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Optimizing Climate-Responsive PCM Integration in Office Buildings for Energy Efficiency and Comfort in Iran

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Abstract

The building sector accounts for a substantial share of global energy demand and greenhouse gas emissions, with space conditioning dominating operational loads. In Iran—a nation spanning five Köppen-Geiger climate zones—designing energy-efficient envelopes that simultaneously ensure occupant comfort remains a formidable challenge. This thesis introduces a reproducible, simulation-based **multi-objective optimization** (**MOO**) framework for the climate-responsive integration of **Phase Change Materials** (**PCMs**) in office buildings.

The workflow couples EnergyPlus with the bespoke **ChameleonPCM** plugin (seamlessly embedded in Rhino/Grasshopper via Honeybee/Ladybug) and the NSGA-II genetic algorithm. Four decision variables—PCM type, melting temperature, layer thickness, and envelope placement—are optimized to minimize annual **Energy Use Intensity (EUI)** while maximizing **Thermal Comfort Percentage (TCP)**, defined per ASHRAE Standard 55 adaptive criteria. Five cities serve as climatic proxies: Yazd (BWh, hot-desert), Kerman (BWk, cold-desert), Mashhad (BSk, cold semi-arid), Rasht (Cfa, humid subtropical), and Bushehr (BSh, hot-humid).

Pareto frontiers reveal stark climatic dependence. In arid and semi-arid zones exhibiting diurnal swings exceeding 15 °C, optimized PCMs reduce EUI by **9–31 %** and sustain or enhance comfort. Peak-performing solutions feature paraffin-based PCMs with melting points of **25–27 °C**, 40–50 mm thicknesses, and mid- or interior-side placements that guarantee complete nightly solidification. In humid coastal cities, where swings fall below 7 °C and latent loads prevail, passive PCMs yield negligible gains (<1.5 % EUI reduction) due to incomplete phase-transition cycles.

Future-climate resilience is assessed under RCP 8.5 (2080 horizon). Arid-region benefits persist despite a 4–5 °C ambient rise, whereas humid-zone performance degrades further, underscoring the need for hybrid strategies—e.g., PCMs paired with nocturnal ventilation or desiccant-assisted cooling.

The open-source **ChameleonPCM** tool and accompanying MOO template empower designers to generate locale-specific guidelines within hours. By quantifying trade-offs and delimiting applicability boundaries, this work bridges the gap between material science and climate-adaptive architecture, furnishing actionable pathways toward net-zero-ready buildings across Iran's diverse thermal regimes.

Keywords: Phase Change Materials (PCMs), Climate-Responsive Building Design, Energy Efficiency, Thermal Comfort, Simulation-Based Optimization.

Nomenclature

Symbol	Description
Acronyms	
PCM	Phase Change Material
NZEBs	Nearly Zero-Energy Buildings
TES	Thermal Energy Storage
SHS	Sensible Heat Storage
LHS	Latent Heat Storage
TCHS	Thermochemical Heat Storage
HVAC	Heating, ventilation, and Air-Conditioning
CO_2	Carbon Dioxide
DERs	Distributed Energy Resources
MOO	Multi-Objective Optimization
PPD	Predicted Percentage of Dissatisfied
WWR	Window-to-Wall Ratio
BPS	Building Performance Simulation
SHGC	Solar Heat Gain Coefficient
PPD	Predicted Percentage of Dissatisfied
BOEC	Building Operational Energy Consumption
LCEB	Lifecycle Economic Benefit
LCCR	Lifecycle Carbon Reduction
NSGA-II	Non-dominated Sorting Genetic Algorithm II
NSGA-III	Non-dominated Sorting Genetic Algorithm III
PSO	Particle Swarm Optimization

XGBoost	eXtreme Gradient Boosting
LCA	Life-Cycle Assessment
BMS	Building Management Systems
MPC	Model-Predictive Control
TMY	Typical Meteorological Year
TCP	Thermal Comfort Percentage

Table of content

1. Introduction and research framework

1.1 Introduction

Buildings are among the largest contributors to global energy use and greenhouse gas emissions, accounting for approximately 40–45 % of total energy consumption worldwide (Alva et al., 2017; Pereira et al., 2025). Much of this energy is devoted to maintaining comfortable indoor conditions through heating and cooling systems, which are particularly strained in regions with extreme climates. In Iran, rapid economic growth, urbanization, and rising living standards have caused a sharp increase in building energy demand and CO_2 emissions over the past two decades (Abedini et al., 2025). This trend underscores the urgent need for climate-responsive building strategies that enhance energy efficiency while ensuring thermal comfort for occupants.

Among the various passive solutions explored in recent years, Phase Change Materials (PCMs) have gained significant attention as an effective approach for moderating indoor temperature fluctuations and reducing energy loads. PCMs can absorb and release large quantities of latent heat during phase transitions, storing excess thermal energy when ambient temperatures rise and releasing it when temperatures fall. This process increases a building's thermal inertia and smooths temperature variations throughout the day, reducing dependence on mechanical heating and cooling systems (Lajimi & Boukadida, 2023).

Studies show that well-designed PCM integration can cut building energy use by up to 30 % while enhancing occupant comfort (Pereira et al., 2025). For example, Arasteh et al. (2023) demonstrated a 44 % reduction in cooling energy and a 34 % increase in comfort hours in a PCM-based retrofit project (Arasteh et al., 2023). However, the effectiveness of PCMs depends strongly on climatic conditions, installation location, and material configuration. Parameters such as the PCM melting point, layer thickness, and placement within the building envelope critically influence its charging and discharging behavior. If the PCM fails to complete its phase cycle within a day, residual heat can accumulate, diminishing performance (Al-Absi, Mohd Isa, et al., 2020). Therefore, climate-specific optimization is essential.

Despite extensive research on PCMs in building applications, significant knowledge gaps remain, especially for regions with diverse climates like Iran. Previous studies have typically focused on a single climate type or limited parametric analyses, leaving a lack of clear guidance for PCM selection and configuration across multiple climatic zones. Iran's climatic diversity—from the hot-dry deserts of Yazd to the humid coastal conditions of Rasht—provides a valuable opportunity to investigate how PCM parameters should be tuned for different environments.

In this context, the present research seeks to optimize PCM integration in office buildings across five representative Iranian cities—Yazd, Kerman, Bushehr, Mashhad, and Rasht—using advanced parametric simulation and multi-objective optimization. By combining the ChameleonPCM plugin (developed by Sangin & Haghighatnejad Chobari, 2025) with EnergyPlus and Honeybee/Ladybug Tools in the Rhino-Grasshopper environment, this study performs comprehensive analyses of energy use and comfort (Sangin & Haghighatnejad Chobari, 2025). The outcomes will provide design-specific guidelines that inform architects and engineers about optimal PCM types, thicknesses, and installation positions for various Iranian climates.

Ultimately, this research contributes to sustainable building design by bridging the gap between material science, energy modeling, and climate adaptation. Its findings are expected to advance both the scientific understanding of PCM behavior and the practical implementation of PCM technologies in energy-efficient, climate-responsive architecture—supporting Iran's and other regions' transition toward low-carbon, resilient built environments.

1.2 Research questions

To guide the investigation, the following research questions are formulated:

1. Which **PCM types** and **melting temperatures** yield the best performance in terms of energy efficiency and comfort across the diverse climate zones of Iran?
2. What is the **optimal PCM layer thickness** that maximizes latent-heat utilization without over-storing heat or limiting phase reversal?
3. Where should **PCMs** be **positioned** within wall or roof assemblies (interior, middle, or exterior layers) to achieve the greatest thermal benefit in each climate?
4. How much **energy reduction** and **comfort improvement** can be achieved by the **optimized PCM configurations** compared with baseline (non-PCM) cases?
5. What are the **trade-offs between energy** and **comfort**, and how can multi-objective optimization (**EUI ↓**, **TCP ↑**) identify balanced solutions?

6. How transferable are these **optimized guidelines** to other regions with similar climatic characteristics?

These questions collectively structure the analytical path of the thesis—from understanding climate-specific PCM behavior to developing practical recommendations for climate-adaptive building envelopes.

1.3 Research objectives and structure

This thesis aims to develop and validate a **systematic framework** for optimizing the integration of Phase Change Materials in office buildings under varying climatic conditions. The specific objectives are:

- **Objective 1**: Identify the most suitable PCM type (melting point and material properties) for each selected city's climate.
- **Objective 2**: Determine the optimal PCM layer thickness that maximizes annual Energy Use Intensity (EUI) reduction while maintaining full phase reversibility.
- **Objective 3**: Evaluate the influence of PCM placement (interior, mid-layer, exterior, or roof application) on energy and comfort outcomes.
- **Objective 4**: Quantify the improvements in energy efficiency, thermal comfort (PMV/PPD, TCP) resulting from optimized PCM configurations.
- **Objective 5**: Formulate design guidelines mapping each climate zone to its optimal PCM strategy, providing actionable insights for architects and engineers.

1.3.1 Research Framework

As illustrated conceptually in **Figure 1**, the research follows a sequential and iterative workflow:

1. **Base Model Development**: A standardized reference office model (ASHRAE 140 Case 600) is prepared in EnergyPlus.
2. **PCM Parameter Definition**: Material properties (melting point, conductivity, density, etc.) and placement options are established based on commercial data (BioPCM, InfiniteR PCM).
3. **Simulation & Validation**: The ChameleonPCM plugin injects PCM definitions into EnergyPlus via Honeybee, and results are validated against benchmark studies.
4. **Multi-Objective Optimization**: Parametric sweeps and evolutionary solvers (Octopus/Wallacei) minimize EUI while maximizing Thermal Comfort Percentage (TCP).
5. **Cross-Climate Analysis**: Optimal configurations are identified for each city and compared to reveal climate-specific design patterns.

Table 1: Thesis organization

Chapter	**Content**
Chapter 1: Introduction	Background, motivation, research gap, objectives, questions, and framework.
Chapter 2: Literature Review	Overview of PCM technologies, thermal-storage principles, prior studies on PCM building integration, and optimization methods.
Chapter 3: Methodology	Overview of PCM technologies, thermal-storage principles, prior studies on PCM building integration, and optimization methods.

Chapter 4: Case Studies	Description of the five Iranian cities, their climatic characteristics, and baseline building performance.
Chapter 5: Results and Discussion	Comparative performance of PCM configurations across climates; analysis of EUI, and comfort results.
Chapter 7: Conclusion	Summary of key findings, policy implications, limitations, and directions for future research.

Also, worth mentioning that as shown in Figure 1, at first, this research methodology primarily utilizes remote sensing to detect high-temperature areas. Subsequently, it analyzes a selected area to identify UHIs. Following this, future scenarios, particularly the worst-case scenario for the year 2050 and 2080, will be examined. Finally, several scenarios aimed at mitigating the effects of climate change will be proposed and analyzed again to arrive at a final decision.

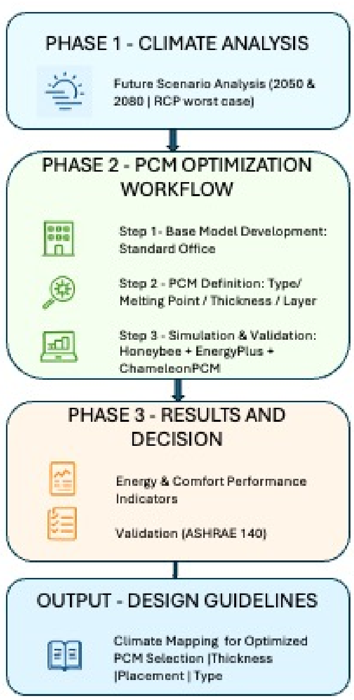


Figure 1: Research overall framework

2. Literature review

2.1 Introduction to Thermal Energy Storage in Buildings

2.1.1 The Critical Role of Buildings in Global Energy and Climate Challenges

Buildings are pivotal in shaping global energy consumption and environmental sustainability, accounting for approximately 40% of global primary energy use and 37% of energy-related carbon dioxide (CO_2) emissions (Agency, 2025a). A significant portion of this energy is dedicated to heating, ventilation, and air-conditioning (HVAC) systems, which dominate operational energy demands, particularly in regions with extreme climates. The escalating energy needs driven by population growth, urbanization, and rising living standards exacerbate peak load pressures on electrical grids, inflating operational costs and environmental impacts (Programme, 2024). These dynamic underscores the urgent need for innovative energy management solutions to enhance building efficiency, reduce greenhouse gas emissions, and support the global transition to a low-carbon energy future.

The integration of renewable energy sources, such as solar and wind, introduces further complexity due to their intermittent nature, creating a temporal mismatch between energy supply and demand (Agency, 2025b). Buildings, traditionally passive energy consumers, have the potential to evolve into active distributed energy resources (DERs) by leveraging advanced technologies like thermal energy storage (TES). TES systems enable buildings to store and manage thermal energy, enhancing grid stability, reducing reliance on fossil fuels, and aligning with climate-responsive design principles (ASHRAE, 2021).

2.1.2 Principles and Strategic Importance of Thermal Energy Storage

Thermal energy storage (TES) technologies capture and store thermal energy—either as heat or cooling—for later use, addressing the temporal disparity between energy generation and consumption. By decoupling energy supply from demand, TES facilitates peak load shaving and load shifting, reducing grid stress during high-demand periods and optimizing the use of cost-effective, low-carbon energy during off-peak times (Taylor et al., 2018). This capability is critical for integrating intermittent renewable energy sources, enabling buildings to act as thermal batteries that store surplus energy and release it when needed (Vérez et al., 2023).

TES systems offer a multifaceted value proposition, delivering economic, environmental, and operational benefits. For building owners, TES reduces electricity costs through lower demand charges and time-of-use rates, while potentially downsizing HVAC equipment requirements (Energy, 2023). For utilities, TES enhances grid reliability by flattening load profiles and deferring infrastructure investments. Environmentally, TES reduces greenhouse gas emissions by maximizing renewable energy utilization and minimizing reliance on carbon-intensive peaker plants. For occupants, TES improves thermal comfort by stabilizing indoor temperatures and enhances building resilience during power outages (ASHRAE, 2021).

2.1.3 Taxonomy of Thermal Energy Storage Systems

TES systems are classified into three primary categories based on their storage mechanisms: sensible heat storage (SHS), latent heat storage (LHS), and thermochemical heat storage (TCHS). Each type offers distinct advantages and challenges, tailored to specific building applications.

Sensible Heat Storage (SHS): SHS stores thermal energy by raising the temperature of a medium, such as water, concrete, or rock, without a phase change. Governed by the equation:

$$Q = mC_p\Delta T$$

where (Q) is the stored energy, (m) is the mass, Cp is the specific heat capacity, and ΔT is the temperature change, SHS is cost-effective (0.1–10 €/kWh_th) and widely deployed due to its simplicity and reliability (Barbhuiya et al., 2024). However, its low energy density (10–50 kWh/m³) necessitates large storage volumes, limiting its applicability in space-constrained environments.

Latent Heat Storage (LHS): LHS utilizes phase change materials (PCMs) to store energy during phase transitions, typically solid-to-liquid, at near-constant temperatures. PCMs, such as paraffins, fatty acids, or salt hydrates, offer 5–14 times higher energy density (50–150 kWh/m³) than SHS, enabling compact systems ideal for building envelopes (Zalba et al., 2003). The isothermal nature of PCMs aligns with thermal comfort requirements, but challenges include higher costs (10–50 €/kWh_th), low thermal conductivity, and issues like supercooling or material degradation (Pereira et al., 2025).

Thermochemical Heat Storage (TCHS): TCHS stores energy via reversible chemical reactions, offering the highest energy density (120–250+ kWh/m³) and potential for loss-free, long-term storage (Kraftblock, 2025). Despite its promise, TCHS remains in early development due to complex system designs, material instability, and high costs (8–100 €/kWh_th) (Saha & Rupam, 2023).

