Coupled Modeling and Monitoring of Phase Change Phenomena in Architectural Practice

Billie Faircloth¹, Ryan Welch¹, Yuliya Sinke², Martin Tamke², Paul Nicholas², Phil Ayres², Erica Eherenbard¹, Mette Ramsgaard Thomsen²

¹ KieranTimberlake
Philadelphia, USA
bfaircloth@kierantimberlake.com

² CITA Centre for IT and Architecture
Copenhagen, Denmark
martin.tamke@kadk.dk

ABSTRACT
Geometries designed with carefully controlled heat absorption and heat transfer profiles often elude designers because of the complexity of thermodynamic phenomena and their associated discipline-specific numerical models. This project examines the behavior and design of geometries associated with non-isolated thermodynamic systems by constructing a material prototype that is fully coupled to a mechanistic modeling interface. The prototype, a facade system of phase change materials, was mounted on an adjustable outdoor testbed. Its baseline geometry was continuously monitored over two seasons and characterized with respect to variation in liquid and solid states. The mechanistic model, which uses a finite element method, incorporates multiple components including geometry, orientation, material properties, context geometry (e.g. buildings and vegetation), weather, climate, and an array of sensors monitoring the real-time temperature distribution of the testbed and phase-change materials. Data were continuously collected from the testbed and used to calibrate, validate, and verify the mechanistic model. In turn, the calibrated mechanistic model provided a platform for the design of new facade geometries and predictions of their behavior. The project demonstrates an integrative modeling approach, orchestrating handshakes and feedback loops between disparate spatial and temporal domains, with the ambition of defining a cogent design framework for practices that are trans-scalar, trans-temporal, and trans-disciplinary.

Author Keywords
Thermodynamics; System boundaries; Phase change materials; Mechanistic model.

ACM Classification Keywords
D.1.7 Visual Programming; D.2.2 Design Tools and Techniques; I.6.4 Model Validation and Analysis.

1 INTRODUCTION
The architectural design community has difficulty integrating methods to manipulate, measure, and model transient phenomena associated with open thermodynamic systems. Phase transition, such as the melting from solid to liquid, is one of these observable phenomena. It is influenced by the nuanced interaction between geometry, context, material properties, weather, and the mechanisms of heat transfer. Whereas the assumption of steady-state conditions provides a well-defined system boundary to study heat transfer; and, whereas numerical and analytical approaches, such as finite element analysis (FEA), discretize heat flow at an unlimited number of points across a given domain in order to identify boundary conditions; these methods are associated with multiple scales and disciplinary-specific workflows [1]. They are limited in their capacity to handle dynamic information flows, presume an analytic, rather than generative, design approach, and are indicative of a complex, multi-scalar, and multi-method modeling and simulation challenge within the design community [8].

Actual material behavior is an entanglement of macro and micro interactions and extensive and intensive properties across spatial and temporal domains [12]. For instance, architectural material assemblies continuously accumulate and dissipate heat which engender small, large, symmetrical, and asymmetrical thermal gradients. Thermal gradients, which are likewise a transient phenomenon, are attributable to the interaction between environment, material properties, local surface features, surface geometry, and overall form. There is, thus, the potential to investigate a multi-scalar, multi-method design and modeling approach for architectural assemblies using methods from the fields of architectural design, thermodynamics, and materials engineering in which (1) using full-scale prototypes, the actual thermal behavior of a material system is continuously measured and characterized; (2) using a mechanistic model of coupled components and real-time measurement, the thermal behavior of the same system is simulated, calibrated, and validated; and (3) using a calibrated and validated simulation platform, designers can author and predict nuanced heat transfer profiles for new surface geometries, and thereby fabricate, measure, and characterize their performance.
Here we present results from a six-month study that implements this modeling approach using organic, paraffin wax phase change materials (PCMs). PCMs undergo a phase transition from solid to liquid, and conversely liquid to solid, at a designated temperature. In doing so, PCMs are capable of maintaining that temperature while absorbing or releasing large quantities of energy. In architecture, PCM-based thermal energy storage systems seek to reduce overall building energy use, reduce peak energy loads, minimize HVAC system sizing, and improve overall thermal comfort [2, 4, 10]. Experimentation with PCM-integrated elements, including walls, floors and ceilings, are systematically reviewed in the literature [3, 6, 13]. PCM applications include microencapsulants (10 - 1000 µm spheres) mixed with materials such as gypsum to create wallboard, or cement to create mortar [7, 9]. They also include macroencapsulants (≅ 4cm x 4cm x 1cm bars) integrated into climate management layers such as the commercially available BioPCM®. PCM glazing experiments include encapsulation between several glass or plastic layers and incorporation into slats, louvers, and shading fins [11].

