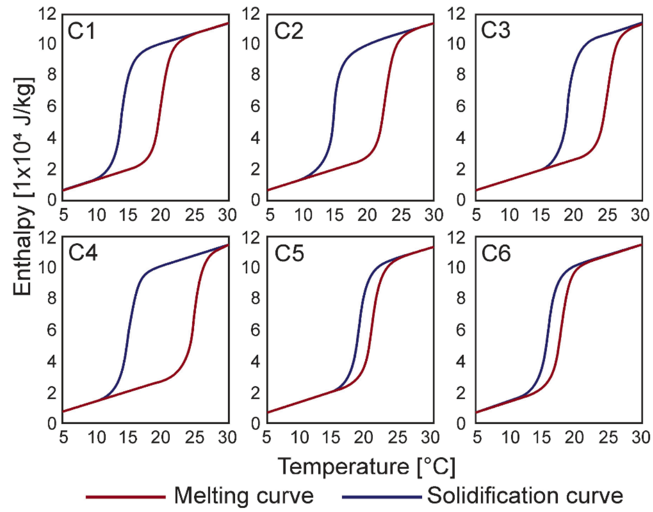

Fig. 14. Enthalpy curves for the analysed configurations of NRG-Panels.

- Hysteresis degree: 0.01 °C, 2 °C, 4 °C, 6 °C, 8 °C, 10 °C.

Other parameters, such as total latent heat and the width of the melting and solidification curves, were kept fixed. Then, a set of virtual materials was generated using all possible combinations of the variable parameters. For each configuration, the final properties of the insulation layer were calculated and an .idf file was created. These files were then used to run EnergyPlus simulations for each material configuration.

In our case, simulations for all configurations were run using six versions of EnergyPlus: four hysteresis models discussed above, and two reference models without hysteresis (EnergyPlus v9.3 and v24.1). For the no-hysteresis models, only the melting curve of the PCM was used. To do so, the PCM parameters of each material configuration were used to build the enthalpy curve, which was then converted into the temperature–enthalpy pair format required by EnergyPlus to be provided in the MaterialProperty:PhaseChange input field of .idf file.

After obtaining the yearly HVAC energy consumption results, the best material configuration according to each model was identified. Table 2 provides an overview of these configurations and Fig. 14 shows the enthalpy curves for each configuration. The resulting parameters of the layer that were used in EnergyPlus are provided in Table 3. The resulting .idf files for each of the configurations can be found in the repository. For each configuration, four different .idf files are included:

- With hysteresis for EnergyPlus v9.3 (used for the Feng et al. model).
- Without hysteresis for EnergyPlus v9.3 (used for the no-hysteresis model v9.3).
- With hysteresis for EnergyPlus v24.1 (used for the current EnergyPlus hysteresis model, modified model with corrected curve switching and the Feng et al. model integrated into EnergyPlus v24.1).
- Without hysteresis for EnergyPlus v24.1 (used for the no-hysteresis model v24.1).

The results of the simulations for each material configuration obtained using the analysed PCM modelling approach are presented in Table 4. As observed in Table 4, the models disagree on which material configuration is the most promising in terms of the optimal energy performance of the demonstrator building: every configuration is ranked as the best according to only one of the models.

The current hysteresis model clearly favours configurations with the lowest porosity, and therefore the highest MPCM content and maximum heat capacity (C1). In contrast, all other models rank this configuration as one of the least preferable. Furthermore, when comparing the energy consumption values obtained from the current model with those from the other EnergyPlus v24.1-based models, it becomes evident that the

Table 2
Overview of the analysed configurations of NRG-Panels.

Configuration	Porosity	MPCM fraction	Panel thickness (m)	PCM peak melting temp. (°C)	Melting curve width (low) (°C)	Melting curve width (high) (°C)	Degree of hysteresis (°C)	Freezing curve width (low) (°C)	Freezing curve width (high) (°C)
C1	0.05	0.6	0.2	20	2	2	6	2	2
C2	0.2	0.6	0.3	23	2	2	8	2	2
C3	0.8	0.6	0.3	25	2	2	6	2	2
C4	0.2	0.6	0.3	25	2	2	10	2	2
C5	0.95	0.6	0.3	21	2	2	2	2	2
C6	0.2	0.6	0.3	18	2	2	2	2	2

Table 3
Resulting calculated properties of NRG-Panels for each analysed configuration.