Table 1: summarizes the characteristics of these TES technologies

Characteristic	SHS	LHS	TCHS
Storage Mechanism	Temperature change	Phase transition	Chemical reactions
Common Media	Water, concrete, rock	PCMs (paraffins, salt hydrates)	Salt hydrates, metal hydrides
Energy Density (kWh/m³)	0–50	50–150	120–250+

Storage Duration	Short-term (diurnal)	Short to medium-term	Long-term (seasonal)
Advantages	Low cost, mature, reliable	High density, isothermal output	Highest density, loss-free
Limitations	Low density, large volume	Higher cost, low conductivity	Low maturity, high complexity

2.1.4 Integration of TES in Climate-Responsive Building Design

TES systems, particularly LHS using PCMs, enhance climate-responsive building design by improving thermal inertia and reducing energy demands. PCMs embedded in building envelopes (e.g., walls, roofs, or glazing) absorb excess heat during high temperatures and release it when temperatures drop, stabilizing indoor environments. In hot climates, PCMs can reduce cooling loads by 10–25%, while in cold climates, they store solar gains to minimize heating needs (Arasteh et al., 2023). Studies demonstrate that PCM wallboards can lower peak indoor temperatures by 4–6 °C and improve thermal comfort hours by over 20% in hot-arid conditions (Liu et al., 2022).

TES also supports nearly zero-energy buildings (NZEBs) and smart grids by enabling demand-side management. By storing surplus renewable energy, TES reduces grid dependency and enhances energy system flexibility, aligning with decarbonization goals (Balliet et al., 2023).

2.1.5 Challenges and Future Research Directions

Despite its potential, TES faces technical, economic, and market barriers. High initial costs, particularly for LHS and TCHS, deter adoption, especially in regions with weak financial incentives (DOE, 2021). Technical challenges include thermal losses, low thermal conductivity in PCMs, and material degradation in TCHS systems. Market barriers, such as a lack of standardized performance metrics and limited stakeholder awareness, further hinder deployment (Balliet et al., 2023).Ongoing research addresses these challenges through advancements in materials (e.g., nano-enhanced PCMs for improved conductivity), hybrid TES systems, and AI-driven control strategies that optimize performance based on real-time data (Arévalo et al., 2024). Policy initiatives, such as those by the U.S. Department of Energy, aim to standardize metrics and foster collaboration to accelerate TES adoption (Energy, 2021).

2.1.6 Synthesis and Future Directions for TES in Building Decarbonization

Thermal energy storage, particularly through PCM-based latent heat storage, is a transformative technology for achieving energy-efficient, climate-resilient, and grid-responsive buildings. By addressing the mismatch between energy supply and demand, TES enhances thermal comfort, reduces operational costs, and supports renewable energy integration. Among TES modalities, LHS strikes a balance between high energy density and practical applicability, making it a cornerstone for low-carbon building design. The subsequent section (2.2) will explore PCMs in greater detail, focusing on their thermal properties, classifications, and integration strategies to provide a foundation for further analysis.

2.2 Principles and Classification of Phase Change Materials (PCMs)

Phase Change Materials (PCMs) are advanced materials designed to store and release thermal energy during phase transitions, typically between solid and liquid states, at a nearly constant temperature. This unique capability makes PCMs highly effective for thermal energy storage (TES) in buildings, enabling enhanced energy efficiency and indoor comfort (Cui et al., 2017). This section explores the fundamental principles of PCMs, their essential properties for building applications, and their classification into organic, inorganic, and eutectic categories.

2.2.1 Principles of Latent Heat Storage

The core principle of PCMs lies in latent heat storage, where energy is absorbed or released during a phase transition without significant temperature variation. This process, driven by the latent heat of fusion, allows PCMs to store substantially more energy per unit mass than sensible heat storage, which relies on temperature changes alone (Wang et al., 2022). When ambient temperatures exceed a PCM's melting point, the material absorbs heat as it transitions from solid to liquid, stabilizing indoor environments by mitigating temperature spikes. Conversely, as temperatures drop below the melting point, the PCM solidifies, releasing stored heat to maintain warmth (Osterman et al., 2012). This reversible cycle of charging (melting) and discharging (solidification) positions PCMs as a passive solution for reducing heating and cooling demands in buildings.

2.2.2 Essential Properties for Building Applications

The efficacy of PCMs in building envelopes hinges on a combination of thermophysical, kinetic, chemical, and economic properties. The following criteria are critical for selecting an appropriate PCM (Madad et al., 2018):

- **Thermal Properties:**
    - **Melting Temperature:** Ideally within the human comfort range (18–30°C) to align with indoor temperature regulation needs.
    - **High Latent Heat of Fusion**: Maximizes energy storage capacity per unit mass or volume.
    - **High Thermal Conductivity**: Facilitates rapid heat transfer during phase transitions, though many PCMs require enhancements like metallic or graphite additives to address low conductivity.
    - **High Specific Heat and Density**: Enhances both latent and sensible heat storage, improving overall energy density.

- **Physical Properties:**

- **Minimal Volume Change:** Reduces mechanical stress on encapsulation systems.
    - **Low Vapor Pressure:** Prevents containment issues under operating conditions.

- **Kinetic Properties:**
    - **Minimal Supercooling:** Ensures reliable heat release at the intended temperature.
    - **High Crystallization Rate:** Supports efficient heat discharge during solidification.

- **Chemical Properties:**
    - **Long-Term Stability:** Maintains performance over numerous thermal cycles.
    - **Congruent Melting:** Prevents phase segregation for consistent behavior.
    - **Non-Corrosive, Non-Toxic, Non-Flammable:** Ensures compatibility with building materials and occupant safety.

- **Economic and Environmental Properties:**
    - **Cost-Effectiveness and Availability:** Supports large-scale adoption.
    - **Sustainability:** Preference for recyclable, environmentally friendly materials.

These properties collectively determine a PCM's suitability for applications such as wallboards, ceilings, or glazing units.

2.2.3 Classification of Phase Change Materials

PCMs are categorized into three primary groups based on their chemical composition: organic, inorganic, and eutectic. Each category offers distinct advantages and challenges, influencing their application in building design (Bao et al., 2019).

Organic PCMs

Organic PCMs, including paraffin waxes, fatty acids, and bio-based materials, are carbon-based compounds valued for their reliability and compatibility. Paraffin waxes (C_nH_{2n+2}) have melting points of 18–35°C and high latent heat (150–250 kJ/kg), making them ideal for indoor temperature regulation (Krupa et al., 2017). Fatty acids, derived from renewable sources like vegetable oils, and bio-based PCMs (e.g., soy or coconut derivatives) offer sustainability and stable phase transitions (Khadiran et al., 2016). Key advantages include chemical stability, negligible supercooling, non-corrosiveness, and ease of encapsulation. However, their low thermal conductivity (≈0.2 W/m·K) and moderate flammability necessitate enhancements for optimal performance (Arasteh et al., 2023).

Inorganic PCMs

Inorganic PCMs, primarily salt hydrates (e.g., $CaCl_2 \cdot 6H_2O$, $Na_2SO_4 \cdot 10H_2O$), provide high latent heat (200–300 kJ/kg), superior thermal conductivity, and cost-effectiveness compared to organic PCMs (Nkwetta & Haghighat, 2014). Their non-flammability and minimal volume change during phase transitions make them attractive for building applications. However, challenges such as supercooling, phase segregation, and corrosiveness require mitigation through nucleating agents or specialized containment (Agyenim et al., 2023). Commercial inorganic PCMs, like InfiniteR, demonstrate improved stability for use in building envelopes (Arasteh et al., 2023).

Eutectic PCMs

Eutectic PCMs are mixtures of organic and/or inorganic compounds designed to melt and solidify at a single, sharp temperature, offering precise thermal control. Their tunable melting points and high energy density make them versatile, but complex synthesis and limited thermophysical data increase costs and require extensive testing (Nkwetta & Haghighat, 2014). Eutectics are less common but hold potential for customized applications.

2.2.4 Encapsulation Techniques

To prevent leakage and enhance heat transfer, PCMs are encapsulated in various forms:

- **Macro-encapsulation**: PCMs are housed in large containers (e.g., tubes, panels) integrated into building elements.
- **Micro-encapsulation**: PCM droplets (1–100 μm) are encased in polymer shells and embedded in materials like plaster or concrete.
- **Shape-Stabilized PCMs**: PCMs are combined with supporting matrices (e.g., graphite, metal foams) to maintain structural integrity (Bao et al., 2019).

These techniques improve mechanical stability, increase heat transfer surface area, and enable seamless integration into construction materials (Khadiran et al., 2016).

2.2.5 Comparative Analysis of PCM Categories

Table 2 summarizes the characteristics, advantages, and limitations of PCM categories for building applications.

Table 2: advantages, and limitations of PCM type

Category	Examples	Advantages	Limitations
Organic	Paraffin, fatty acids, bio-PCMs	Chemically stable, non-corrosive, negligible supercooling, easy encapsulation	Low thermal conductivity, flammability, moderate cost
Inorganic	Salt hydrates ($CaCl_2 \cdot 6H_2O$, $Na_2SO_4 \cdot 10H_2O$)	High latent heat, good conductivity, non-flammable, low cost	Supercooling, phase segregation, corrosiveness
Eutectic	Organic–inorganic mixtures	Sharp melting point, high storage density, tunable composition	Complex synthesis, limited data, higher cost

2.3 PCM Integration Strategies in Building Envelopes

The integration of Phase Change Materials (PCMs) into building envelopes represents a transformative approach to enhancing thermal performance, improving occupant comfort, and reducing energy consumption for heating and cooling. The efficacy of PCMs hinges not only on material selection but also on strategic incorporation within the building fabric, which dictates the efficiency of thermal energy storage and release (Pomianowski et al., 2013). This section synthesizes key strategies for PCM integration, encompassing passive and active systems, optimal placement within building components, encapsulation techniques, and considerations for climatic and operational contexts.

2.3.1 Overview of Integration Approaches

PCM integration strategies are broadly classified into passive and active systems. Passive systems leverage PCMs embedded within the building envelope to naturally absorb, store, and release thermal energy through conduction, convection, and radiation, requiring no mechanical intervention (Nkwetta & Haghighat, 2014). These systems are favored for their simplicity, cost-effectiveness, and low maintenance. Active systems, conversely, couple PCMs with mechanical components, such as HVAC or hydronic systems, to actively control charging and discharging cycles, offering greater precision but at the cost of increased complexity and maintenance (Khadiran et al., 2016). The choice between passive and active strategies depends on project goals, building typology, and local climate, with passive systems being the primary focus of this thesis due to their sustainability and scalability.

Effective PCM integration requires optimizing thermal coupling between the PCM and its surrounding environment to ensure efficient heat exchange during phase transitions. Critical design parameters include PCM placement, layer thickness, encapsulation method, building orientation, and climatic conditions, all of which profoundly influence thermal performance (Nkwetta & Haghighat, 2014).

2.3.2 Integration within Building Components

PCMs can be incorporated into various building envelope components, each offering unique thermal regulation benefits. The following subsections detail integration strategies for walls, roofs, floors, ceilings, and glazing systems.

a) Walls

Walls are a primary focus for PCM integration due to their significant role in heat transfer. PCMs can be embedded in plasterboards, gypsum panels, cement composites, or insulation layers to stabilize indoor temperatures and reduce energy loads (Arasteh et al., 2023). Studies indicate that wall-integrated PCMs can reduce indoor temperature fluctuations by up to 4°C and peak cooling loads by 15–30% (Jelle & Kalnæs, 2017). For instance, micro-encapsulated paraffin PCMs in gypsum boards have been shown to reduce annual cooling energy by 12% in warm climates (Xie et al., 2018).

The placement of PCM layers within walls is critical:

- **Inner-surface placement** enhances nighttime heat release, improving comfort in cooling-dominated climates.
- **Mid-layer placement** maximizes thermal lag, stabilizing diurnal temperature swings.

- **Exterior placement** bolsters insulation but may limit PCM activation if exposed to extreme outdoor conditions (Parameshwaran et al., 2012).

Wall-integrated PCMs are particularly effective in lightweight constructions, where low thermal mass exacerbates temperature fluctuations (Sharma & Sagara, 2005).

b) Roofs

Roofs, exposed to intense solar radiation, are ideal for PCM integration to mitigate heat gain. PCM layers in roofing systems, such as insulation panels or cool roofs, can reduce peak roof temperatures by 15–20°C and cooling demand by up to 25% (Nkwetta & Haghighat, 2014). In hot-arid climates, where large diurnal temperature swings facilitate complete PCM phase transitions, roof-integrated PCMs demonstrate superior performance (Xamán et al., 2020). Configurations include PCM-embedded insulation, roof ponds with reflective membranes, or PCM layers under metal roofing, each tailored to specific climatic and structural requirements (Ramakrishnan et al., 2017).

c) Floors and Ceilings

Floors and ceilings with integrated PCMs support uniform temperature distribution and complement radiant heating or cooling systems. Macro-encapsulated PCMs in floors store daytime heat for nighttime release, reducing heating energy in cold climates (Khadiran et al., 2016). Ceiling panels with micro-encapsulated PCMs, commonly used in offices and educational buildings, can reduce operative temperature variations by up to 2.5°C and increase thermal comfort hours by 18% (Karwacki, 2021). These systems are particularly suitable for retrofitting, offering flexibility for both new and existing buildings.

d) Glazing and Windows

PCM integration in glazing systems is an innovative approach to managing solar gains while preserving daylighting. PCM-glazing units absorb excess solar radiation during the day and release stored heat at night, reducing HVAC loads by up to 44% and increasing comfort hours by 34% compared to conventional glazing (Arasteh et al., 2023). Advanced designs incorporate thermochromic or photochromic PCMs, which adapt optical properties with temperature, enabling dynamic solar control (Khadiran et al., 2016). These systems require PCMs with high optical transparency to balance thermal performance and daylight transmission.

2.3.3 Integration Techniques

PCM integration techniques are categorized into direct and indirect methods, each with distinct advantages and challenges.

2.3.4 Direct Incorporation

Direct incorporation involves mixing PCMs with construction materials such as concrete, mortar, or gypsum, creating thermally active building components (Mishra et al., 2022). This method ensures high thermal coupling but risks compromising mechanical strength and material compatibility, making it less suitable for load-bearing structures (Wang et al., 2022). It is commonly applied in wallboards and plaster layers for non-structural elements.

2.3.5 Indirect Incorporation

Indirect incorporation uses encapsulated PCMs housed in panels, tubes, or cavities, thermally coupled to the building envelope. This approach prevents leakage, simplifies maintenance, and allows for targeted PCM placement (Zhou et al., 2012). Encapsulation methods include:

- **Micro-encapsulation**: PCM droplets encased in polymer shells, offering high surface area and compatibility with paints or plasters (Jelle & Kalnæs, 2017).
- **Macro-encapsulation**: Larger PCM-filled containers or panels, ideal for walls, roofs, or floors (Arévalo et al., 2024).
- **Shape-stabilized composites**: PCMs combined with polymers or porous matrices to maintain structural integrity during phase transitions (Nkwetta & Haghighat, 2014).

Micro-encapsulation is increasingly preferred for its homogeneous distribution and durability, minimizing leakage risks.

2.3.6 Active Integration Systems

Active systems enhance PCM performance by integrating with mechanical systems, such as PCM-air heat exchangers or hydronic systems coupled with solar collectors or chillers (Nkwetta & Haghighat, 2014). These systems enable precise control of PCM charging and discharging, optimizing energy use during off-peak periods. For example, PCM-air heat exchangers cool daytime air by passing it over solidified PCM, while nighttime ventilation solidifies the PCM for the next cycle (Zalba et al., 2003). Despite their efficiency, active systems entail higher costs and complexity compared to passive approaches.