Ours is a non-normative application of PCMs: they are bulk-cast into formed panels and exposed to direct solar radiation and extreme differences in temperature. While absorption and release of energy is the primary interest of PCM wall applications, our interest in PCMs stems from their capacity to act as a visual register of thermodynamic behavior and, correspondingly, as a tool for qualitative validation of predictive modeling methods. Used thus, they offer the possibility to connect behavior at the material scale to a nested series of larger length and time scales; and the opportunity to calibrate, via design, these larger scales to steer phase transitions within the PCM for the purpose of achieving particular desired visual effects and expressions.

2 METHODS

In order to study the relationship between model geometry and PCM melting behavior, an adjustable apparatus consisting of 23 rhombic panels was fabricated, assembled, and monitored on-site in Copenhagen, DK for a period of six months. An accompanying digital mechanistic model was developed to form predictions of melting behavior based on empirical data for internal calibration.

2.1 Panel Geometry

Variations in panel geometry were explored to test the hypothesis that local differences in the quantity of PCM (in terms of surface area to volume ratio) and exposure to solar radiation should yield measurable differences in the local rate of melting. Five panel designs were developed as mesh geometries in Rhinoceros3D using the Grasshopper visual scripting environment. A baseline geometry was established based on a bi-directional sinusoidal pattern applied to the outside surface, with a total depth of 40mm. Two variations employed horizontal and vertical displacements, respectively, to the baseline pattern in order to study the effect of varied solar exposure on melting behavior, under the constraint of constant PCM volume. A third variation reduced the amplitude of the sinusoidal pattern by 50%, and a fourth variation reduced the overall scale of the sinusoidal pattern in all dimensions by 50%.

These last two variations permit study of how volume and surface area influence melting behavior; each has half the overall PCM volume of the baseline, while the latter has significantly greater exposed surface area than the former.

Figure 1. Panel geometries: (top row, l-r) baseline, horizontal shift, vertical shift, (bottom row, l-r) shallow, dense.

2.2 Panel Fabrication

To encapsulate the fluid volume of each PCM panel, a vacuum-formed thermoplastic shell was constructed. Panels were assembled from two layers of 1mm thick Vivak® polyethylene terephthalate glycol-modified (PETG) sheet. PETG was selected based on its ability to take on complex geometries when thermoformed and for its visual transparency, which permits direct visual observation and video recording of melting behavior. The outer layer of each shell was thermoformed onto a medium density fiberboard (MDF) surface, milled to form the positive of the digitally-modeled PCM pattern. After thermoforming, the outer layer of PETG was heat-press bonded along its perimeter onto a flat, inner PETG surface, and additional mechanical through-fasteners were added periodically at sinusoidal valleys to prevent buckling under static PCM pressure.

Two types of PCM, Rubitherm® RT 6 and RT 10, were selected for study based on nominal melting points of 6°C and 10°C falling slightly above typical dry bulb temperatures experienced in Copenhagen during the initial study period. Hence, the combination of daytime solar radiation and nighttime conductive heat loss would offer a high likelihood of complete cycling between solid and liquid state over a typical 24-hour period. The two PCM types were distributed
among the 23 panels such that every unique combination of panel geometry and material occurred at least twice.

One panel of each unique type was furnished with an array of Maxim DS2438 1-Wire™ temperature sensors (±0.5°C accuracy) to monitor the state of the PCM over the duration of the experiment. Sensors were conformally coated to protect from moisture, affixed to the interior of the panel with epoxy cement, and wired with conductive tape to an interface port at the edge of each panel for connection to a Wi-Fi enabled node.

