Optical and Thermodynamic Relationships of an Emerging Class of Organic Phase Change Materials

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Abstract: Architects, building scientists and sustainability engineers are committed to lowering energy consumption and decreasing carbon footprint while increasing the qualitative human experience of the built environment. This paper summarizes a set of design prototypes that characterize the thermal and visual nature of an emerging class of organic phase change materials (PCMs) with high thermal storage density. A novel packaging system designed for liquid to solid phase transition is described that reveals the intrinsic qualities of PCM's by making nucleation and crystal growth patterns visual during transition. The current design extracts the PCM from its normative location within the wall section and positions the material as a separate element for application on the interior of curtain walls. It is envisioned that this application, in addition to providing effective thermal self-regulation and lowering the reliance on mechanical conditioning, can engender occupant behavioral change towards energy consumption. This argument is based on the connected domains of sensory pattern recognition, reasoning and decision-making as the sustainable technology is made visible. A case study is also presented with the quantitative energy results of PCM application.

Keywords: Thermal storage, phase change material, design, environment, social impact

1 INTRODUCTION

Sustainability research in architecture increasingly relies on high-technology solutions to lower overall carbon footprint and energy use. Less studied and perhaps more effective, are inquiries that draw upon the intrinsic qualities of responsive materials and advance the prospect of architecture to act passively in response to environmental fluctuation. The history of building has historically embodied sensitive building siting, climatically appropriate building form and local material sourcing to achieve a symbiotic relationship with the local environment. Knowledge to construct environmentally responsive buildings has traditionally been local, derived from regional practices and handed down over time. Until relatively recently, nearly all construction revealed directness to geography, climate and by extension, the progression of cultural values. In this rich history of tuning building technology to local conditions, there is experiential evidence that construction technique in tandem with the sensorial qualities of building materials have been an important agent of human cultural development. Arguably, it is our relationship with architecture and the environment that enables shifts in understanding, imaginative speculation, informed decision making and behavioral change. A goal of this study is to continue this cultural and technological trajectory through visual engagement with thermally reactive phase change materials (PCMs) to instill an awareness of the thermal cycles of our local environment. This premise arises from a lineage of ecological thinking and is insightfully expressed in architect Richard Kroeker’s words: “In a context dedicated to the notion of progress, as measured from the distance covered from the point of origin, we risk losing contact with origins.”

The etymological origin of technology comes from the Greek root “technē" meaning artful and skillful, and in Classical Greece, technological achievements in the building arts embodied beauty as an ideal. This was a time before the western separation of art and science, and prior to the separation of intellectual and physical dexterity. Technology was seamlessly intertwined with design and served as litmus for the state of cultural prowess of a nation. Contemporary building technologies have evolved that sense our presence, monitor our biorhythms, anticipate our climatic expectations and deliver an appropriate quantity of mechanical condi-

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tioning to suit our needs. In this experiment, we are left to wonder if there is a behavioral and cultural consequence of separating ourselves from the tangible nature of technology.

In Heidegger’s words, it is far more useful to reveal the essence of technology than to hopelessly rebel against it. The attitude adopted in this study is not cautionary, but rooted in the essence of technology. A position is taken that the end of modern sustainable building technology is not solely human comfort and environmental best practices but a nuanced understanding of our relationship to the environment. As humans, we derive deep knowledge and understanding of our environment through direct experience; it is this depth of experience - through contact and observation - that we interact with the world fully. In this study, techne is a material lens that can serve to amplify direct experience.

2 MATERIAL PROPERTIES AND CHARACTERIZATION

PCMs are classified as materials with high heat of fusion with the ability to transfer substantial amounts of energy during liquid/solid phase transition. Sometimes described as thermal batteries, PCMs serve as energy storage sources similar to thermal mass in buildings, though are far more effective than stone or concrete per unit volume. The main advantage of PCM occurs upon phase transition when significantly more energy is absorbed/released than in traditional high-mass materials (see Figure 1). During phase transition the bonding energy between molecules varies while the average kinetic energy remains constant resulting in constant temperature. In the case of most high-mass materials, heat is transferred linearly until their melting point is reached. Then, there is a significant increase in latent heat storage capacity, as the addition of heat to a substance causes an increase in temperature or a change in phase. High thermal energy storage capacity per unit volume is driving PCM development for building application in regions with high diurnal temperature swings. A thermodynamic property of materials that undergo phase transition is the characteristic to maintain near constant temperature during the absorption and discharge of thermal energy, thus contributing to thermal balance when used in building applications.