2.3.7 Climatic and Orientation Considerations

PCM performance is highly sensitive to building orientation and climate. In hot–humid climates, interior PCM placement mitigates excessive heat accumulation, while in cold climates, exterior placement captures solar gains (Parameshwaran et al., 2012). Climates with small diurnal temperature ranges may hinder complete phase transitions, reducing storage efficiency (Arasteh et al., 2023). Simulation-based optimization, incorporating local solar radiation profiles, temperature swings, and occupancy schedules, is essential to ensure effective PCM performance (Al-Absi, Mohd Isa, et al., 2020).

2.3.8 Synergy with Renewable and Passive Systems

PCMs can be integrated with passive systems, such as ventilated façades or green roofs, to enhance thermal regulation. Coupling PCMs with night ventilation accelerates cooling, ensuring complete solidification for daytime heat absorption (Nkwetta & Haghighat, 2014). Similarly, PCMs in building-integrated photovoltaic (BIPV) systems or solar collectors store excess thermal energy, mitigating overheating and balancing energy supply (Ramakrishnan et al., 2017). These hybrid approaches exemplify the potential of PCMs to synergize with renewable and passive technologies, advancing sustainable building design.

2.4 Influencing Parameters on PCM Performance

The efficacy of Phase Change Materials (PCMs) in enhancing building energy efficiency and thermal comfort hinges on a complex interplay of material properties, integration strategies, and environmental conditions. Optimizing PCM performance requires careful consideration of thermophysical characteristics, design parameters, and operational contexts. This section elucidates the key factors influencing PCM performance, including melting temperature, layer thickness, placement within the building envelope, thermal conductivity, phase reversibility, climatic conditions, and operational cycles.

2.4.1 Melting Temperature and Thermal Compatibility

The melting temperature (Tm) of a PCM is paramount, as it must align with the building's indoor comfort range (typically 20–27 °C) to ensure effective thermal regulation (Soares et al., 2021). A Tm too high or low results in incomplete phase transitions, rendering the PCM either perpetually solid or liquid, thus undermining its latent heat storage capacity (Baetens et al., 2010). For instance, in hot climates, PCMs with lower melting points (21–23 °C) are optimal for capturing daytime heat gains, while higher melting points (25–27 °C) suit colder climates to facilitate nighttime heat release (Parameshwaran et al., 2012). Research indicates that a Tm within ±2 °C of the mean indoor temperature maximizes energy savings and comfort (Arasteh et al., 2023). Climate-responsive selection of Tm is thus critical to ensure complete phase cycling and optimal performance.

2.4.2 Layer Thickness and PCM Quantity

The thickness of the PCM layer directly influences its latent heat storage capacity and thermal response. Layers between 10–30 mm typically balance storage capacity with responsiveness, enabling complete phase transitions within daily cycles (Xie et al., 2018). Excessive thickness (e.g., >40 mm) can lead to thermal stratification and incomplete solidification, reducing efficiency due to delayed heat transfer (Baetens et al., 2010). Conversely, overly thin layers (<10 mm) may limit thermal mass, compromising storage potential (Khadiran et al., 2016). Simulation tools like EnergyPlus and TRNSYS have demonstrated that optimal thickness depends on wall composition, solar exposure, and operational schedules, necessitating case-specific design (Ramakrishnan et al., 2017).

2.4.3 Placement within the Building Envelope

The positioning of PCMs within the building envelope significantly affects their thermal performance. Inner-surface placement enhances direct interaction with indoor air, promoting effective nighttime discharge in cooling-dominated climates. Mid-layer placement balances heat storage from indoor and outdoor sources, maximizing thermal lag, while outer-surface integration mitigates solar gains but may hinder solidification in hot climates (Al-Absi, Mohd Isa, et al., 2020). Studies show mid-layer PCMs achieve up to 18% annual energy savings in hot-arid conditions, whereas inner-layer placement excels in moderate climates (Arasteh et al., 2023). Optimal placement is thus climate-specific and must align with the building's thermal objectives.

2.4.4 Thermal Conductivity and Enhancement

Low thermal conductivity (0.2–0.3 W/m·K) in organic PCMs, such as paraffin, limits heat transfer rates, slowing phase transitions (Mishra et al., 2022). Incorporating thermal conductivity enhancers (TCEs) like graphite nanoparticles or metal foams can increase conductivity by 200–300%, accelerating melting and solidification (Ramakrishnan et al., 2017). However, excessive additives may reduce latent heat capacity and increase costs, necessitating a balance between conductivity enhancement and storage efficiency (Nkwetta & Haghighat, 2014). Advanced encapsulation techniques and composite materials further improve heat diffusion, enhancing overall system performance (Arévalo et al., 2024).

2.4.5 Phase Reversibility and Hysteresis

Complete phase reversibility—repeated melting and solidification without degradation—is essential for sustained PCM performance. Incomplete cycling, often due to insufficient diurnal temperature swings, results in residual liquid fractions and reduced storage capacity (Sharma & Sagara, 2005). Hysteresis, the temperature difference between melting and solidification points, further complicates performance, particularly in salt-hydrate PCMs, where differences of 3–5 °C can delay solidification (Alva et al., 2017). Organic PCMs exhibit lower hysteresis (0.5–1 °C), but their lower conductivity requires careful management. Stabilization agents and precise temperature control are critical to minimize hysteresis and ensure long-term reliability (Jiao et al., 2024).

2.4.6 Climatic and Operational Influences

PCM performance is highly sensitive to local climate, particularly diurnal temperature amplitude, solar radiation, and humidity. Large diurnal swings, common in hot-arid regions, enable full phase cycling, significantly reducing cooling loads (Xie et al., 2018). In contrast, humid or mild climates with narrow temperature ranges may prevent complete solidification, diminishing efficiency (Jelle & Kalnæs, 2017). Operational factors, such as occupancy patterns and HVAC schedules, also influence PCM behavior by dictating internal heat gains. Dynamic simulation tools reveal that integrating PCMs with adaptive controls, such as night ventilation or active regeneration, enhances performance under varying conditions (Arasteh et al., 2023). Seasonal calibration is equally vital, as PCM efficacy varies between summer and winter due to differences in solar exposure and indoor setpoints (Parameshwaran et al., 2012).

2.5 Experimental and Simulation Studies on PCM-Integrated Buildings

The integration of Phase Change Materials (PCMs) into building envelopes has been extensively studied through experimental and simulation-based approaches to evaluate their thermal performance and energy-saving potential. These investigations provide critical insights into PCM behavior under diverse climatic conditions, validate predictive models, and guide the optimization of PCM-enhanced designs. By combining empirical testing with advanced computational tools, researchers have quantified energy savings, thermal comfort improvements, and phase transition efficiencies, paving the way for practical implementation strategies in energy-efficient buildings.

2.5.1 Experimental Investigations

Experimental studies have been pivotal in characterizing the thermal performance of PCMs under controlled and real-world conditions. Foundational work by Zalba et al. (2003) and Sharma and Sagara (2005) established laboratory protocols for measuring key PCM properties, including latent heat, phase transition temperature, and thermal cycling stability (Zalba et al., 2003). Recent studies have advanced to full-scale testing of PCM-integrated wall and roof assemblies to assess dynamic heat transfer. For instance, Ramakrishnan et al. (2017) conducted laboratory and field experiments on PCM-cement composites, reporting a 16% reduction in peak indoor temperatures and a 12% decrease in cooling energy demand (Ramakrishnan et al., 2017). Similarly, Liu et al. (2022) investigated lightweight building walls with paraffin-based PCMs, achieving temperature reductions of 4–6°C and over 20% improvement in comfort hours across various orientations (Liu et al., 2022).

Field experiments underscore the influence of climatic context on PCM performance. Ahmad et al. (2025) demonstrated that roof-integrated PCM systems in hot-arid climate reduced cooling loads by 25% (Ahmad & Dang, 2025), while Lajimi and Boukadida (2023) found that inner-wall PCM placement in Tunisian summer conditions minimized temperature oscillations and delayed heat penetration (Lajimi & Boukadida, 2023). Karwacki (2021) tested PCM ceiling panels in an office setting, achieving enhanced thermal stability with simulation predictions validated within a ±5% margin. These studies highlight the importance of installation location, PCM layer thickness, and sufficient diurnal temperature swings (typically >10°C) to ensure complete phase cycling (Karwacki, 2021).

2.5.2 Numerical and Simulation Studies

Numerical simulations complement experimental work by enabling parametric analyses of PCM performance across diverse scenarios. Tools such as EnergyPlus, TRNSYS, and ESP-r model PCM thermal properties, hysteresis, and heat transfer dynamics, facilitating long-term performance assessments (Jelle & Kalnæs, 2017; Zhou et al., 2012). Xie et al. (2018) used simulations to evaluate PCM-integrated wallboards, identifying a 20 mm layer with a 24°C melting point as optimal for balancing storage capacity and phase reversibility (Xie et al., 2018). Parameshwaran et al. (2012) employed TRNSYS to simulate PCM layers in multi-zone buildings, reporting up to 18% energy savings in cooling-dominated climates (Parameshwaran et al., 2012). Baetens et al. (2010) noted diminishing returns for PCM thicknesses exceeding 40 mm due to incomplete solidification (Baetens et al., 2010).

Hybrid experimental–simulation approaches enhance model accuracy and practical applicability. Arasteh et al. (2023) combined laboratory testing with EnergyPlus simulations to study PCM-glazing systems, achieving a 44% reduction in cooling energy and a 34% increase in comfort hours (Arasteh et al., 2023). Similarly, Al-Absi et al. (2020) used coupled experiments and modeling to determine that mid-layer PCM placement optimizes annual performance in hot-arid climates. These integrated approaches bridge theoretical predictions with real-world outcomes, informing robust design strategies (Al-Absi, Mohd Isa, et al., 2020).

2.5.3 Multi-Climate and Optimization-Based Studies

Recent advancements have extended PCM research optimization-driven frameworks. Sangin and Haghighatnejad Chobari (2025) developed the ChameleonPCM plugin for EnergyPlus, enabling automated PCM parameterization (Sangin & Haghighatnejad Chobari, 2025). Their tools enable multi-objective optimization (MOO) tools, such as Octopus and Wallacei. Studies by Jiao et al. (2024) and Arévalo et al. (2024) demonstrated EUI reductions of 10–30% and comfort hour improvements of 15–25%, depending on climate and operational schedules (Arévalo et al., 2024; Jiao et al., 2024).

2.5.4 Discussion and Key Insights

The collective findings from experimental and simulation studies reveal several critical insights:

- PCM performance is highly sensitive to climate, layer placement, and alignment of melting temperature with indoor conditions.
- Optimal PCM thickness typically ranges from 10–30 mm, beyond which incomplete phase cycling reduces efficiency.
- Synergistic benefits arise from combining PCMs with passive strategies, such as night ventilation or reflective coatings.
- Validated simulation models, calibrated with precise thermophysical data from experiments, accurately predict PCM behavior.

These insights underscore the need for holistic, climate-specific optimization of PCM parameters (type, thickness, and location). Subsequent sections of this thesis leverage the ChameleonPCM–EnergyPlus framework to perform multi-objective optimization across Iranian climates, addressing gaps in case-specific studies and advancing practical design guidelines for PCM-integrated buildings.

2.6 PCM Applications and Research in Iran and Similar Climates

Phase Change Materials (PCMs) have emerged as a promising solution for enhancing energy efficiency and thermal comfort in buildings, particularly in regions with diverse and extreme climatic conditions like Iran. With its varied climate zones—ranging from hot-dry deserts (e.g., Yazd), humid coastal areas (e.g., Bandar Abbas), to cold-arid regions (e.g., Tabriz)—Iran provides a unique context for evaluating PCM performance. Research in Iran and comparable climates, such as those in the Middle East and North Africa, has demonstrated PCMs' potential to reduce energy consumption, stabilize indoor temperatures, and enhance resilience to climate variability. This section synthesizes key findings from experimental and simulation-based studies, identifies critical insights, and highlights research gaps to inform future investigations.

2.6.1 PCM Research in Iran

Iranian research has increasingly focused on optimizing PCM applications across the country's diverse climates, leveraging both experimental and numerical approaches to assess their impact on building energy performance.

In Tehran's semi-arid climate, Soleimani Dashtaki et al. (2019) conducted a numerical study on PCM integration in residential building walls. Their transient heat-transfer simulations revealed that placing PCM layers in the middle of the wall optimized heat storage and release, reducing energy consumption. However, overly thick PCM layers led to incomplete solidification, diminishing performance (Dashtaki et al., 2019). Similarly, Refahi et al. (2023) simulated double-layer PCM wallboard systems across five Iranian cities (Tehran, Isfahan, Shiraz, Tabriz, and Bandar Abbas), finding that climate-specific PCM selection could reduce annual energy consumption by up to 6.6%, with optimal melting temperatures ranging from 23°C to 27°C (Refahi et al., 2023).

In the hot-dry climate of Yazd, Rabani et al. (2025) experimentally evaluated a PCM-based ceiling cooling system, achieving a 3.2°C reduction in peak indoor temperatures and a 10% decrease in cooling energy demand. Their findings underscored the importance of selecting PCMs with melting points aligned with indoor comfort ranges to ensure complete daily phase transitions (Rabani et al., 2025). Similarly, Solgi et al. (2025) reported that PCM-integrated ceilings in Yazd reduced ceiling temperatures by 5–10°C, highlighting significant cooling cost savings in extreme heat conditions (Solgi et al., 2017).

For colder climates like Tabriz, Moradinia et al. (2024) used EnergyPlus and BIM-based modeling to assess PCM integration in double-skin façades under future climate scenarios. Their results showed a modest 4–6% reduction in annual energy demand but significant improvements in thermal stability and reduced overheating hours, demonstrating PCMs' resilience benefits (Moradinia et al., 2024). Baybourdy et al. (2020) further reported that combining PCM with insulation in Tabriz's cold-dry climate yielded up to 42% savings in heating loads and 32.5% in total annual energy consumption (Baybourdy et al., 2020).

Innovative applications have also been explored. Sedaghat et al. (2024) investigated PCM-enhanced photovoltaic (PV) façades at Shahid Beheshti University in Tehran, finding that PCM integration reduced PV panel temperatures by up to 12°C and improved system efficiency by 8% (Sedaghat et al., 2024). Saeedian (2025) demonstrated that PCM-coupled free-cooling HVAC systems with night ventilation in southern Iran's hot climates enhanced cooling potential by 25–30%, particularly when solidification occurred during cooler nighttime periods (Saeedian et al., 2025).

2.6.2 Insights from Comparable Climates

Research in regions with similar climatic profiles, such as Saudi Arabia, the UAE, Iraq, and North Africa, reinforces Iran's findings. In hot-humid climates like Jeddah, Bagazi et al. (2021) found that encapsulated PCMs reduced cooling energy consumption, provided careful selection of melting points and encapsulation ensured complete phase cycling (Bagazi et al., 2021). However, Al-Absi and Hafizal (2020) noted that small diurnal temperature swings in hot-humid climates, similar to Bushehr, can limit PCM effectiveness unless paired with night ventilation (Al-Absi, Hafizal, et al., 2020). In hot-arid climates like Mexico, Xamán et al. (2020) reported that roof-integrated PCMs reduced cooling loads by up to 25%, emphasizing the importance of large diurnal temperature swings for optimal PCM performance (Xamán et al., 2020). Similarly, Lajimi and Boukadida (2023) found that PCM placement near inner wall surfaces in Tunisia delayed heat transfer, reducing peak indoor temperature fluctuations (Lajimi & Boukadida, 2023).