2.3 Testbed and Instrumentation
Encapsulated PCM panels were mounted to the front face of the adjustable testbed enclosure and placed in an exterior courtyard where they remained for the duration of the experiment. The testbed measured approximately 1.2m x 2m x 2.5m and consisted of a plywood frame with infill expanded polystyrene (EPS) foam insulation. The frame was affixed to a plywood and polyisocyanurate (PIR) foam base that was anchored to earth screws and sat slightly above the ground. The base incorporated a horizontal hinge along its front face to permit changing the vertical orientation of the PCM panels. This allowed incident solar radiation to be maximized in response to changing solar altitude across seasons. The narrow ends of the testbed were sealed with Thinsulate™ fabric to permit maintenance access to the otherwise fully enclosed interior. As the interior was unconditioned and normally unoccupied, it operated in a passive, free-run condition based on climatic forces.

A second set of 19 1-Wire temperature sensors was arrayed across the inside face of the PCM panels and throughout the
testbed interior to monitor the interior environment of the apparatus and its contribution to PCM melting behavior.

The array of temperature sensors was connected to a Wi-Fi-enabled node running Pointelist®, an ecosystem for wireless collection of high-density sensor data. The node logged readings from each sensor in five-minute intervals and sent data to the Pointelist web API for subsequent viewing and analysis.

Ambient conditions at the testbed site were monitored by a local weather station (Ambient Weather® WS-1400-IP) and reported to the Personal Weather Station service of Weather Underground. This device was mounted adjacent to the testbed at a 4m elevation and gathered various relevant quantities, including dry bulb temperature, humidity, wind speed and direction, and total horizontal radiation.

A time-lapse camera (WansView®) was mounted in front of the testbed to monitor changes in PCM state, direct sunlight, and cloud cover in five-minute intervals to coincide with temperature recordings.

### 2.4 Mechanistic Model

A mechanistic model was developed to predict the behavior of PCM under varying environmental conditions and calibrate predictions against observed behavior. The model comprises a series of custom Grasshopper components that cover the following modules: climate, context, sensor, material, geometry, simulation, and results.

The climate module describes the ambient environmental conditions surrounding the physical testbed in terms of dry bulb temperature, wind speed, diffuse horizontal radiation, direct normal radiation, and solar angle. These are sourced variously from typical meteorological data, airport data, and local weather station data, depending on the time-frame of the simulation and the availability of data from each source.

The context module represents the geometry of neighboring structures and vegetation that would potentially shade the physical model from direct or diffuse radiation. It accounts for both permanent structures and vegetation with a variable shading coefficient.

The sensor module connects the mechanistic model to the array of temperature sensors describing the interior conditions of the testbed as well as to the sensors embedded within the PCM medium. The former serves to define the interior boundary condition of the simulation while the latter serves as calibration points against which the predicted behavior can be validated.

The material module describes the thermodynamic properties of PCM for use in the run-time simulation. These include the heat of fusion, melting point range, and liquid-and-solid-state properties of density, heat capacity, thermal conductivity, and albedo.

The geometry module translates the bounding surfaces of the encapsulated PCM form into a 3D polyhedral finite element mesh, whose resolution may be defined through an input parameter. The module pre-computes the direct and diffuse shading coefficients for each mesh face of the exterior boundary, which frees the run-time simulation from the burden of occlusion calculations. Neighbor-neighbor relations are automatically generated so that at any point during the simulation, the heat flow between neighboring elements may be computed based on the local temperature gradient and the area of their common face and cached at each time step. Due to the nonlinear diffusion behavior in the phase-change regime the complete set of heat flows are calculated at each time-step and subsequently applied to each element, which—depending on the element’s current phase—may have the effect of changing its temperature, phase, or both. Hence storing the heat flows independently permits parallelization of the run-time computation.

![Figure 6. Grasshopper components of mechanistic model](image-url)
2.5 Interaction Between Testbed and Model
The mechanistic model serves a dual purpose: it offers a platform for design iteration and material selection; and it provides a means of validating its predictions using empirical data gathered from sensors embedded in the PCM medium. Prior to engaging in physical prototyping, one may begin with a set of preliminary simulation settings (e.g. spatial and temporal resolution, time frame, etc.) and simulate the expected behavior of a given PCM, geometry, and siting. Based on initial predictions one may choose to modify material properties, such as selecting a PCM with a higher melting point or greater heat of fusion. Alternatively, one may choose to modify geometry or siting to enhance the frequency and variety of predicted melting behavior in response to design goals. Likewise, one may compare the relative effects of systematically changing geometric properties (depth, surface area, or orientation) in order to guide the refinement and selection of panel types for subsequent fabrication.