Conf.	Latent heat of fusion (J/kg)	Specific heat (J/kgK)	Density (kg/m^3)	Thermal conductivity (W/mK)
C1	7.50E+04	1.29E+03	1.16E+03	2.90E-01
C2	7.50E+04	1.29E+03	9.80E+02	2.29E-01
C3	7.47E+04	1.29E+03	2.46E+02	5.81E-02
C4	7.50E+04	1.29E+03	9.80E+02	2.29E-01
C5	7.36E+04	1.29E+03	6.24E+01	3.04E-02
C6	7.50E+04	1.29E+03	9.80E+02	2.29E-01

Table 4
The final HVAC energy demand for the demonstrator building with every analysed configuration of NRG-Panels. Each building configuration has been simulated using every PCM model considered in this study. For each PCM model, the results of energy simulations were ranked and those ranks are also provided in the table. For example, for the current hysteresis model in EnergyPlus, the configuration C1 is the best ranked since it has the lowest energy consumption compared to other configurations.

Conf.	Heating and cooling demand, kWh/a						Configuration rank					
	Original	Curve-switch	Feng et al. v9.3	Feng et al. v24.1	No Hysteresis 9.3	No Hysteresis 24.1	Original	Curve-switch	Feng et al. v9.3	Feng et al. v24.1	No Hysteresis 9.3	No Hysteresis 24.1
C1	964	1667	995	1674	1008	1703	1	4	6	4	6	4
C2	1186	1545	896	1549	928	1626	2	1	4	2	4	2
C3	1770	1780	843	1781	853	1796	5	5	1	5	2	5
C4	1298	1576	892	1543	934	1638	3	2	3	1	5	3
C5	1916	1936	845	1932	844	1934	6	6	2	6	1	6
C6	1372	1601	919	1600	905	1575	4	3	5	3	3	1

current model significantly overestimates the effect of PCM inclusion: configuration C1, which has the highest total amount of PC, shows an HVAC energy consumption of less than 1000 kWh/a according to the original model while it never drops below 1500 kWh/a according to the rest of EnergyPlus v24.1-based models.

The no-hysteresis EnergyPlus v9.3 model is at the opposite extreme, identifying the configuration with the highest porosity of 0.95 (C5) as optimal. However, this configuration is poorly ranked by all other models, including the version of the Feng et al. [27] model integrated into EnergyPlus v24.1. The only other model aligned with it is the original Feng et al. model that also favours high porosities and identifies NRG-Panels with 0.8 porosity as optimal. However, these two models do not agree on the optimal melting temperature of PCM.

It is also important to note the differences in results caused by the EnergyPlus version. The no-hysteresis models in EnergyPlus v9.3 and EnergyPlus v24.1 disagree on the optimal configuration, highlighting that the results of simulations are strongly influenced not only by the PCM hysteresis modelling but also by other changes made to EnergyPlus between the versions. This has a major impact on material design decisions, as the optimal configuration varies significantly depending on the version of EnergyPlus used. The changes between EnergyPlus versions also affect the results obtained from hysteresis models, leading to situations where the original Feng et al. [27] model and its version implemented in EnergyPlus v24.1 produce contradictory results. For example, the two models disagree on how the porosity of NRG-Panels influences HVAC energy demand. To illustrate this disagreement, let us fix all the parameters of NRG-Panels except for porosity (0.6 MPCM fraction, 0.2 m thickness, 23 °C melting temperature, 5 °C hysteresis). The .idf files used for simulations are provided in the repository. Fig. 15 compares the resulting energy consumption according to both models.