2.6.3 Synthesis of Key Findings

The reviewed studies highlight several critical insights for PCM applications in Iran and similar climates:

- Climate-Specific Optimization: PCM melting points should be within ±2°C of the average indoor operative temperature to ensure complete phase cycling, particularly in climates with large diurnal variations (e.g., Yazd, Kerman).
- Strategic Placement: Mid-wall PCM placement is most effective in arid climates, while roof or inner-surface placement performs better in humid or mixed climates.
- Energy Savings: PCMs typically achieve 5–15% reductions in annual energy consumption, with higher benefits in cooling-dominated climates.

- Synergistic Strategies: Combining PCMs with passive (e.g., night ventilation, shading) or active systems (e.g., HVAC, BIPV) significantly enhances energy efficiency and thermal comfort.
- Experimental Validation Needs: While simulation-based studies dominate, large-scale experimental validation under real operating conditions remains limited.

2.6.4 Research Gaps and Future Directions

Despite significant progress, several gaps persist in the literature:

- **Long-Term Performance**: Limited data exist on the cyclic stability feasibility of PCMs under Iran's extreme climatic conditions.
- **Comprehensive Optimization**: Multi-objective optimization studies comparing PCM type, thickness, and placement across Iran's diverse climates using consistent methodologies are scarce.

This thesis aims to address these gaps by developing a simulation-based optimization framework to identify climate-specific PCM configurations for office buildings, extending findings to regions with analogous climatic characteristics.

2.7 Multi-Objective Optimization Approaches for PCM Design

2.7.1 Introduction and Rationale

Phase Change Materials (PCMs) are increasingly integrated into building envelopes and thermal energy storage systems due to their ability to store and release latent heat at near-constant temperatures. This property enables PCMs to moderate indoor temperature fluctuations, shift peak energy loads, and enhance overall energy efficiency. However, designing PCM-enhanced systems involves balancing multiple, often conflicting objectives, such as minimizing energy consumption, lifecycle costs, and carbon emissions while maximizing occupant thermal comfort. These competing goals transform PCM design into a complex multi-objective optimization (MOO) problem, necessitating advanced computational frameworks to identify trade-off solutions, commonly represented as a Pareto front. Unlike single-objective optimization, which yields a single "optimal" solution, MOO provides a set of non-dominated solutions, allowing designers to make informed decisions based on project priorities.

Recent studies, such as Yang et al. (2023), highlight the efficacy of MOO in PCM design by simultaneously optimizing building operational energy consumption (BOEC), lifecycle economic benefit (LCEB), and lifecycle carbon reduction (LCCR) using a coupled machine learning and evolutionary algorithm approach (Stacking model + Non-dominated Sorting Genetic Algorithm III (NSGA-III)). Such research underscores the need for MOO to address the multifaceted nature of PCM integration, considering factors like cost, carbon footprint, and system durability alongside energy performance (Yang et al., 2023).

2.7.2 Decision Variables and Objective Functions in PCM Design

2.7.2.1 Decision Variables

The performance of PCM-integrated systems depends on carefully selected design variables that define their thermal and operational behavior. Common decision variables include:

- **PCM Layer Thickness**: Influences latent heat storage capacity but increases costs, weight, and spatial constraints. Thicker layers enhance energy storage but may not always be cost-effective (Yang et al., 2023).
- **Phase Transition Temperature**: Determines the temperature at which PCMs change phase, affecting thermal lag, indoor temperature stability, and load shifting.
- **Thermal Conductivity Enhancements**: Additives like graphite or metal matrices improve charging/discharging rates but increase cost and complexity.
- **PCM Placement**: The location within the building envelope (e.g., walls, roof, floor) impacts solar gain utilization and HVAC integration. Yang et al. (2023) found east/west wall placements particularly effective in certain contexts.
- **Building Envelope Parameters**: When PCM design is part of broader envelope optimization, variables such as window-to-wall ratio (WWR), glazing U-value, and solar heat gain coefficient (SHGC) are included (Yang et al., 2023).
- **Other Parameters:** Insulation thickness, wall materials, orientation, air infiltration rates, and HVAC setpoints are often considered in integrated building optimization.

2.7.2.2 Objective Functions

MOO frameworks typically address the following objectives, reflecting trade-offs in PCM design:

- Minimize **Building Operational Energy Consumption (BOEC)**: Measured as annual energy use intensity (kWh/m^2·year), this is a primary objective in studies like Yang et al. (2023).
- Maximize **Lifecycle Economic Benefit (LCEB)**: Balances installation, maintenance, and operational costs against energy savings over the system's lifespan (Yang et al., 2023).

- Maximize **Lifecycle Carbon Reduction (LCCR)**: Targets reductions in greenhouse gas emissions, including operational and embodied carbon (Yang et al., 2023).
- Maximize **Thermal Comfort**: Quantified through metrics like the Predicted Percentage of Dissatisfied (PPD) or hours within a comfort range.
- Minimize **Peak Loads** or **Payback Time**: Reduces peak heating/cooling demands or accelerates return on investment.

These objectives are inherently conflicting. For instance, thicker PCM layers may reduce energy consumption but increase costs and embodied carbon, necessitating MOO to map trade-offs effectively.

2.7.3 Methodological Frameworks

The MOO process for PCM design typically follows a structured workflow:

- **Parametric Simulation or Experimental Data Generation**: Building performance simulation (BPS) tools like EnergyPlus or TRNSYS are used to evaluate design variable combinations. For example, Yang et al. (2023) used DesignBuilder to generate 315 simulation points for a building in Shenzhen, China.
- **Surrogate Model Development**: To reduce computational costs, machine learning-based surrogate models (e.g., Random Forest, XGBoost (eXtreme Gradient Boosting), or Stacking ensembles) approximate the relationship between decision variables and objectives. Yang et al. (2023) achieved an $R^2 \approx 0.97$ for BOEC predictions using a Stacking model with eight heterogeneous algorithms.
- **Multi-Objective Optimization**: Evolutionary algorithms like Non-dominated Sorting Genetic Algorithm II (NSGA-II) or NSGA-III explore the decision space to identify

Pareto-optimal solutions. Yang et al. (2023) employed NSGA-III, yielding 67 Pareto solutions with significant energy reductions (39.7–47.1 kWh/m² vs. 77.6 kWh/m² baseline, ~45% reduction).

- **Pareto Front Analysis** and **Decision-Making**: The resulting Pareto front is analyzed to understand trade-offs, often using visualization tools like scatter plots. Sensitivity analyses identify influential variables, such as glazing U-value and WWR in Yang et al. (2023).

2.7.4 Multi-Objective Algorithms

Evolutionary and heuristic algorithms dominate MOO for PCM design due to their ability to handle non-linear, non-convex problems:

- NSGA-II: A widely used algorithm for building energy optimization, effective for two to three objectives (Kabiri & Maftouni, 2024).
- NSGA-III: Suitable for problems with three or more objectives, maintaining diversity in the Pareto front (Yang et al., 2023).
- Particle Swarm Optimization (PSO): Applied for continuous variable spaces with computational constraints.
- Hybrid Approaches: Combine surrogate models with evolutionary algorithms to reduce computational costs.
- Model Predictive Control (MPC): Frameworks like Distributed MPC (DMPC) integrate PCM scheduling with energy, comfort, and service life objectives (Xin et al., 2025).

The non-linear thermal behavior of PCMs, including phase change hysteresis and time-lag effects, requires algorithms that can navigate complex solution spaces. Studies like Brehm et al. (2023) emphasize the need to account for varying melting temperatures across climates.

2.7.5 Limitations and Research Gaps

Despite advancements, several challenges persist:

- **Computational Cost**: High-fidelity simulations (e.g., CFD for PCM dynamics) are computationally intensive, necessitating surrogate models (Yang et al., 2023).
- **Limited PCM-Specific Focus**: Many studies treat PCMs as one of many variables, with fewer dedicated to optimizing PCM properties like melting temperature or encapsulation.
- **Incomplete Lifecycle Analysis**: While operational energy is well-studied, embodied carbon, maintenance, and end-of-life impacts are often overlooked (Yang et al., 2023).
- **Uncertainty and Robustness**: Deterministic assumptions about climate, occupancy, or PCM degradation limit real-world applicability. Robust optimization under uncertainty is rare.
- **Climate Variability**: Most studies focus on specific climates, with limited generalization across diverse zones (e.g., Yang et al.’s focus on Shenzhen).
- **Real-World Validation**: Experimental validation of optimized PCM systems remains scarce, hindering practical adoption.
- **Integration with Smart Systems**: Interactions with HVAC controls, renewable energy, and demand response are underexplored.

2.8 Comparative Assessment with Other Passive Techniques

Passive design strategies are pivotal for enhancing building energy performance and thermal comfort while minimizing reliance on active systems. As discussed in Section 2.7, the multi-objective optimization of Phase Change Materials (PCMs) leverages their latent heat storage (LHS) capabilities to improve thermal regulation within building envelopes. However, PCMs represent only one of many passive approaches. This section provides a comparative assessment of PCMs against other prominent passive strategies, including high thermal mass (sensible heat storage, SHS), heat avoidance (e.g., shading, reflective surfaces, advanced glazing), heat dissipation (e.g., natural ventilation, night flushing), and green systems (e.g., green roofs and façades). By evaluating their energy-saving potential, flexibility, cost, climate suitability, and synergies, this assessment aims to position PCM-based designs within the broader spectrum of passive techniques and highlight their unique contributions to building performance optimization.

2.8.1 Overview of Key Passive Design Strategies

Several passive design strategies are widely adopted to enhance building energy efficiency and thermal comfort:

1. **High Thermal Mass (Sensible Heat Storage)**: Materials such as concrete, brick, or stone absorb and store heat through temperature changes, stabilizing indoor conditions by releasing heat during cooler periods. Monis and Rastogi (2022) identify thermal mass as a critical passive design factor, particularly effective in climates with significant diurnal temperature swings (Monis & Rastogi, 2022).
2. **Enhanced Insulation** and **High-Performance Envelopes**: Insulation materials reduce thermal conductivity, minimizing heat transfer through walls, roofs, and floors. Kitsopoulou et al. (2024) note that insulation is among the most commonly deployed

passive retrofit strategies due to its simplicity and effectiveness (Kitsopoulou et al., 2024).

3. **Advanced Glazing** and **Shading Systems**: Low-emissivity (low-e) coatings, optimized window-to-wall ratios (WWR), and external shading devices (e.g., overhangs, louvers) reduce solar heat gain. Al-Tamimi report that such measures can reduce annual energy consumption by up to 23.6% in hot arid climates (Al-Tamimi, 2022).
4. **Natural Ventilation** and **Night Flushing**: These techniques utilize ambient air movement or cool night air to dissipate internal heat gains, reducing cooling loads. Earth-to-air heat exchangers further enhance passive cooling by leveraging ground temperatures (Okba, 2005).
5. **Green Roofs** and **Façades**: Vegetative systems provide evaporative cooling, reduce solar gains, and enhance envelope performance. Kitsopoulou et al. (2024) classify these as effective passive retrofit solutions, particularly in urban settings (Kitsopoulou et al., 2024).

2.8.2 Comparative Analysis: PCMs vs. Other Passive Strategies

2.8.2.1 Energy-Saving Potential

Passive envelope strategies, such as insulation, advanced glazing, and shading, are well-documented for their energy-saving potential. For instance, Al-Tamimi report energy reductions of 21–37% in residential buildings in hot desert climates through envelope modifications. PCMs, by contrast, provide latent heat storage, enabling peak load shifting and enhanced thermal stability (Al-Tamimi, 2022). Unlike insulation, which primarily reduces heat flow, PCMs absorb and release heat during phase transitions, complementing envelope upgrades by managing residual thermal loads. Studies, such as Hadded et al. (2025), indicate that PCMs, when integrated with night ventilation, can enhance cooling performance by 22–26% compared to sealed buildings (Hadded et al., 2025).

2.8.2.2 Flexibility and Functionality

Traditional passive strategies like insulation and shading focus on reducing heat transfer and solar gain. PCMs, however, offer a unique advantage through their high energy density (5–14 times greater than SHS), enabling thermal inertia in lightweight or retrofit applications where heavy thermal mass is impractical (Gauthier et al., 2017). For example, PCMs integrated into gypsum boards can provide significant thermal storage without structural modifications. However, PCMs require effective heat discharge (e.g., via night ventilation) to remain functional over multiple cycles, as un-discharged heat can render them ineffective (Sarri et al.).

2.8.2.3 Cost and Implementation Complexity

Envelope upgrades, such as adding insulation or installing shading devices, are typically straightforward and cost-effective. PCM integration, however, involves additional complexities, including material selection, encapsulation, performance modeling, and durability considerations. Kitsopoulou et al. (2024) emphasize that passive technologies must be evaluated for investment cost and retrofit applicability. While PCMs offer enhanced functionality, their higher initial costs and technical risks may limit their adoption compared to simpler envelope solutions (Kitsopoulou et al., 2024).

2.8.2.4 Climate and Site Specificity

The efficacy of passive strategies is highly climate-dependent. High thermal mass and night ventilation excel in regions with large diurnal temperature variations, while shading is critical in hot climates. PCM performance hinges on aligning their melting/solidification temperatures with local climate and load profiles. Monis and Rastogi (2022) underscore the importance of contextual factors, such as building orientation and envelope properties, in determining passive strategy effectiveness. PCMs require careful tuning to outperform conventional strategies in specific climates (Monis & Rastogi, 2022).

2.8.3 Synergies and Hybrid Systems

Rather than competing, PCMs and other passive strategies are highly synergistic. For instance, combining PCMs with shading reduces peak solar loads, allowing PCMs to manage diffuse and internal heat gains more effectively (Sarri et al., 2019). Similarly, integrating PCMs with night ventilation or mechanical free-cooling systems enhances their heat discharge, improving long-term performance (Alam et al., 2017). Hybrid approaches, such as PCM layers within insulated envelopes or cool roofs, can outperform standalone strategies, particularly when optimized for energy, cost, and comfort objectives (Lassandro & Di Turi, 2017). In retrofit scenarios, PCMs can provide significant benefits when paired with moderate envelope upgrades, though diminishing returns may occur in highly optimized envelopes.

2.9 Knowledge Gaps and Research Opportunities

Despite significant advancements in the development, characterization, and simulation of Phase Change Materials (PCMs) for building applications, critical knowledge gaps persist that hinder their scalable, climate-adaptive, and sustainable implementation. These gaps span material science, building integration, computational modeling, life-cycle assessment, and socio-economic domains. Addressing these challenges presents transformative opportunities to advance PCM-based building design toward carbon-neutral, energy-efficient, and occupant-centric solutions. This section synthesizes the limitations identified in the literature (Sections 2.1–2.8) and proposes a cohesive research agenda to bridge these gaps, with a particular focus on cross-climatic applicability and practical design outcomes.

2.9.1 Material-Level Knowledge Gaps

Long-Term Thermal Reliability and Aging. Current research on PCM durability is limited to short-term laboratory testing, typically under 1,000 thermal cycles, whereas building applications require stability over decades (approximately 10,000 cycles). Issues such as thermal degradation, supercooling, and phase segregation, particularly in inorganic and eutectic PCMs, remain unresolved (Bao et al., 2019). Comprehensive studies evaluating long-term performance under realistic indoor-outdoor temperature fluctuations are critically needed to ensure material reliability.

Thermal Conductivity Enhancement Trade-Offs. Additives like graphite, carbon nanotubes, or metal foams enhance PCM thermal conductivity but often compromise latent heat capacity or induce non-uniform melting (Mishra et al., 2022; Ramakrishnan et al., 2017). Future research should employ coupled experimental-numerical approaches to quantify these trade-offs and optimize additive concentrations for durability, cost-effectiveness, and recyclability.