Following a phase of prototyping and data collection, the time-series temperature values predicted by the mechanistic model are compared to the corresponding empirical temperature data collected by the calibration sensors embedded in the PCM medium. Standard deviations between predicted and observed behavior are calculated automatically within the simulation component, provided calibration sensor data is available for the chosen time period. Hence, numerical refinements to the material properties and simulation settings may be automated through optimization tools such as Grasshopper’s Galapagos GA solver. Where numerical refinements fail to resolve differences between predicted and observed behavior, time-series graphical comparisons and video footage are employed to discover systematic deviations due to real-world phenomena not adequately represented in the model (see further discussion of buoyant effects).

Findings from this calibration exercise establish the range over which the mechanistic model yields accurate predictions and thus permits further design iteration and material selection. Thus, one can alternate between these two modes of operation with each series of prototypes.
3 FINDINGS AND DISCUSSION

Two sets of experiments conducted between March and September of 2017 attempted to prove the viability of the design and calibration workflow described above.

3.1 Initial Experiment

The initial experiment using the five aforementioned panel types was conducted from March 15th to April 18th, 2017 and attempted to validate three hypotheses: different PCMs should exhibit similar patterns of melting in panels of the same geometry, but at distinct temperatures and times; variations in panel surface geometry should exhibit local variations in melting rate; and the mechanistic model should correctly predict these trends.

Time series temperature data and video recordings confirmed that panels containing RT 6 PCM exhibited melting behavior before their counterpart panels containing RT 10, which has a higher melting point temperature. While the precise duration of these phase transitions differed slightly between predictions and observations, the mechanistic model correctly predicted the start time of melting in both cases as well as the relative difference in complete melting between the two materials.

At the local scale of the surface texture, it was observed that the melting occurs first at the shallowest areas of the panel. This behavior is expected because these regions have the highest surface area to volume ratio, and hence the least heat capacity per unit of conductive and radiative heat gain. This observation was also correctly predicted by the mechanistic model.

By extension, the shallow panel types (4 and 5), which contain less PCM per unit of surface area, completed melting significantly earlier than the other three panel types. Embedded sensors inside the PCM also confirmed that the shallower panels exhibited a higher rate of temperature change than their deeper counterparts during these phase transitions.

Comparison of the deeper panel types, which differ in the displacement rather than depth of sinusoidal pattern, yields less pronounced differences than in comparison to shallower panels. Since these three panel types have approximately equivalent surface area and volume, their principle difference lies in the orientation of particular surfaces toward or away from direct sunlight. Hence, the differences ought to be perceived only at a highly localized scale, not comprehensively for an entire panel. Indeed, footage reveals that the panel with a vertical shift, which has roughly half of its peaks oriented with a broad surface toward midday sun, begins melting somewhat earlier than the other two panel types.

One important feature of the observed behavior that was not captured in the mechanistic model was the buoyant convection of the liquid PCM during the later stages of the melting regime. The PCMs under investigation exhibit significant thermal expansion when they transition from solid to liquid. At the onset of melting, this is not problematic because the liquid is confined to small regions and the surface texture remains the dominant factor driving melting behavior. However, as more of the material transitions into the liquid state, the buoyant effects begin to dominate as the lower density liquid finds a continuous path for rising to the top where it accelerates the melting of any residual solid PCM. At this point, any trace of effects due to panel geometry is confined to the bottom of the panel where solid material remains.

While in principle, the finite element method employed in the mechanistic model could be extended to consider buoyant convection, the visual effects of this buoyancy were considered undesirable, and in subsequent design iterations (discussed further), effort was made to compartmentalize the PCM medium and limit the degree to which liquid-state PCM could rise to the top.

In contrast to melting behavior, the process of solidification was much more gradual and uniformly distributed throughout the PCM medium, suggesting little dependence on surface geometry. The solidification regime was characterized by local crystal formation throughout the PCM, suggesting that the liquid medium was at internal equilibrium prior to changing phase. This can be understood...
based on two observations: the liquid state permits more rapid heat diffusion via convective flow; and the nighttime ambient temperatures tend to fall gradually compared with the rapid daytime temperature rise brought on by solar radiation. Furthermore, it is likely that microscopic effects below the resolution of the FEM contribute to the observed hysteresis, as observed by others [8]. Due to this feature, and the fact that solidification typically occurred at night when no one was present to observe it, further analyses and design iterations focused exclusively on melting behavior.