Traditional thermal mass materials, such as concrete or water, either do not undergo phase transitions or the melting point is too low to balance interior temperatures. The properties of two commercially available organic PCMs, one manufactured from fatty acids (BIOPCM) and the other from paraffin (Rubitherm), are shown for comparison in Table 1.

Table 1. Differing properties of commercially available PCMs (fatty acid and paraffinic) and water

<table>
<thead>
<tr>
<th>Property</th>
<th>BIOPCM</th>
<th>GR27</th>
<th>Water</th>
</tr>
</thead>
<tbody>
<tr>
<td>Melting Point (°C)</td>
<td>29</td>
<td>28</td>
<td>0</td>
</tr>
<tr>
<td>Density (kg/m³)</td>
<td>860</td>
<td>710</td>
<td>1000</td>
</tr>
<tr>
<td>Specific Heat (kJ/kg)</td>
<td>1.97</td>
<td>1.125</td>
<td>4.179</td>
</tr>
<tr>
<td>Latent Heat (kJ/kg)</td>
<td>219</td>
<td>72</td>
<td>334</td>
</tr>
</tbody>
</table>

2.1 Types

PCMs are classified as exhibiting solid-liquid transitions and further as organic or inorganic. The inorganic materials are salt-based and the organic are composed of paraffin or fatty acids. The melting point, heat of fusion, thermal conductivity and density are key contributors to the value of PCMs for building technology applications. Significant literature exists on the comparison of different materials and the main issues surrounding PCMs are their cost, toxicity, flammability, corrosiveness, chemical instability, fatigue life and knowledge base. New companies, including developments at
Oak Ridge National Labs, have produced fatty acid PCMs that address the above concerns, and notably they are considerably less flammable than paraffinic types. Current manufacturers are packaging organic materials that perform well in flame-spread tests and have a reduced smoke index and toxin release relative to a comparable wall without the PCM product. Organic PCMs are less corrosive and more chemically stable than salts, melt more evenly and have proved to have a very low freeze/thaw fatigue cycle rate, increasing their durability and reliability in building products. A key material advancement has been targetable melting points, thus increasing PCM application to diverse building types. These attributes contributed to specifying organic PCMs for this project.

2.2 Encapsulation

To be used effectively in buildings, PCMs are either micro or macro-encapsulated. Micro-encapsulation is the method of trapping the material (typically a 1-3 mm sphere) within a polymer skin that contains the material in both solid and liquid phases, enabling the PCM to be added to concrete or plaster, and giving the new composite material heightened latent thermal storage capacity. Plaster with embedded microencapsulated PCMs has been commercially available since 2004 and much research has been conducted on the application of the material to concrete, gypsum wallboard, particleboard, cellulose insulation and composite roofing systems. Macro-encapsulation is the practice of encapsulating significant amounts of PCM within a single container. This method is becoming more viable with the emergence of organic PCM with low corrosive properties (Zalba et al. 2003), making container composition less exacting and degradation less of an issue. In both instances of micro and macro-encapsulation the material operates in the background and the phase change attributes are not visible. In the current study, a wall system is proposed that reveals the visual properties of PCMs by removing them from traditional encapsulation methods and containing them between glass sheets.