Sustainable PCM Development. While paraffins dominate commercial applications, bio-based PCMs (e.g., fatty acids) offer renewable alternatives (Khadiran et al., 2016). However, their biodegradability, life-cycle emissions, and compatibility with building composites are underexplored. Developing recyclable encapsulation materials and low-impact synthesis pathways represents a key sustainability opportunity.

2.9.2 Building-Integration Gaps

System-Level PCM–Envelope Interactions. Most studies focus on isolated building elements (e.g., walls or roofs) rather than whole-building dynamics (Arasteh et al., 2023; Liu et al., 2022). Integrated modeling frameworks combining tools like EnergyPlus or TRNSYS with computational fluid dynamics (CFD) are needed to capture localized heat transfer, airflow interactions, and the influence of windows, infiltration, and occupant behavior.

Retrofit Feasibility and Standardization. Limited field data exist on PCM retrofit installation, maintenance, and long-term performance, particularly in diverse climatic and economic contexts (Rabani et al., 2025). Standardized protocols for PCM-integrated components (e.g., walls, ceilings, glazing) and practical retrofit guidelines would accelerate market adoption, especially in developing regions.

Cross-Climatic Validation. Experimental studies often rely on single-zone test cells under controlled conditions, lacking large-scale, multi-zone demonstrations in operational buildings across diverse climates (e.g., arid, humid, coastal, continental) (Bagazi et al., 2021). Multi-site experimental campaigns, particularly in underrepresented regions like Iran's varied Köppen zones, are essential for validating simulation results and ensuring generalizability.

2.9.3 Modeling and Optimization Gaps

Computational Efficiency and Surrogate Modeling. High-fidelity PCM simulations are computationally intensive. While machine-learning-based surrogate models (e.g., XGBoost, stacking ensembles) reduce runtimes (Yang et al., 2023), standardized workflows for data generation, training, and validation are absent. Open-access benchmark datasets would enhance reproducibility and enable robust algorithm comparisons.

Uncertainty-Aware Optimization. Current multi-objective optimization (MOO) frameworks often assume deterministic inputs for climate and occupancy (Kabiri & Maftouni, 2024). Integrating uncertainty quantification, Monte Carlo sampling, and robust optimization techniques would improve reliability under variable future climate scenarios and occupant behaviors. Smart Control Integration. Few studies explore PCM integration with real-time building management systems (BMS) or model-predictive control (MPC). Distributed MPC frameworks could dynamically coordinate PCM operation with HVAC schedules, renewable energy inputs, and demand-response signals, transforming PCMs into semi-active energy storage solutions (Xin et al., 2025).

2.9.4 Environmental and Life-Cycle Assessment Gaps

Comprehensive Life-Cycle Assessment (LCA). While operational energy savings are well-documented, embodied energy, manufacturing emissions, and end-of-life impacts of PCMs remain understudied (Yang et al., 2023). Comparative LCAs based on functional units (e.g., 1 m^2 of wall or 1 kWh of thermal storage) are needed to evaluate environmental trade-offs across PCM formulations.

Circular Economy Pathways. Recycling and reusability of PCMs and their encapsulation systems are rarely addressed. Developing bio-based PCM composites with recyclable shells and quantifying their environmental benefits represent a critical research frontier (Arévalo et al., 2024).

2.9.5 Socio-Economic and Policy Gaps

Market and Regulatory Barriers. High initial costs, limited incentives, and the absence of performance standards hinder PCM adoption (Balliet et al., 2023). Developing certification protocols aligned with existing standards (e.g., ASHRAE, ISO) and conducting region-specific cost-benefit analyses incorporating energy tariffs, carbon pricing, and occupant comfort would enhance economic viability.

Socio-Climatic Integration. Optimization studies rarely incorporate occupant feedback or adaptive comfort models. Integrating thermal comfort surveys with simulation results would bridge technical and behavioral dimensions, ensuring PCM solutions align with user needs across diverse climates.

2.9.6 Research Opportunities

To address these gaps, the following research directions are proposed:

1. Standardized Durability Testing. Develop protocols for long-term thermal cycling and aging tests for both bio-based and synthetic PCMs to ensure stability across decades.
2. Open-Source Data and Tools. Create accessible PCM databases and simulation libraries to support cross-study comparisons and AI-driven meta-analyses.
3. AI-Enabled Digital Twins. Integrate PCM models with AI-based building digital twins for real-time energy and comfort optimization.
4. Cross-Climatic Experimental Campaigns. Conduct multi-site validations across diverse Köppen zones (e.g., hot-dry, cold-arid, temperate) to ensure climate-adaptive performance.
5. Holistic Optimization Frameworks. Couple MOO with LCA and techno-economic assessments to balance energy, environmental, and economic objectives.

6. Hybrid PCM Systems. Explore combinations of latent and thermochemical storage to enable seasonal energy balancing.
7. Integrated Renewable Systems. Investigate PCM coupling with photovoltaic and ventilated façades for simultaneous heat recovery and renewable energy generation.
8. Climate-Specific Design Guidelines. Synthesize optimization results into practical, evidence-based guidelines for PCM type, thickness, and placement tailored to specific climates, such as Iran's diverse regions.

These research opportunities form the foundation for this thesis, which employs a simulation-based MOO framework using the novel ChameleonPCM plugin within EnergyPlus to systematically analyze PCM performance across five representative Iranian climate zones. The findings will be distilled into actionable design guidelines, bridging the gap between academic research and professional practice. The next chapter synthesizes key literature insights, highlighting trends, benchmarks, and remaining challenges to contextualize this work.

2.10 Summary of Key Literature Findings

The reviewed literature confirms that Phase Change Materials (PCMs) are among the most effective latent-heat thermal-energy-storage (TES) technologies for improving building energy performance and occupant comfort. Synthesizing evidence from Sections 2.1 to 2.9 reveals consistent progress in PCM research but also exposes notable gaps that this thesis seeks to address.

2.10.1 Thermal Energy Storage and Building Efficiency.

Buildings consume nearly 40–45 % of global primary energy and produce over one-third of CO_2 emissions, mainly due to heating and cooling (Agency, 2025a). TES systems, especially latent-heat storage using PCMs, mitigate the temporal mismatch between energy supply and demand, enabling load shifting and enhanced grid flexibility (Vérez et al., 2023). Compared with sensible-heat storage, PCMs offer 5–14 times higher energy density and maintain near-isothermal operation, achieving up to 30 % reductions in heating or cooling energy use (Pereira et al., 2025; Zalba et al., 2003).

2.10.2 Material Properties and Classification.

PCM performance depends on thermophysical, kinetic, and chemical stability. Organic PCMs (paraffins, fatty acids, bio-based materials) provide long-term stability and minimal supercooling but require thermal-conductivity enhancement (Khadiran et al., 2016). Inorganic PCMs (salt hydrates) feature higher conductivity and energy density but face corrosion and phase segregation (Nkwetta & Haghighat, 2014). Eutectic mixtures offer tunable melting points but remain costly and less mature. Encapsulation methods—micro, macro, or shape-stabilized—prevent leakage and enhance reliability (Bao et al., 2019). A melting range between 20 and 27 °C is generally optimal for indoor thermal regulation (Wang et al., 2022).

2.10.3 Integration within Building Envelopes.

Integrating PCMs into walls, roofs, ceilings, or glazing provides passive temperature stabilization (Pomianowski et al., 2013). Wall-embedded PCMs can reduce cooling loads by 15–30 % and limit indoor-temperature peaks by 4–6 °C (Jelle & Kalnæs, 2017). Roof applications perform best in hot-arid regions, lowering roof temperature by 15–20 °C (Xamán et al., 2020). Ceiling and floor panels improve comfort hours by 15–20 % (Karwacki, 2021), while PCM-glazing units combine daylight control with 30–40 % energy savings (Arasteh et al., 2023). Placement is climate-specific:

inner or mid-layer positions favor cooling-dominated climates, whereas outer layers assist heating-dominated ones (Parameshwaran et al., 2012).

2.10.4 Influencing Parameters.

PCM behavior is controlled by melting temperature, layer thickness, conductivity, and diurnal-temperature amplitude. Optimal thickness ranges between 10 and 30 mm; greater thickness hinders solidification and reduces efficiency (Baetens et al., 2010; Xie et al., 2018). Thermal-conductivity enhancers (graphite, metal foams) can increase heat-transfer rates by 200–300 % (Mishra et al., 2022). Organic PCMs show better cycling stability and lower hysteresis (Alva et al., 2017). Large diurnal temperature swings enable complete phase transitions, while humid or temperate conditions require hybrid solutions such as night ventilation (Jelle & Kalnæs, 2017).

2.10.5 Experimental and Simulation Findings.

Both experimental and computational research confirm that climate-specific design is essential. Laboratory tests and field experiments report 10–25 % reductions in cooling energy and 20–30 % improvements in thermal comfort (Ramakrishnan et al., 2017). Simulation platforms like EnergyPlus and TRNSYS extend these results to different envelopes and weather conditions. Recent hybrid studies (Al-Absi, Hafizal, et al., 2020; Arasteh et al., 2023) show that aligning PCM melting temperature within ± 2 °C of mean indoor temperature and ensuring daily phase cycling maximize benefits. The new ChameleonPCM plugin (Sangin & Haghighatnejad Chobari, 2025) automates PCM definition within EnergyPlus, enabling multi-objective optimization across climates.

2.10.6 Applications in Iran and Comparable Climates.

Iran's varied Köppen zones make it an ideal context for PCM evaluation. In Tehran and Isfahan, mid-wall placement reduced annual energy use by 5–7 % (Refahi et al., 2023). In Yazd, ceiling-integrated PCMs lowered peak temperatures by 3–5 °C and cut cooling demand by ≈ 10 % (Rabani et al., 2025; Solgi et al., 2017). In Tabriz, PCM-insulated façades achieved ≈ 40 % heating-load savings (Baybourdy et al., 2020). Comparable studies from Saudi Arabia, Tunisia, and Mexico confirm that arid regions yield the highest PCM benefits, while humid zones require supplementary ventilation (Lajimi & Boukadida, 2023; Xamán et al., 2020).

2.10.7 Optimization and Comparative Perspectives.

Multi-objective optimization (MOO) methods that combine evolutionary algorithms (NSGA-II/III, PSO) with machine-learning models (e.g., XGBoost) identify trade-offs between energy, comfort, and carbon objectives (Yang et al., 2023; Kabiri & Maftouni, 2024). Optimized PCM configurations can reduce EUI by 40–50 % and enhance comfort by 15–25 %. When compared with other passive strategies—insulation, shading, thermal mass, green roofs—PCMs stand out for their latent heat capacity and load-shifting capability. Hybrid designs (PCM + night ventilation or PCM + cool roof) achieve the highest synergies (Hadded et al., 2025; Sarri et al., 2019).

2.10.8 Concluding Remark.

Overall, the literature demonstrates that PCM performance is highly climate-specific and sensitive to material and design parameters. However, no comprehensive study has simultaneously optimized PCM type, thickness, and placement across multiple Iranian climates using a consistent multi-objective framework. This represents a clear methodological gap. The present research directly addresses this deficiency by developing and applying a simulation-based optimization approach through the ChameleonPCM–EnergyPlus integration, thereby providing climate-specific design guidelines for PCM applications in office buildings and contributing novel knowledge to bridge the existing gap between theoretical advancement and practical implementation.

3. Methodology

This chapter presents a rigorous and systematic methodology to evaluate and optimize the integration of Phase Change Materials (PCMs) in office building envelopes across diverse Iranian climates. The research framework combines advanced building performance simulation with multi-objective optimization (MOO) to identify optimal PCM configurations that minimize Energy Use Intensity (EUI) while maximizing Thermal Comfort Percentage (TCP). The methodology is structured into distinct phases, leveraging state-of-the-art computational tools and standardized protocols to ensure reproducibility and robustness. Figure 2 illustrates the overall workflow, encompassing climate analysis, case study definition, parametric simulation, optimization, and the derivation of climate-specific design guidelines.

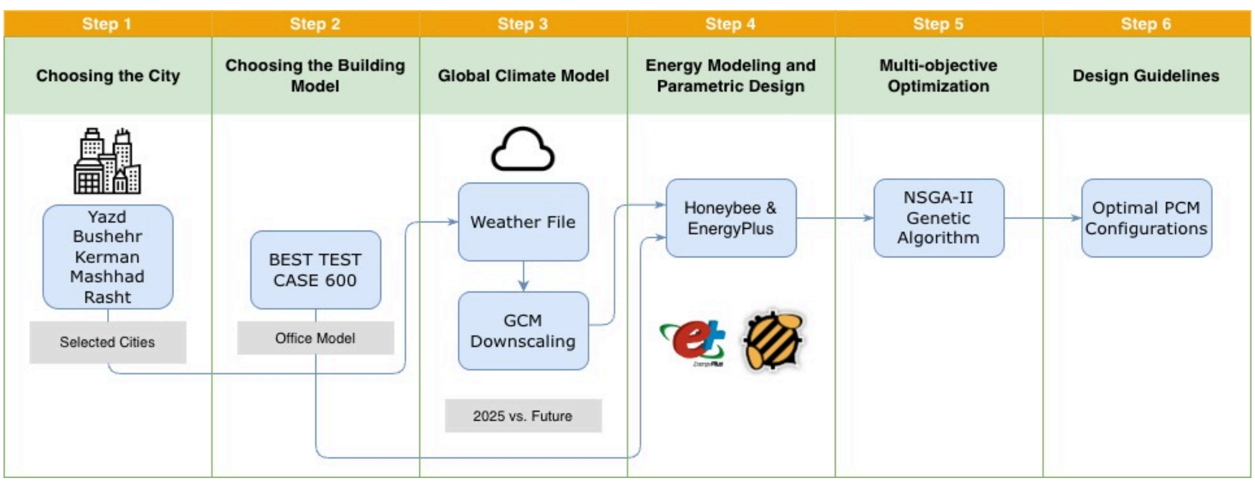


Figure 2: Research workflow for PCM optimization across Iranian climates.

3.1 Research Framework and Design

The methodological framework integrates simulation-based building performance analysis with evolutionary optimization to systematically explore PCM-enhanced building envelopes. The study employs a multi-phase approach:

1. **Climate and Case Study Definition**: Selection of five representative Iranian cities spanning distinct Köppen–Geiger climate zones and definition of a standardized office building model.
2. **Parametric Simulation Workflow**: Use of Rhino/Grasshopper, coupled with EnergyPlus and the ChameleonPCM plugin, to simulate PCM-integrated envelopes under varying parameters.
3. **Multi-Objective Optimization**: Application of evolutionary algorithms to identify Pareto-optimal PCM configurations balancing energy efficiency and thermal comfort.
4. **Analysis and Guidelines**: Post-processing of simulation results to derive climate-specific PCM design strategies, validated against baseline models.

This framework ensures a comprehensive evaluation of PCM performance across diverse climatic conditions, providing actionable insights for energy-efficient building design.

3.2 Reference Office Building Model

A reference medium-sized office building is adopted as the case study for all simulations and optimization analyses. The building is based on the ASHRAE 140 Case 600 benchmark, which is widely used for validation and comparative assessment of building energy performance models. The use of a standardized reference building ensures methodological robustness and allows the effects of PCM integration and climatic variation to be evaluated independently of architectural form.

The baseline model is adapted from ASHRAE Standard 140 Case 600, a single-zone office building selected for its standardized geometry and suitability for comparative energy studies. The model was modified to reflect typical Iranian office prototypes, ensuring relevance to the local context.