3.2 Model Verification and Calibration

Model verification was performed in the results module of the mechanistic model. Following each simulation, a graph of predicted and observed behavior was generated to identify systematic variations at each calibration sensor location. In the solid phase and during the initial melting, these graphs typically showed agreement between predicted and measured values within the reported accuracy of the sensor. However, wider discrepancies arose toward the end of the melting regime and persisted throughout the liquid phase. The initial deviation is likely due to the aforementioned effects of buoyancy, which were observed in the physical testbed but not represented in the mechanistic model. Subsequent deviations in the liquid phase tended to show that measured values were significantly higher than predicted. One possible explanation for this observation is the sensors may be exposed to direct solar radiation in the liquid phase due to the transparency of the PCM. Hence, measured values may not accurately reflect the local temperature of the medium.

3.3 Model Conversion

Following calibration of the mechanistic model and determination of appropriate simulation parameters and range of predictive capacity, a second round of design iteration was conducted. In order to maximize the frequency and duration of the melting phase and to account for the warmer season of this experiment, Rubitherm RT 18 HC was selected as the PCM for all 23 panels. This material has a nominal melting point of 18°C and a higher heat of fusion (260 kJ/kg) compared to both RT 6 and RT 10 (160 kJ/kg). This study began with a routine for linearly varying PCM depth as a height-field based on distance from a set of control points, resulting in a form resembling a voronoi diagram. The mechanistic model predicted that melting would begin at each control point and expand radially. Indeed, this behavior was observed at the onset of melting. However, the continuity of the PCM material in this panel geometry exacerbated the buoyant effects observed previously.

A subsequent exercise attempted to explicitly resolve the top-down melting of the voronoi experiment by compartmentalizing the fluid volume and limiting buoyant flow. It also sought to demonstrate more refined design control of material behavior by introducing a set of panels whose variation was not apparent in the exterior form, but revealed itself through the melting process. Therefore, the inner surface of PETG was thermoformed to establish varying material depth while the exterior surface was molded to a uniform cross-hatch. Under this modification, the testbed appears undifferentiated in the solid phase, while the melting reveals transient directional patterns of dashes and dots according to varying depth of the inner surface. Four panel types incorporating variations on lines, dashes, and dots were

![Figure 13. Validation of melting behavior for panel type 4.](image)

![Figure 14. Voronoi panel with sequential predictions of radial melting behavior](image)

![Figure 15. Array of panels types whose melting behavior intends to reveal lines, dashes, deep dashes, and dots.](image)
distributed across the testbed and monitored from June through September of 2017.

The results of this concluding exercise were largely successful. Melting occurred first in the intermittent regions of minimal material depth, leaving behind discontinuous patterns of solid material. Thus, for the brief period of melting, the selected patterns were observable at the scale of the entire 23-panel facade.

**Figure 16.** Variations in panel behavior in situ as compared to simulation.

### 4 CONCLUSION

A multi-scalar, multi-method design and modeling approach couples the behavior of full-scale material prototypes to a mechanistic modeling framework through continuous cycles of measurement and calibration. This approach recognizes that material behavior cannot be accurately captured, controlled, or manipulated through a single disciplinary method and that physical prototyping and simulation can work together to integrate multiple methods. This research is motivated by the aim to provide designers with the means and methods to work directly with complex transient phenomena, such as heat transfer, which normally lie beyond their purview. Individuals with backgrounds in architectural detailing, architectural computation, computer science, chemical physics, materials engineering, and sculpture jointly engaged processes to author surface geometry and predict PCM melting behavior.

A mechanistic model can be internally calibrated and remain only partially validated due to its inability to account for all transient behavior. Comprehensive modeling of PCMs remains a formidable challenge [5]. A highly localized process of phase change is driven by heat transfer mechanisms that occur at multiple scales. On account of the complexity of these phenomena and the non-standard and dynamic conditions of our application, our mechanistic model did not attempt to address buoyancy effects or sub-millimeter scale heat transfer. This points to conditions that must be placed on mechanistic model specifications, and to the value of continuous observation in building tacit knowledge of material behavior. Control of transient behavior was achieved to a degree, indicating opportunities elsewhere for designers to engage in complex modeling and feedback through the coupling of models and prototypes.

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### REFERENCES