2.3 A Note on Composition, Nutrition and Transportation

Most commercially available organic fatty acid PCMs are composed of palm oils. Palm oil is derived from the fruit of palm trees, does not contain cholesterol and is common used as cooking oil throughout much of Southeast Asia, Africa and Brazil. Palm oil is also used for biodiesel and a 2007 Malaysian law (80% of all palm oil is produced in Indonesia and Malaysia) directed all domestic diesel fuel to contain a 5% minimum of palm oil; this is commensurate with the global shift to turn food products into fuel. The food vs. fuel debate has proponents on both sides with some scientific estimates claiming that there is potential to increase palm oil production to meet both nutrition and transportation needs. This is tempered by the World Food Programs’ estimate that 1/6 of the world population is underfed. This again is countered by the fact that there is enough overall supply of food though many do not have the land to grow or income to purchase food according to the World Hunger Education Service. One certain statistic is that significant tropical deforestation is occurring as a result of the demand for palm oil. These thoughts are conveyed as it is necessary for architects and building scientists to make ethical choices in materials specification as the embodied energy, carbon footprint, chain of custody and material ethics are often variable or difficult to track.

3 PROTOTYPES AND OBSERVATIONS

Organic PCMs are characterized by their low thermal conductivity (0.2 W/m/K) and it is this property, in combination with an interest to make the phase change visible, that underlies this study. To address the issue of conductivity, the material is packaged with a high ratio of PCM to air contact and this condition allows the visual properties of the material to emerge. It was observed that the organic PCM transitioned from opaque to near clear at the melting point and ideas were generated about the potential of this temperature controlled optical “switching” action. During the construction of the prototypes, it was also observed that nucleation and crystal growth could be both directed and made macroscopically visible by adjusting the dimension of the PCM within the container. The purpose of this ongoing study is to characterize the relationship between crystal nucleation, crystal growth and thickness of the PCM.

Prototypes were constructed to gain a working sense of the potential of the material and the PCM was packaged to better visualize phase transitions. Prototypes 1 - 4 are constructed from three sheets of acrylic, two outer layers and one variable interlayer ranging in thicknesses from 2.5 mm - 7.5 mm. Each chamber is filled with organic PCM with a thermal storage capacity of 209 joules/gram (i.e., 198 Btu/kg). The thickness of the interlayer determines the thickness, volume and thermal storage capacity of the prototype.

It was expected that rate of crystallization would vary relative to the thickness of the PCM. This was the case as seen in time difference in prototypes 1-3 as shown in Figures 2, 3 and 4. It is speculated this could be applied to varying rates of temperature-dependent opacity of building envelopes when the “PCM tiles” are positioned on the interior of a glass façade, the intended location for this work. It was expected that the manner in which crystallization occurred and the resulting visual effect would vary as a result of the thickness of PCM material within the container. This was not the case, though prototype 2, at 5 mm interlayer, has
smoother crystalline transition boundaries than prototypes 1 and 3. It is possible that this prototype has less contaminants on the inner acrylic surface and therefore less nucleation sites enabling a more even crystal growth pattern. In all cases the PCM material was poured into the chamber in its melted state then allowed to freeze. Crystallization began at the bottom and progressed upward in response to the thermal vari-

Figure 2. Prototype 1, 2.5mm interlayer, Organic PCM, Specific Heat 197 kJ/kg, Melting Point 29 °C, 6-minute transition

Figure 3. Prototype 2, 5mm interlayer, Organic PCM, Specific Heat 197 kJ/kg, Melting Point 29 °C, 9-minute transition

Figure 4. Prototype 3, 7.5mm interlayer, Organic PCM, Specific Heat 197 kJ/kg, Melting Point 29 °C, 15-minute transition
ation in the chamber.

Initial experiments with prototype 4 show a dendritic crystalline growth pattern (see Figures 5 and 6). The material is slightly different in formulation that the PCM in prototypes 1-3, containing an additive that supports a solid/gel phase change as opposed to a solid/liquid transition. The prototype also shows the propensity of the material to nucleate at predetermined sites, increasing the overall rate of crystallization. In order for a liquid to crystallize (transition from liquid to solid) it must first nucleate. In the simplest of case homogenous nucleation, crystals form without a "seed" or specific nucleation site. The introduction of an impurity, or seed, causes directed nucleation and is known as heterogeneous nucleation. After nucleation, crystal growth emerges at a macroscopic level. It is assumed that for all prototypes, most nucleation is heterogeneous due to the significant surface area of the PCM in contact with the container, which contains microscopic imperfections. The presence of more nucleation sites increases the rate of total crystallization, which increases the rate of latent heat absorption. The transition from clear to opaque is shown in Figure 6.