3.2.1 Geometry and Materials

The building is a rectangular prism measuring 8.0 m (width) × 7.0 m (depth) × 3.5 m (height), resulting in a total floor area of 56 m². A three-dimensional visualization of the baseline office model, developed in Rhino, is presented in Figure 3, while Figure 4 illustrates the isometric south view of the base building case (Case 600), highlighting the south-facing façade with a 40% Window-to-Wall Ratio (WWR). Table 3 summarizes the envelope construction and associated thermophysical properties, which are derived from typical Iranian building practices and DRES classroom configurations.

Table 3: Baseline Model Construction and Material Properties

Building Element	Composition	Thickness (m)	Thermal Conductivity (W/m·K)	Specific Heat (J/kg·K)	Density (kg/m³)
External Wall	Brick + EPS + Concrete + Plaster	0.30	0.84 / 0.038 / 1.94 / 0.70	800 / 1200 / 899 / 1000	1700 / 30 / 2240 / 1400
Roof	Asphalt + Air Gap + Concrete + Plaster	0.34	0.70 / – / 1.94 / 0.70	0.70 / – / 1.94 / 0.70	2100 / – / 2240 / 1400
Floor	Tile + Concrete + EPS + Plaster	0.28	0.06 / 1.06 / 0.038 / 0.70	589 / 1000 / 1200 / 1000	368 / 2000 / 30 / 1400

Window	Double Glazing (3 mm/6 mm Air)	–	U = 2.72 W/m²·K	SHGC = 0.76, VT = 0.81	–

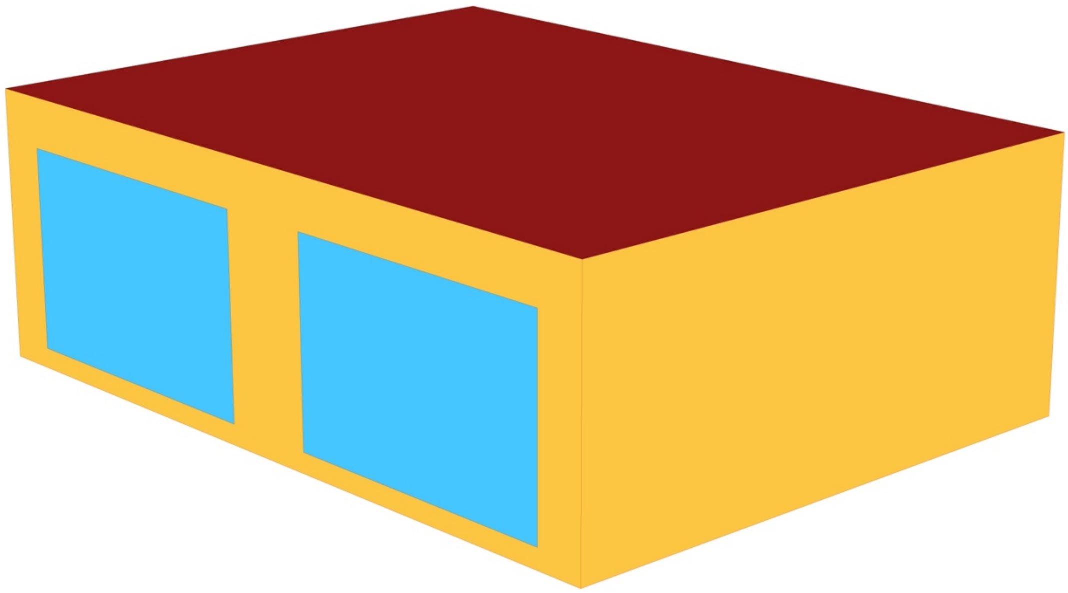


Figure 3: 3D visualization of the baseline office model in Rhino.

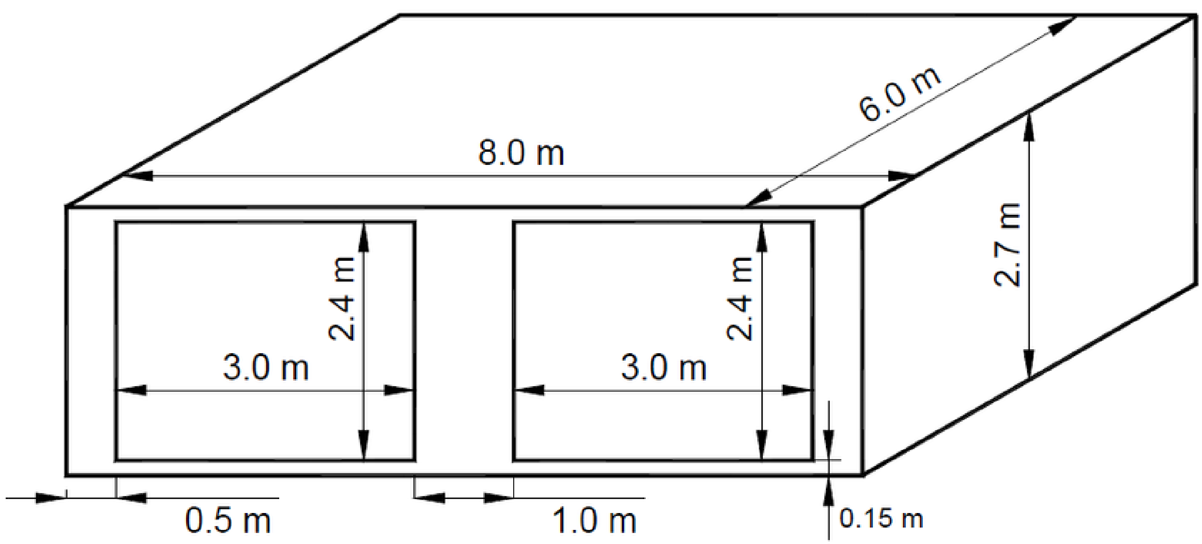


Figure 4: Isometric South View: Base Building Case 600 showing South Wall Glazing.

3.2.2 Internal Loads and Schedules

Occupancy, lighting, and HVAC schedules align with INB (2019) standards for Iranian office buildings. Heating and cooling setpoints are 20 °C and 28 °C, respectively, with an infiltration rate of 0.0003 $m^3/s \cdot m^2$ per ASHRAE guidelines for medium-tight buildings. Schedules differentiate between active weekdays (Wednesday–Saturday) and inactive days (Sunday–Tuesday), as detailed in Table 4

Table 4: Internal Loads and HVAC Schedules

Time	Occupancy (Sat–Wed)	Occupancy (Thu–Fri)	Lighting (Sat–Wed)	Lighting (Thu–Fri)	Heating (°C, Sat–Wed)	Cooling (°C, Sat–Wed)
00:00–07:00	0	0	0.1	0.1	15	32
07:00–08:00	0.7	0	0.9	0.1	17	30
08:00–12:00	0.95	0	0.9	0.1	20	28
12:00–13:00	0.95	0	0.9	0.1	17	28
13:00–14:00	0.2	0	0.9	0.1	17	30
14:00–24:00	0	0	0.1	0.1	15	32

3.3 Climatic Context

To capture Iran's climatic diversity, five cities representing major Köppen–Geiger climate zones were selected:

Table 5: Selected Cities and Climate Types

City	Climate Type	Köppen Code
Yazd	Hot-dry desert	BWh

Bushehr	Hot-humid	BSh
Kerman	Cold-arid	BWk
Mashhad	Cold-semi-arid	BSk
Rasht	Humid-temperate	Cfa

Typical Meteorological Year (TMY) weather files in EPW format were sourced from the Ladybug EPW Map and validated against EnergyPlus Weather Data, ensuring consistency and accuracy in boundary conditions.

3.4 PCM Parameterization

Two commercial PCM families were evaluated using the ChameleonPCM v0.2 plugin within Grasshopper:

- **BioPCM (Organic):** Melting points = 21 °C, 23 °C, 25 °C, 27 °C, 29 °C
- **InfiniteR PCM (Inorganic):** Melting points = 18 °C, 21 °C, 23 °C, 25 °C, 29 °C

Table 6: Thermophysical Properties of PCMs

Property	BioPCM	InfiniteR PCM
Latent Heat (J/kg)	100,000	200,000
Conductivity (solid/liquid, W/m·K)	1.8 / 1.5	1.0 / 0.54

Density (solid/liquid, kg/m³)	2300 / 2200	1540 / 1540
Specific Heat (J/kg·K)	2000	3140
Hysteresis Range (ΔT)	±1 °C	±1 °C

PCM layer thicknesses ranged from 0.00 m to 0.2 m (0.05 m increments), with placement options including inner surface, mid-layer, outer surface, and roof layer (Figure 5).

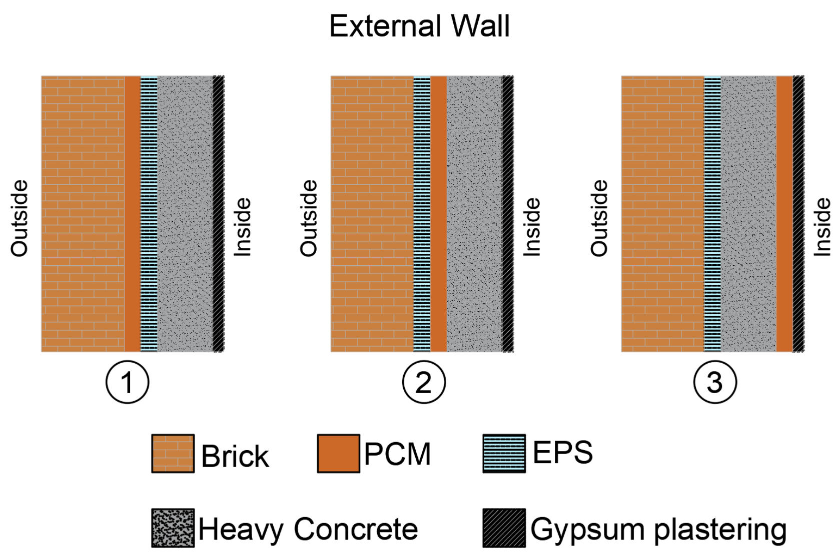


Figure 5: PCM placement configurations within the building envelope.

Each PCM melting temperature evaluated in this study corresponds to a specific commercial product from BioPCM® (Phase Change Energy Solutions Inc.) and InfiniteR PCM (Infinite R Technologies), with thermophysical properties derived directly from the respective manufacturer technical datasheets, as documented in Appendix A.

3.5 Simulation and Optimization Environment

The study adopts a reproducible simulation–optimization workflow that integrates parametric modeling, dynamic building performance simulation, and evolutionary multi-objective optimization. The workflow is designed to be generalizable and independent of specific climatic contexts, which are introduced later in the case study chapter.

3.5.1 Simulation Workflow

Building geometry and envelope configurations are developed parametrically within the Rhino/Grasshopper environment. The Honeybee plugin is used to translate the parametric building model into EnergyPlus-compatible input data files (IDF), including geometry, constructions, schedules, and boundary conditions.

Phase Change Materials (PCMs) are implemented through the ChameleonPCM plugin, which dynamically modifies EnergyPlus material definitions by injecting PCM thermophysical properties and enthalpy–temperature curves directly into the IDF files. This approach enables systematic variation of PCM properties without manual intervention and ensures consistency across simulations.

EnergyPlus performs annual dynamic simulations using the Conduction Finite Difference (CondFD) algorithm to accurately capture transient heat transfer and latent heat effects associated with PCM phase transitions.

Each simulation is conducted over a full year at an hourly time step.

3.5.2 Simulation Outputs and Performance Metrics

For each simulated configuration, the following outputs are extracted:

- Annual Energy Use Intensity (EUI) expressed in kWh/m²·year
- Thermal comfort indicators, expressed by Thermal Comfort Percentage (TCP), defined as the percentage of occupied hours within the ASHRAE 55 adaptive comfort range

Simulation outputs are automatically parsed and structured to enable comparative analysis and subsequent optimization.

3.5.3 Multi-Objective Optimization Coupling

The extracted performance metrics serve as objective function inputs to a multi-objective optimization engine. The optimization process is conducted using an evolutionary algorithm (NSGA-II), which iteratively explores the predefined parametric space by evaluating trade-offs between energy efficiency and thermal comfort.

The optimization framework does not seek a single optimal solution but rather identifies a set of non-dominated (Pareto-optimal) solutions, forming the basis for trade-off analysis and design interpretation. The formal definition of objective functions and optimization logic is presented in Section 3.7.

3.5.4 Computational Tools and Software Environment

All simulations and optimization processes are carried out within the following integrated computational environment:

- Rhino 8 + Grasshopper: Parametric modeling and workflow orchestration
- Honeybee 1.8: EnergyPlus model generation and simulation management

- Ladybug 1.8: Weather data preprocessing and environmental visualization
- ChameleonPCM v0.2: Automated PCM parameterization and EnergyPlus material injection
- EnergyPlus v9.4: Dynamic thermal and energy simulation engine
- Octopus 1.5: Multi-objective evolutionary optimization platform implementing NSGA-II

3.5.5 Model Validation

The baseline simulation setup is validated against ASHRAE Standard 140 benchmark cases and relevant literature. Annual energy demand results exhibit deviations within ±5% of reference values, confirming the reliability of the simulation framework for comparative and optimization-based analyses.

To ensure methodological consistency across simulations and optimization analyses, all model configurations are evaluated using two primary Key Performance Indicators (KPIs), selected to represent energy efficiency and long-term thermal comfort.

Energy performance is assessed using Energy Use Intensity (EUI), expressed in kWh/m^2·year, which quantifies annual operational energy demand normalized by floor area.

Thermal comfort performance is evaluated using Thermal Comfort Percentage (TCP), defined as the percentage of occupied hours during which indoor operative temperature complies with the ASHRAE 55 adaptive comfort criteria. TCP is employed as an aggregate, annual comfort indicator rather than an instantaneous metric.

These two KPIs constitute the objective functions of the multi-objective optimization framework and form the basis for all comparative analyses presented in Chapter 5.

Throughout this thesis, variations in Thermal Comfort Percentage (TCP) are reported as absolute differences expressed in percentage points (pp) to avoid ambiguity between relative and absolute performance changes. Accordingly, an increase of 0.8 pp in TCP indicates that the share of comfort-compliant occupied hours rises, for example, from 72.4% in the baseline case to 73.2% in the corresponding PCM-enhanced configuration.

3.6 Definition of Decision Variables and Optimization Space

This research investigates the effectiveness of Phase Change Materials (PCMs) integrated into building envelopes through a clearly defined multi-objective parametric framework. The central research question addressed in this study is:

"Is the integration of Phase Change Materials in office building envelopes beneficial from both an energy efficiency and a thermal comfort perspective across different Iranian climates?"

To answer this question in a rigorous and reproducible manner, the PCM-enhanced building envelope is formulated as a discrete optimization problem. A finite set of decision variables is defined to capture the most influential design parameters governing PCM thermal behavior, phase-change effectiveness, and interaction with climatic conditions. These variables are selected based on the literature review (Chapter 2) and practical constructability constraints.

The PCM melting temperature values included in the optimization represent distinct commercially available PCM products, ensuring that each simulation case corresponds to a physically realizable material with documented manufacturer specifications (see Appendix A).

3.6.1 Decision Variables

Four decision variables are explicitly defined and parametrically explored:

(1) PCM Type

Two commercially representative PCM categories are considered:

- **BioPCM** (Organic PCM / paraffin-based), characterized by chemical stability, negligible supercooling, and widespread use in building applications.
- **InfiniteR PCM** (Inorganic PCM / salt-hydrate-based), selected for its higher thermal conductivity and latent heat capacity.

These two categories allow for a comparative assessment of PCM material behavior while maintaining realistic implementation assumptions.