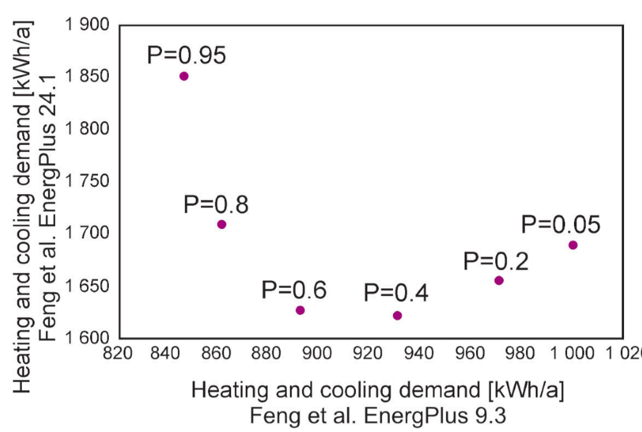

Fig. 15. Comparison of heating and cooling energy demand according to the original Feng et al. hysteresis model in EnergyPlus 9.3 and the same model integrated into EnergyPlus 24.1 at different NRG-Panel porosities.

As depicted in Fig. 15, a porosity of 0.95 is optimal according to the original Feng et al. model, yet it is the worst according to the Feng et al. v24.1 model, which favours a porosity of 0.4. Physically, this implies that in EnergyPlus v9.3, reduced thermal conductivity is seen as more beneficial than increased thermal storage capacity. Within the NRG-Storage project, this balance between thermal conductivity and heat storage was a key factor guiding material development. The situation where different models provide contradictory directions has a major impact on decision-making, essentially eliminating its sole foundation.

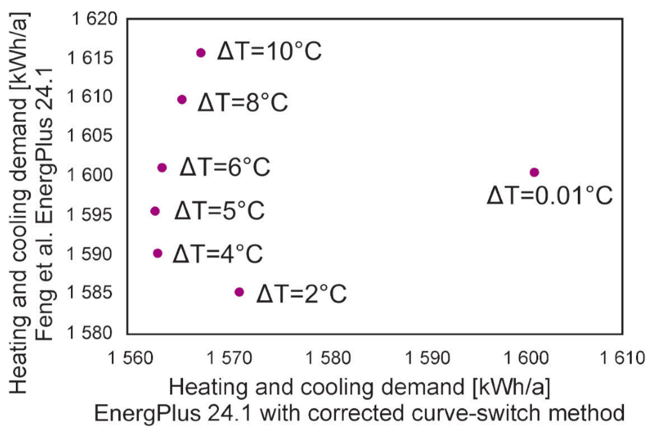

Fig. 16. Comparison of heating and cooling energy demand between the corrected curve-switch model and the Feng et al. v24.1 model at different degrees of hysteresis.

The contradictions related to the material design arise not only due to the differences in the EnergyPlus version. Comparison among the models based on EnergyPlus v24.1 shows that there is also a degree of disagreement between them. The best configuration of NRG-Panels according to the no-hysteresis model v24.1 contains PCM with the melting temperature of 18 °C, which is significantly lower than in the case of other models. Thus, if the decision regarding the choice of PCM for NRG-Panels was to be made based on the simplified simulation without taking hysteresis into account, a PCM with a low melting temperature would be selected. However, this might be a suboptimal design decision if hysteresis is taken into account. And when it comes to the two analysed models with hysteresis based on EnergyPlus v24.1, curve-switch and Feng et al. v24.1, while they generally provide similar results, there are also differences in regard to how some PCM parameters impact the HVAC energy demand. One of such parameters is the degree of hysteresis, and Fig. 16 provides an illustration of one of such cases where all the parameters of NRG-Panels are fixed (0.4 porosity, 0.6 MPCM fraction, 0.3 m thickness, 20 °C melting temperature) and the models are compared across different levels of PCM hysteresis. The .idf files used for simulations are provided in the repository.