3.1 Usefulness

The current study is aimed towards interior standalone encapsulation systems that visually demonstrate

![Figure 5. Prototype 4, 2.5mm interlayer, Organic PCM, Specific Heat 197 kJ/kg, Melting Point 29 °C](image)

![Figure 6. Prototype 4, Time-lapse close-up dendrite crystallization](image)
the crystalline behavior of the PCM. It is speculated that these systems could have a high adoption rate by providing a cost-effective complement to existing energy-related building retrofit strategies. The application of PCM retrofit technology has been proved to contribute to building energy balance. Application of PCM in cooling dominated climates (roof/floor/ceiling - location Phoenix, Arizona) has been shown to lower heating and cooling loads. Muruganantham et al. (2010) demonstrated a reduction in overall energy consumption by 25% and a shift of peak loads to off-demand times.

3.2 Solid State

Many designers are working in response to the trend of increasing complexity in building technology in favor of simple and effective mechanics that visually communicate their mode of operation. As solid-state materials, PCMs exhibit reliability and durability, two important factors for the successful adoption of new building materials. As designers, we are often engaged in applied research and are “middle users” of technology, neither the inventor nor the selector from a catalogue, but active in furthering the potential of basic research. This widening area of sustainable materials research offers potential for architects and building scientists to tune the compelling visual attributes of solid-state materials to specific outcomes (structural, optical and/or thermal) and advance the communicative potential of energy efficient building technologies.

4 CASE STUDY

The PCM system illustrated by the initial prototypes is planned for inclusion in the new Frick Park Environmental Center in Pittsburgh, Pennsylvania as a strategy to help meet the energy petal of the Living Building Challenge. Simulations were run in the US Department of Energy’s Energy Plus (version 6) to help quantify the energy savings associated with PCM application. The default PCM data embedded within Energy Plus was reconfigured to meet the PCM manufactures specifications, as they are significantly higher in terms of energy density. The energy model evaluates the PCM’s effectiveness at maintaining a thermal comfort temperature range of 20-25 °C during the heating and cooling seasons for the heating dominated Pittsburgh climate (see Figure 7).

The enthalpy versus temperature curve of the organic PCM provided by manufacturers, was added to the Energy Plus simulation, and indicates that the material out-performs salt hydrate or paraffinic materials. At this early stage of design, the simulation results verified that the first cost of the PCM is worth the investment given the improvement of energy performance of the building, especially during the long heating season of Pittsburgh. For the model, PCM was applied to the interior surface of the south façade (see Figures 8) (area 18.5 m²) at 6.35 mm thickness. Initial results indicate that PCM application on the south façade reduces annual heating loads by 10-15% reduction in and a 5-10% reduction in annual cooling loads. More refined analysis predicted 13.8% reduction in annual heating load.

![Figure 7. Annual temperature profiles for Pittsburgh](image)
5.2% reduction in annual cooling load (Clifford and Jones 2012). The addition of PCM along the south facade allows for a 10% reduction in mechanical system sizing and subsequent reduction in energy use by that system. Downstream, lowering reliance on the mechanical system, translates to a reduction in the photovoltaic array size for the building.

4.1 Behavioral Change

Writer Susan Griffith has expressed that “though it is the nature of the mind to create and delineate, and though forms are never perfectly consonant with reality, still there is a crucial difference between a form which closes off experience and a form which evokes and opens it.” This observation recognizes the latent power of architecture which is the speculative component of this study. The PCM modules could serve as environmentally responsive cues that trigger awareness of architectural thermodynamics, and heightened awareness of our surroundings can influence attitudes toward energy consumption and contribute to the transformation of social norms that influence individual behavior. The theory that reasoned behavior combines intent, attitude and social norms as indicators to predict behavior (Fishbein and Ajzen 1975; Ajzen and Fishbein 1980) has been proved valuable to predict consumer intent in the field of product marketing. In terms of behavioral change towards energy consumption, it is imperative that occupants become aware of measures they can take to maintain physiological and psychological comfort while consuming less energy. It is speculative intent of this work that awareness and understanding of our interior environment is central to shift our attitudes toward consumption. If one of the goals of education itself is behavioral change, then perhaps the visualization of building technologies will contribute to a heightened environmental sensibility.