(2) PCM Melting Temperature

The PCM melting temperature is a critical parameter governing phase-change activation and thermal comfort compatibility. Discrete melting points of:

a) **BioPCM (Organic)**

- **21 °C**
- **23 °C**
- **25 °C**
- **27 °C**
- **29 °C**

b) **InfiniteR PCM (Inorganic)**

- **18 °C**
- **21 °C**
- **23 °C**
- **25 °C**

- **29 °C**

are selected to span the adaptive thermal comfort range defined by ASHRAE Standard 55 and to account for seasonal and climatic variability across Iranian climate zones.

(3) PCM Layer Thickness

PCM layer thickness directly influences latent heat storage capacity, charging/discharging duration, and constructability. Four thickness levels are investigated:

- **10 mm**
- **20 mm**
- **30 mm**
- **40 mm**
- **50 mm**

This range reflects realistic envelope integration limits and avoids excessive thicknesses that may lead to incomplete phase reversal.

(4) PCM Placement within the Envelope

The position of the PCM layer within the wall assembly affects thermal coupling with indoor and outdoor environments. Three placement configurations are analyzed:

- Interior-side placement, directly interacting with indoor air temperature
- Mid-layer placement, embedded within the wall stratigraphy
- Exterior-side placement, closer to outdoor climatic excitation

These configurations enable the investigation of thermal lag, storage effectiveness, and phase-change reversibility under different climatic conditions.

3.6.2 Optimization Space Definition

The combination of the four decision variables defines a discrete and fully enumerable optimization space. For each climatic context, the total number of unique PCM configurations is:

2 PCM types × 5 melting temperatures × 5 thickness levels × 3 placements = 150 configurations per climate

This explicitly defined optimization space ensures:

- Full transparency of the parametric scope
- Reproducibility of the methodology
- Traceability between input variables and output performance
- A clear foundation for multi-objective optimization and Pareto analysis

The defined solution space is subsequently explored using a multi-objective optimization framework, as detailed in Section 3.7, with the objective of minimizing annual Energy Use Intensity (EUI) while maximizing Thermal Comfort Percentage (TCP).

3.7 Multi-Objective Optimization

The optimization process employed the Non-Dominated Sorting Genetic Algorithm II (NSGA-II) within Octopus to identify Pareto-optimal PCM configurations. The objective functions were formalized as:

$$\mathbf{MOO} = \begin{cases} Minimize \;\; \boldsymbol{EUI} \\ Maximize \;\; \boldsymbol{TCP} \end{cases}$$

Decision Variables:

- PCM Type: BioPCM or InfiniteR PCM
- Melting Point: 18–29 °C
- Thickness: 0.01–0.05 m
- Placement: Inner, mid or outer layer

Optimization parameters included a population size of 100, 200 generations, crossover rate of 0.8, and mutation rate of 0.2.

3.8 Data Analysis and Visualization

Simulation outputs were processed using Grasshopper data trees and Python scripts to extract EUI and TCP. Visualizations included:

- 2D Pareto fronts illustrating trade-offs between EUI and TCP.
- Bar charts comparing optimized versus baseline performance across climates.
- Sensitivity analyses highlighting the influence of PCM parameters (type, thickness, melting point, placement).

3.9 Validation and Cross-Climate Analysis

Optimized configurations were validated against baseline (non-PCM) models to quantify improvements in EUI and TCP. Cross-climate comparisons identified patterns and informed the development of climate-specific PCM design guidelines, detailed in Chapter 6.

3.10 Limitations and Assumptions

The methodology assumes steady occupancy and TMY weather conditions, excluding occupant variability and stochastic weather fluctuations. PCM modeling simplifies complex phenomena like hysteresis and subcooling. The single-zone model limits generalizability to multi-zone or differently oriented buildings. Cost and embodied carbon were excluded due to limited manufacturer data, and thermal conductivity enhancements (e.g., nano-additives) were not validated experimentally.

3.11 Summary

This methodology establishes a robust, reproducible framework for evaluating PCM integration in office buildings across diverse Iranian climates. By leveraging EnergyPlus, the ChameleonPCM plugin, and NSGA-II optimization within Rhino/Grasshopper, it enables a systematic assessment of energy efficiency and thermal comfort. The following chapters apply this framework to the five selected case studies, presenting climate-specific results and actionable design guidelines.

4. Case Studies

4.1 Introduction

This chapter examines the climatic and environmental profiles of five representative Iranian cities—Yazd, Bushehr, Kerman, Mashhad, and Rasht—selected to encompass the predominant Köppen-Geiger climate classifications in Iran. These cities correspond to Hot Desert (BWh), Hot Semi-Arid (BSh), Cold Desert (BWk), Cold Semi-Arid (BSk), and Humid Subtropical (Cfa) zones, respectively, which collectively cover over 98% of the country's land area. Climatic data were derived from Typical Meteorological Year (TMY) files in EPW format, processed using Climate Consultant and Meteonorm software. Key parameters include dry-bulb temperature, relative humidity, global horizontal radiation, wind speed and direction, and comfort indices such as the Universal Thermal Climate Index (UTCI). The analysis establishes baseline environmental conditions and thermal challenges, informing the evaluation of Phase Change Material (PCM) integration for enhancing building energy efficiency and occupant comfort. Future climate projections (2050 and 2080) under representative concentration pathways will be incorporated in subsequent simulations via Meteonorm 8.2.0. Figure 6 illustrates Iran's Köppen-Geiger classifications with the selected cities highlighted.

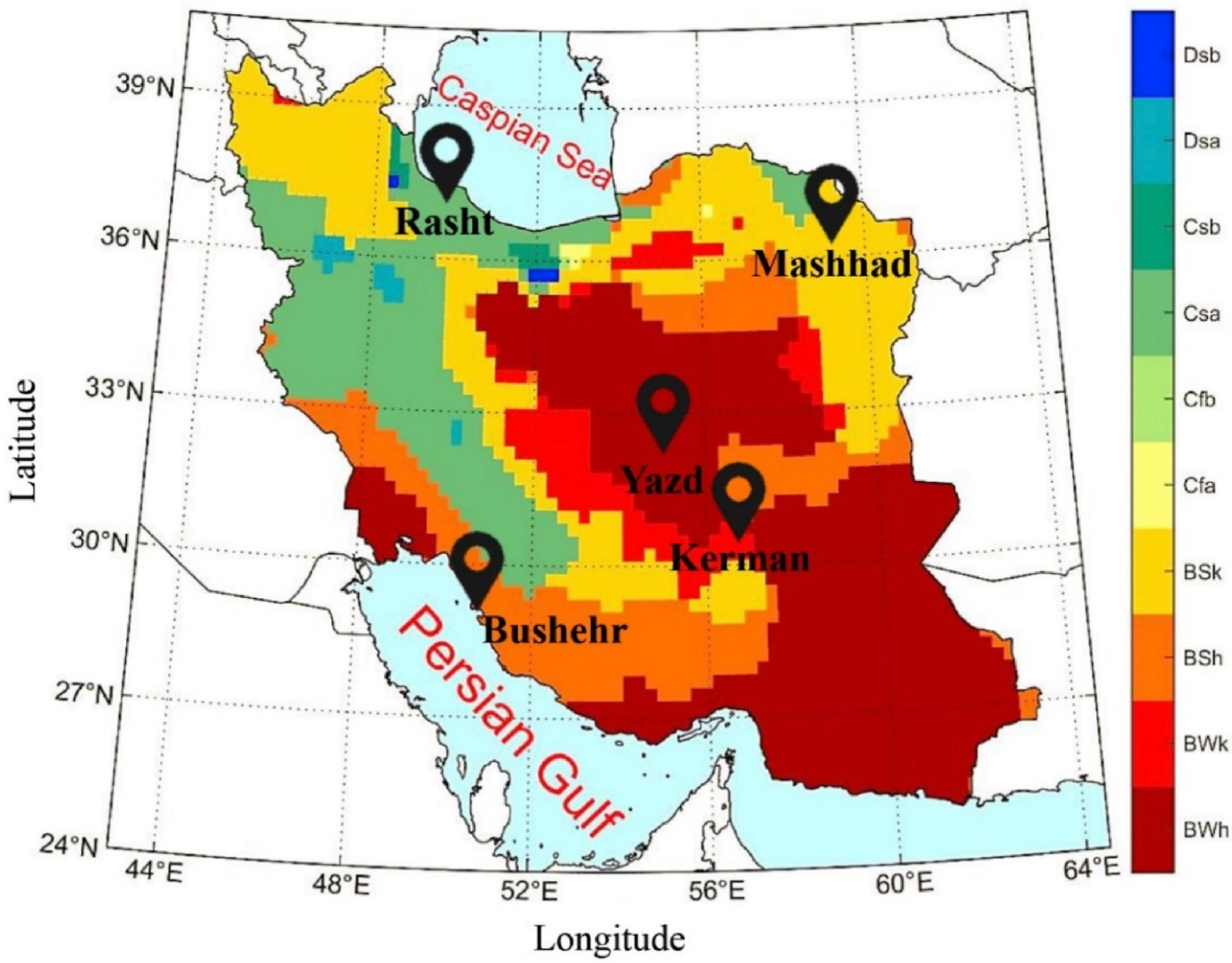


Figure 6: Map of Iran showing Köppen-Geiger climate classifications and the five case study cities (Talaei & Sangin, 2024).

All subsequent analyses are conducted on a standardized reference office building, selected to ensure consistency and comparability across climatic contexts. While climatic conditions vary between cities, the building geometry, internal loads, occupancy schedules, and envelope stratigraphy remain identical across all case studies. This approach isolates the influence of climate and PCM configuration on energy and comfort performance.

4.2 Methodology for Climate Analysis

Psychrometric charts and climate analysis diagrams were generated using Climate Consultant software (UCLA Energy Design Tools Group, 2024), based on Typical Meteorological Year (TMY) weather files obtained from Climate.OneBuilding.org. These charts were used to evaluate passive thermal potential and to support the climate-responsive selection of PCM melting temperatures.

Climatic data were sourced from EnergyPlus weather files and analyzed using Climate Consultant for psychrometric charting, passive strategy identification, and hourly visualizations, supplemented by Meteonorm for radiation and wind profiles. Psychrometric charts delineate comfort zones per ASHRAE Standard 55, while UTCI assessments quantify thermal stress levels. Wind roses and radiation plots guide ventilation and solar control strategies. A comparative summary of annual climatic indicators is provided in Table 7.

Table 7: Summary of Key Climatic Parameters for Selected Cities (Source: EnergyPlus weather data (Climate.onebuilding.org, 2025)).

Parameter	Statistic	Yazd (BWh)	Kerman (BWk)	Bushehr (BSh)	Mashhad (BSk)	Rasht (Cfa)
Dry-Bulb Temperature (°C)	Monthly Min	8.2	4.5	16.0	3.3	7.7
	Monthly Max	34.7	29.5	34.1	28.9	26.4
	Annual Avg	21.5	17.0	25.1	16.2	16.6
Relative Humidity (%)	Monthly Min	12.2	13.2	51.4	20.6	72.0
	Monthly Max	47.6	58.2	77.1	74.0	88.6
	Annual Avg	29.9	35.7	64.3	47.3	80.3
Global Horizontal	-	2,200	2,000	1,950	1,900	1,600

Radiation (kWh/m²·year)						
Wind Speed (m/s)	Monthly Avg Range	2.0–3.2	2.3–3.9	2.5–4.7	2.3–4.4	1.5–2.1
Coordinates	Lat, Long	31.9°N, 54.4°E	30.3°N, 57.1°E	28.9°N, 50.8°E	36.3°N, 59.6°E	37.3°N, 49.6°E
Elevation (m)	-	1,216	1,755	9	995	7

4.3 City Profiles

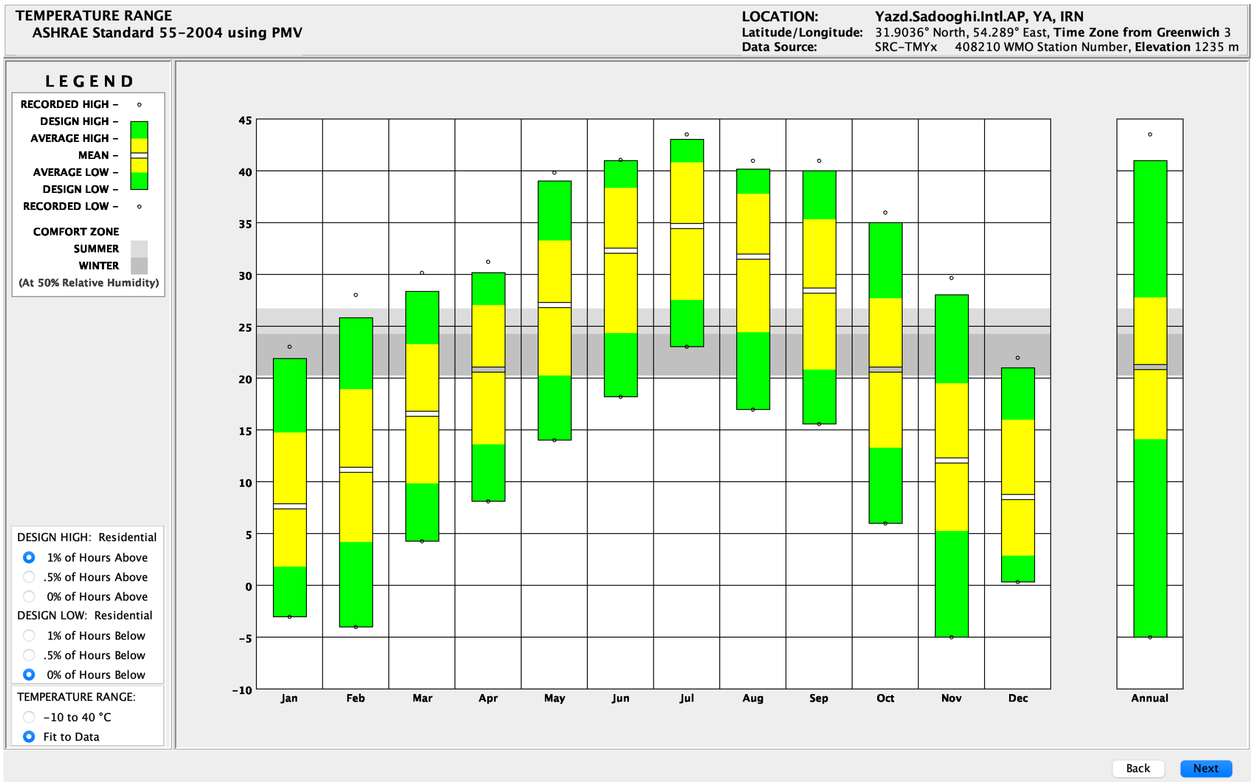
4.3.1 Yazd – Hot Desert Climate (BWh)