As Fig. 16 shows, the degree of hysteresis that results in the minimum HVAC energy demand differs between the models: for the corrected curve-switch method, the optimal hysteresis is around 5 °C, while for the Feng et al. 24.1 model it is around 2 °C. While the degree of hysteresis is not a design parameter that can be easily modified, it can still influence material design decision-making. For example, depending on what the optimal value of hysteresis is for minimised building energy consumption, a different type of PCM can be chosen (organic or inorganic, bio-based or petroleum-based), a product from a different producer could be prioritised (there are differences between PCM hysteresis depending on the producer and the production process), or different encapsulation techniques of MPCM particles can be selected (hysteresis degree can be influenced by the encapsulation process). Contradicting results related to the optimal degree of hysteresis could thus also be a major complication for a decision-making process and the selection of the optimal material configuration. Furthermore, although the demonstrated energy consumption differences between the analysed models are not very large in the case of a small and simple building used for illustrative examples in this work, in real-world scenarios involving larger or more complex buildings, they can be significantly larger.

4. Discussion

The analysis of different EnergyPlus hysteresis models presented in this work highlights that there is currently no model without limitations that could be used without any reservations. The built-in EnergyPlus model is clearly not implemented correctly and cannot be recommended to be used for PCM modelling. A corrected curve-switch model presented in this study has resolved multiple issues of the original EnergyPlus hysteresis model and has been shown to be stable when it comes to the simulation of a variety of PCM configurations. However, it is also based on a simplified approach to PCM modelling and has not been validated against a real-world case. The two-phase hysteresis model by Feng et al. is the most comprehensive and realistic among all the PCM models analysed in this work. Unfortunately, it is also not completely free of limitations and is susceptible to intermittent stability issues. Furthermore, the original model of Feng et al. is implemented in a relatively old version of EnergyPlus v.9.3 and switching to a newer version leads to significantly different and often contradicting results. Finally, there is currently no EnergyPlus hysteresis model that allows for modelling of supercooling effects. Practitioners should be fully aware of those limitations of the existing models when making a choice between them and be sure not to take the results of the simulations at face value, no matter which model is used. Based on a thorough analysis of the working principles and limitations of hysteresis models presented in this study, a set of practical recommendations has been compiled for the practitioners working with PCM modelling in EnergyPlus:

- Be careful with the CondFD algorithm parameters. The default values of those parameters are not suitable for PCM hysteresis modelling, especially when using the two-phase hysteresis model.
- In order to avoid the issues with model stability, decrease the space discretisation constant or the relaxation factor. Increasing the time step of the simulation is beneficial as well. In our tests, decreasing the discretisation constant to 1, relaxation factor to 0.5 and increasing the time step to 30 or more steps per hour usually was enough to prevent model instability issues. Those values, however, vary per case and might need to be significantly different in some instances.
- Thoroughly check the energy simulation outputs at the level of nodes. Output the temperature and specific heat capacity for several nodes in the PCM layers and check the consistency of those outputs. The intermittent stability issues can often go unnoticed if only the final top-level results (e.g., building energy demand) are analysed.
- In the case of an optimisation study, be sure to save the results at every iteration of the optimisation algorithm. E.g., if genetic algorithm is used to minimise the energy demand of a building, the population and corresponding objective functions' values should be saved for each generation. After the optimisation is finished, it is often possible to spot outliers (e.g., abnormally high or low energy demand) by analysing the collected intermediate data. Those outliers should then be analysed more thoroughly since they could represent the cases where the model failed to initialise or became frozen during energy simulation.
- Be aware of the differences in results caused by EnergyPlus versions. The default assumption is that newer versions are more reliable. The results obtained previously using an older version of EnergyPlus might need to be re-evaluated using a newer version.