4.2 Thermal Delight

Constructing temperate interior environments recalls the very source of architecture itself and solar driven sensible thermal storage has played a key role in vernacular design strategies. Over time, and in nearly all climates, buildings have become lighter, more layered and more transparent, and have traded their mass for insulation. The thermal consequence of lightweight construction is increased susceptibility to diurnal and seasonal temperature swings, and thermal effectiveness, that is, the technological trend towards lightness demands low air infiltration, high R-value and on-demand heating/cooling sources. Before the advent of centralized and distributed mechanical heating, direct radiation was the primary source of warmth, either from fire, other warm bodies, or the sun. Associated social behavioral patterns emerged from the direct proximity of these thermal sources. An example is the Japanese Kotatsu, dating to the 14th century, which is simply a low table fitted with a blanket and a heating source under the tabletop. The Kotatsu generates a local thermal zone that, similar to the hearth, satisfies our need to maintain temperature and provides for the intimacy of social interaction. In contrast, it is generally acknowledged that reliance on technologically sophisticated heating, ventilation, and air conditioning systems has distanced both designer and inhabitant from direct association with the nature of a thermal source. Many argue that reliance on mechanical conditioning decreases social interaction and disassociates us from the environment itself.

This acknowledgement is drawn from Lisa Heschong’s critical analysis of heating technology in her book “Thermal Delight in Architecture” (Heschong 1979). Heschong perceptively observes that humans have a “thermal” sense independent from all others but most often associated with the sense of touch and that
not only is this sense real, it is also highly sensitive. She goes further to refer the sensorial interconnectedness and cites instances when the triggering of one sense heightens others. Continuing, she characterizes our social and imaginative estrangement as the result of a loss of contact with physical phenomena, specifically as a result of modern building thermal control. The current study attempts to reverse this trend by tapping the properties of responsive materials to make building technology more visually communicative of thermal ability.

5 CONCLUSIONS

In science, we have sought to eliminate subjectivity via increasingly accurate measuring devices that stand in for the senses, and to effectively control for the relativity of human perception. Sensorial, cognitive and cultural biases in architecture, on the other hand, are arguably significant drivers in the design process. The position of this study is to engage cognitive biases and address the cultural consequences of technology by engaging building users in the combined thermodynamic and visual properties commercialized organic PCMs. Materials, in their process of formation and change, contribute to the dynamic and responsive nature of experiencing a building and position building technology in a demonstrative and educational context. In this light, it is posited that increased environmental communication by the built environment may heighten imaginative, intellectual and bodily awareness and invoke a more profound relationship with materials themselves. Perhaps it is not romantic, and potentially very effective to speculate that energy related behavioral change of building occupants can occur through phenomenal material-based communication of the visual/thermal relationship of energy storage and consumption.

The deliverable of this study is a building technology product that inspires a deep appreciation of sustainable and ecological principles. And that, at times, problems can be solved simply, by being cognizant of the ebb and flow of natural forces - in this case, the visual properties of phase change. In the end, this work is an argument for increasing cultural values through design thinking and sensorial cognition.

One of the things that we value is our relationship to our environment, often through the sensorial information transmitted through direct contact with materials. This work is positioned within a behavioral change/educational context and draws its underpinning in how we learn and come to know the world. In the words of Montessori educational theory: “the purpose and aim of sensorial work is for the child to acquire clear, conscious, information and to be able to then make classifications in his/her environment.” The theory further identifies that the ability to understand one’s relation to the environment serves to orchestrate intelligence. The learning principles are based on discovery through qualitative sensory experience. The underlying premise of this PCM study is to convey the prospect of behavioral change - visual nature of sustainable technologies - through sensation as it is theorized that sensations provide a direct route to understanding as they are not derived from symbols but from our perception of reality itself.

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REFERENCES