The results of this work also suggest that there is still a need for the improvement of the existing hysteresis models as well as for the development of new ones. From the literature, it can be observed that while the theoretical and micro-level modelling of PCM is rapidly evolving [17,23,44–51], the practical implementation of those models in the building energy simulation software is lagging behind. Furthermore, it is also observed that when a new practical PCM model is introduced into EnergyPlus, the validation of this model is usually limited to a very small number of cases. E.g., the performance of the model is tested against one or a couple of PCM types, usually in the laboratory setting and using small-scale cases. Such a narrow approach to the model testing and validation possesses potential risks, that while the model performs well under selected conditions, it might not be the case if other PCM configurations, building case, weather conditions, etc., are considered. While it is understandable that extensive large-scale experimental testing of multiple possible PCM, buildings, and weather conditions for model validation is physically unfeasible, we encourage model developers to at least perform stress-testing of their models. For that, the model is run using a wide gamut of possible PCM parameters, EnergyPlus parameters, as well as using different building models and weather conditions, and the output of the models is cross-checked for consistency. Such testing could generally help uncover hidden and intermittent issues that might only appear under a particular combination of input and model parameters. Beyond the necessity for the further development of hysteresis models, EnergyPlus can also benefit from additional modifications that would allow to better integrate PCM models, improve user awareness and help uncover possible hidden and intermittent issues when they occur. Based on the performed tests and observations resulting from this study, we identify the following possible improvements that could be implemented:

- There is a need for an automated consistency check of the simulation results. At the moment, EnergyPlus has no tools to detect the intermittent issues that were described in detail in the Results Section 3.4.1 of this work. Those intermittent issues can be identified by, for example, monitoring the temperature of the nodes inside the PCM layer. If temperature does not change over a defined number of time steps, the simulation can either be terminated with an error, or the warning can be output into the console or EnergyPlus error file.
- Introducing the uncertainty levels of the results depending on which EnergyPlus components are used. Some of the components included in EnergyPlus are more refined and thus have lower uncertainty, while others (like PCM hysteresis modelling) are more experimental and high-uncertainty. If the user is warned when using a module with high uncertainty, it might help raise their awareness and encourage a more thorough and critical evaluation of the simulation results.
- Better documentation of relevant EnergyPlus parameters is necessary for practitioners, as well as for advanced users and model developers. This applies to both user-definable parameters as well as built-in parameters that can only be modified by changing the source code and compiling a custom version of EnergyPlus. For the user-definable parameters, while the documentation typically provides basic definitions, it often lacks more detailed but necessary information, such as how default values are selected, when they should be changed, and how different parameters are interconnected and influence each other. For example, it is acknowledged in the EnergyPlus documentation that the relaxation factor and inside face surface temperature convergence criteria of the CondFD algorithm should be changed if numerical instabilities are detected. However, the documentation does not mention in which cases the default values might be insufficient, what exactly the numerical instabilities imply, and how they could be detected. Furthermore, the impact of the space discretisation constant on numerical stability or its connection to other stability-impacting parameters is not addressed in the documentation at all. Improving the documentation of the relevant parameters will improve user awareness, help users avoid model instability pitfalls, improving the reliability of the results obtained.

  For the built-in parameters that users cannot easily modify, the source code needs better documentation with an explanation of the relevant parameters and the reasoning behind the selection of their values, especially for those parameters that have a high impact on the simulation results and model stability. One such parameter is the initialisation temperature that has been shown in this work to have a major impact on model stability in some situations. Yet, this parameter is introduced in the code without any description and is not mentioned in the documentation either. Providing better code documentation would help the researchers and developers, and make the improvement of existing PCM models and the implementation of the new ones a significantly easier task.

From a broader perspective, the observed differences in the results obtained using different models have far-reaching implications for research and decision-making related to the use of PCM in construction and the potential benefits of PCM for energy savings. In case we see the benefits of PCM use from energy simulations, can we be sure that those are actual benefits and not the consequences of the PCM model selection and the parameters used? And since all the studies analysing the benefits of PCM to date are not harmonised and rely on a variety of different PCM models, EnergyPlus versions, and chosen simulation parameters, is it possible to make any conclusions at all about PCM applicability as an energy-saving material? In the current situation, there does not seem to be a definitive answer to these questions. It can be argued that conclusions about the benefits of PCM could be drawn from experimental studies that do not rely on computational simulations. However, as discussed before, those studies are limited, and it is hard to draw far-reaching and generalised conclusions based on them. The decision-making related to PCM use in construction is thus currently essentially a shot in the dark: the supporting information is scarce, uncertain, and often contradicting, yet decisions still have to be made.

5. Conclusions

This study highlights the critical importance of correctly modelling PCM hysteresis in full-building energy simulations. Four hysteresis models were tested and compared: the current built-in model, a corrected curve-switch model, and two implementations of a two-phase model. The analysis of the built-in hysteresis model uncovered a flawed implementation of the curve-switch logic, leading to inconsistent results during partial phase transitions. The corrected curve-switch model has fixed multiple issues of the original implementation and has been demonstrated to be stable, but remains limited by its simplified formulation and lack of experimental validation. The two-phase hysteresis model by Feng et al. provides a more realistic representation of PCM behaviour, but is susceptible to intermittent stability issues and is sensitive to the conduction finite difference algorithm settings. Additionally, the same two-phase model re-implemented in a newer EnergyPlus version produces results that diverge significantly from those of its original implementation, pointing to version-related inconsistencies. Furthermore, none of the available models currently supports the modelling of supercooling effects. These limitations highlight the urgent need for the improvement of existing hysteresis models, as well as for the development and integration of new ones.

The observed limitations and issues of PCM modelling emphasise the need for a more thorough and cautious approach to the simulation of buildings including PCM. It is important to check initial conditions and boundary definitions, since even minor changes can lead to significantly different results. The parameters of the CondFD algorithm should be carefully adjusted, and running a few test cases with varied PCM parameters can help detect issues and physical inconsistencies. Reducing the space discretisation constant and the relaxation factor, and increasing the number of time steps per hour, all tend to improve stability in most cases. The output variables for PCM nodes, such as temperature and specific heat, should be carefully monitored to ensure the consistency and reliability of the results. In the case of optimisation studies, saving intermediate results and their subsequent analysis can help identify outliers that might point towards intermittent issues. Finally, the observed differences between the results obtained from the same PCM model in different EnergyPlus versions might require a reconsideration of all PCM-related results obtained using older versions of EnergyPlus.

From the perspective of decision-makers, the current situation with PCM modelling is challenging. As this work has shown, the choice of the PCM model in EnergyPlus has a major impact on the results of simulations and, consequently, on the decisions related to material, component or building design. In some situations, when PCM is not expected to have a large degree of hysteresis (e.g., in the case of some organic PCM), it might be advisable to refrain from using hysteresis models and use a simplified but more reliable single enthalpy curve method. However, in the case of inorganic or encapsulated PCM that are characterised by higher levels of hysteresis, ignoring the associated effects might not be possible. If the number of necessary simulations is not large and the results can be manually validated for possible inconsistencies, the model by Feng et al. is the most advanced and realistic of the available options. However, due to the intermittent stability issues presented in this work, when there is a need to run hundreds or thousands of simulations in an automated manner (optimisations, sensitivity analysis, etc.), curve-switch might be a better alternative due to higher stability. It might also be advisable to use multiple models and compare the results before making final decisions. And no matter which PCM model is used, we encourage practitioners and decision-makers working with PCM in EnergyPlus to be critical, thoroughly analyse the simulation outputs, and take time with adjusting relevant parameters that might influence the outcomes.

EnergyPlus is an irreplaceable tool and NREL has done a commendable job developing it and keeping it open source for all the practitioners to use and build upon. However, like any other complex and actively developing open source project, it might have some issues and limitations. And while PCM modelling in EnergyPlus definitely requires more attention – especially since it is lagging behind the theoretical developments in the field – it is not only in the hands of EnergyPlus developers but also of the academic community to advance it further and make it more comprehensive, realistic, and reliable.

CRediT authorship contribution statement

Dmitry Zhilyaev: Writing – review & editing, Writing – original draft, Visualization, Software, Methodology, Formal analysis, Data curation; **Alejandro E. Albanesi:** Writing – review & editing, Software, Formal analysis; **M. Cecilia Demarchi:** Writing – review & editing, Visualization, Software; **Víctor D. Fachinotti:** Software, Supervision; **Hans L.M. Bakker:** Writing – review & editing, Supervision; **Henk M. Jonkers:** Writing – review & editing, Supervision, Funding acquisition.

Data availability

The files needed to replicate this study are found in the repository: https://doi.org/10.5281/zenodo.15320290

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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