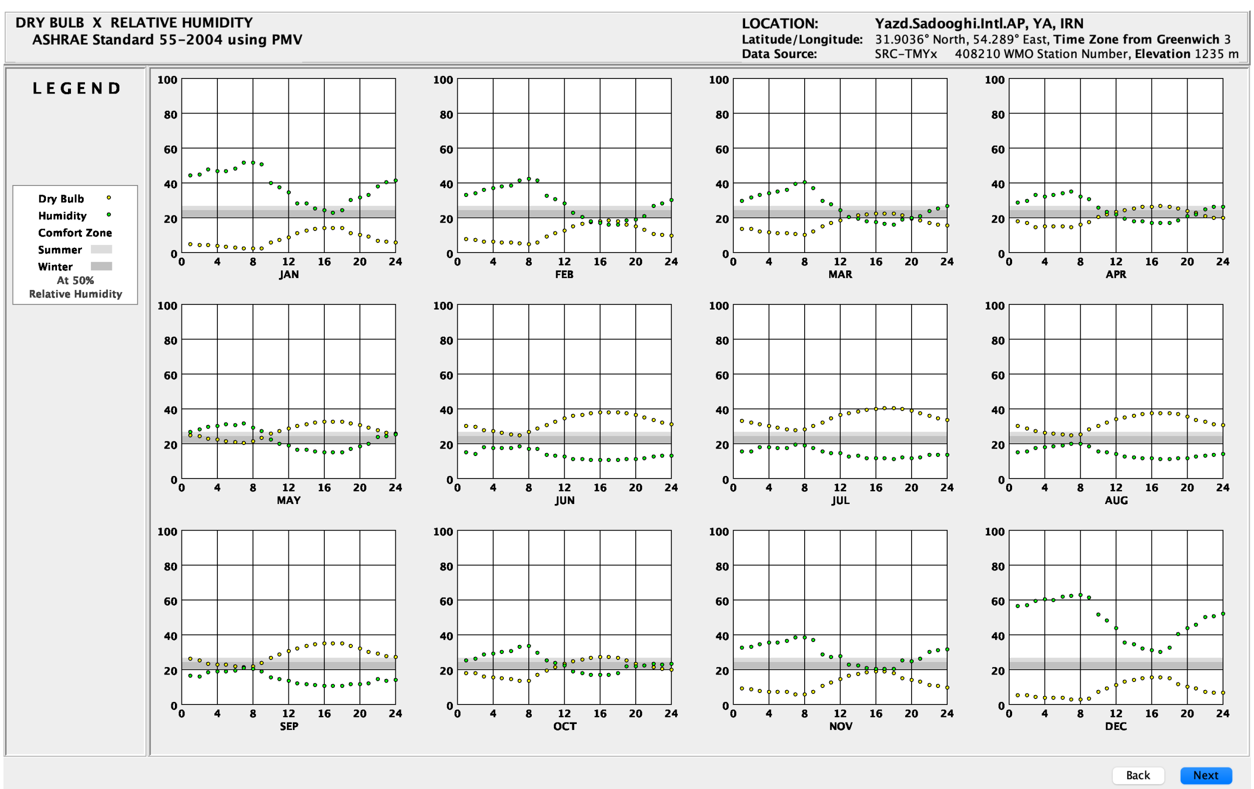
Geographic and Climatic Context

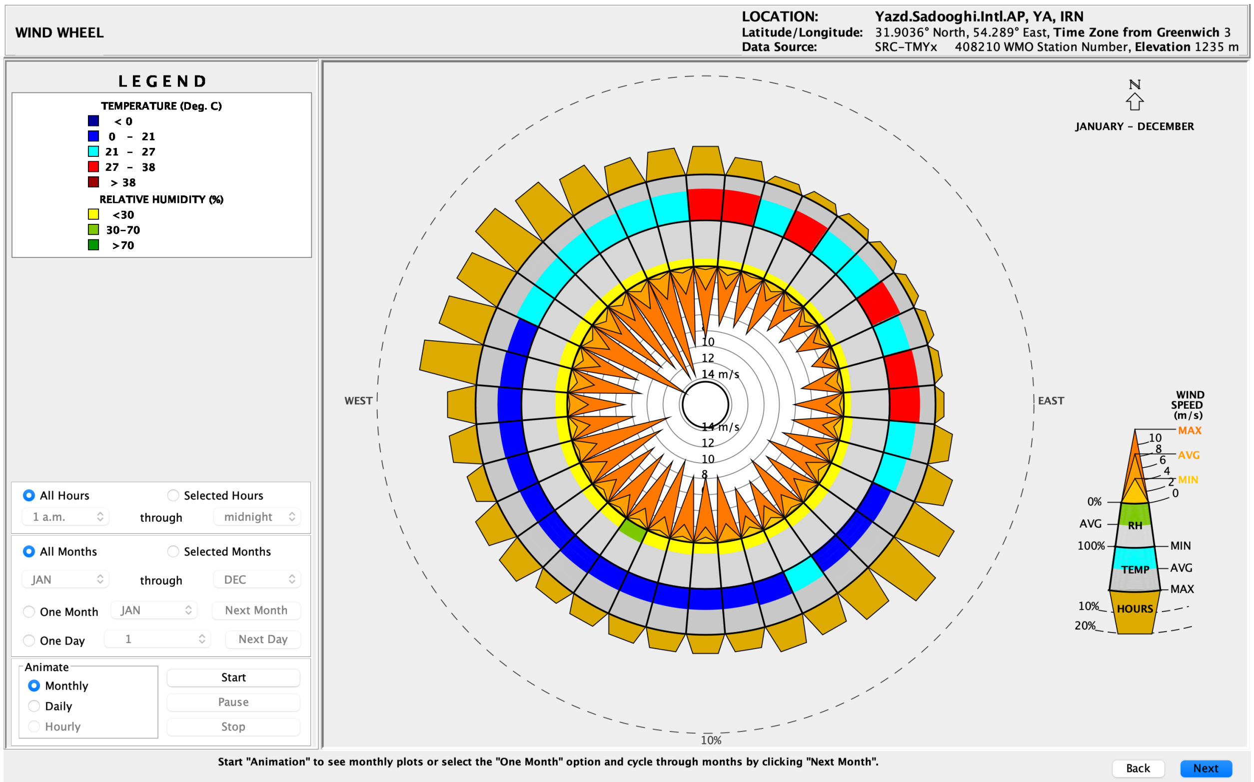
Yazd, the capital of Yazd Province, is centrally located on the Iranian plateau at an elevation of 1,216 m, between the Dasht-e Kavir and Dasht-e Lut deserts. This geographical setting results in a classic hot-desert climate characterized by minimal annual precipitation (<50 mm), low relative humidity, and intense solar exposure. The hourly profiles of dry-bulb temperature, relative humidity, prevailing wind patterns, and global horizontal and direct normal solar radiation for Yazd are presented in Figures 7–9, as generated using Climate Consultant.

Key Climatic Features

- **Temperature**: Extreme diurnal swings (>15–20°C) are hallmark, with summer peaks >40°C and winter minima near 0°C.
- **Humidity**: Consistently <30% annually, enabling evaporative strategies.
- **Wind**: Prevailing northwesterly winds (2–3 m/s) facilitate night flushing.
- **Solar Radiation**: High clear-sky insolation (~2,200 kWh/m²·year).


TEMPERATURE RANGE
ASHRAE Standard 55-2004 using PMV
LOCATION: Yazd.Sadooghi.Intl.AP, YA, IRN
Latitude/Longitude: 31.9036° North, 54.289° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408210 WMO Station Number, Elevation 1235 m
LEGEND
RECORDED HIGH –
DESIGN HIGH –
AVERAGE HIGH –
MEAN –
AVERAGE LOW –
DESIGN LOW –
RECORDED LOW –
COMFORT ZONE
SUMMER
WINTER
(At 50% Relative Humidity)
DESIGN HIGH: Residential
1% of Hours Above
.5% of Hours Above
0% of Hours Above
DESIGN LOW: Residential
1% of Hours Below
.5% of Hours Below
0% of Hours Below
TEMPERATURE RANGE:
-10 to 40 °C
Fit to Data
Jan
Feb
Mar
Apr
May
Jun
Jul
Aug
Sep
Oct
Nov
Dec
Annual
Back
Next


DRY BULB X RELATIVE HUMIDITY
ASHRAE Standard 55-2004 using PMV
LOCATION: Yazd.Sadooghi.Intl.AP, YA, IRN
Latitude/Longitude: 31.9036° North, 54.289° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408210 WMO Station Number, Elevation 1235 m
LEGEND
Dry Bulb
Humidity
Comfort Zone
Summer
Winter
At 50%
Relative Humidity
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC
Back
Next



WIND WHEEL
LOCATION: Yazd.Sadooghi.Intl.AP, YA, IRN
Latitude/Longitude: 31.9036° North, 54.289° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408210 WMO Station Number, Elevation 1235 m
LEGEND
TEMPERATURE (Deg. C)
< 0
0 - 21
21 - 27
27 - 38
> 38
RELATIVE HUMIDITY (%)
<30
30-70
>70
All Hours
Selected Hours
1 a.m.
through
midnight
All Months
Selected Months
JAN
through
DEC
One Month
JAN
Next Month
One Day
1
Next Day
Animate
Monthly
Daily
Hourly
Start
Pause
Stop
N
JANUARY - DECEMBER
WEST
EAST
10%
14 m/s
12
10
8
WIND SPEED (m/s)
MAX
AVG
MIN
0%
AVG
RH
100%
TEMP
MIN
AVG
MAX
10%
20%
HOURS
Start "Animation" to see monthly plots or select the "One Month" option and cycle through months by clicking "Next Month".
Back
Next

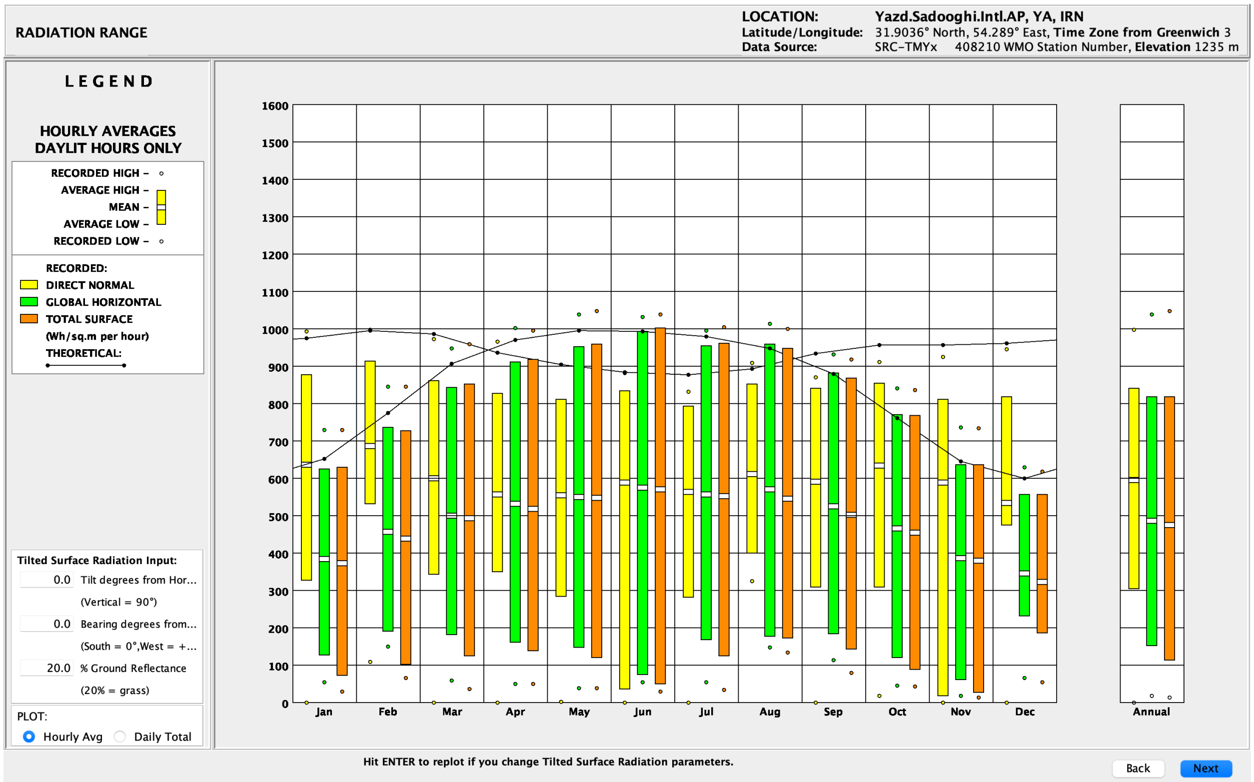


Figure 7 -10: Hourly dry-bulb temperature, relative humidity, wind rose, and global horizontal/direct normal radiation profiles for Yazd (generated via Climate Consultant).

Thermal Comfort and PCM Implications

The psychrometric analysis for Yazd (Figure 11) shows that only 20.4 % of the annual hours fall within the comfort zone, while most conditions lie in the hot-dry region, indicating a significant need for passive cooling strategies. The chart highlights that direct and two-stage evaporative cooling, night ventilation, and high thermal mass are the most effective methods for improving comfort. Given Yazd's wide diurnal temperature range, Phase Change Materials (PCMs) with melting points around 23–25 °C are particularly suitable, as they can store excess heat during the day and release it at night when temperatures drop. Integrating PCMs within walls or roofs in combination with night flushing and natural ventilation can thus maximize latent heat storage and enhance indoor thermal comfort in this hot-dry climate.

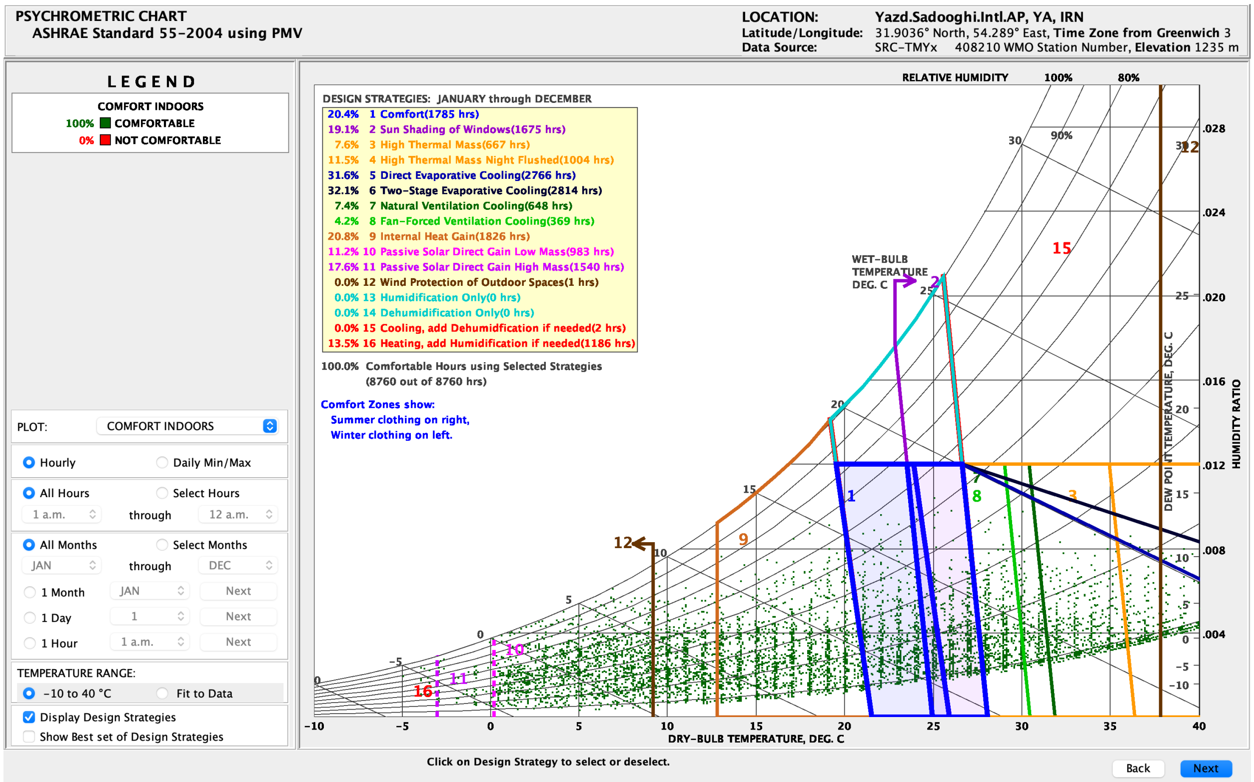


Figure 11: Psychrometric chart with passive strategies for Yazd, generated using Climate Consultant software (UCLA Energy Design Tools Group, 2024).

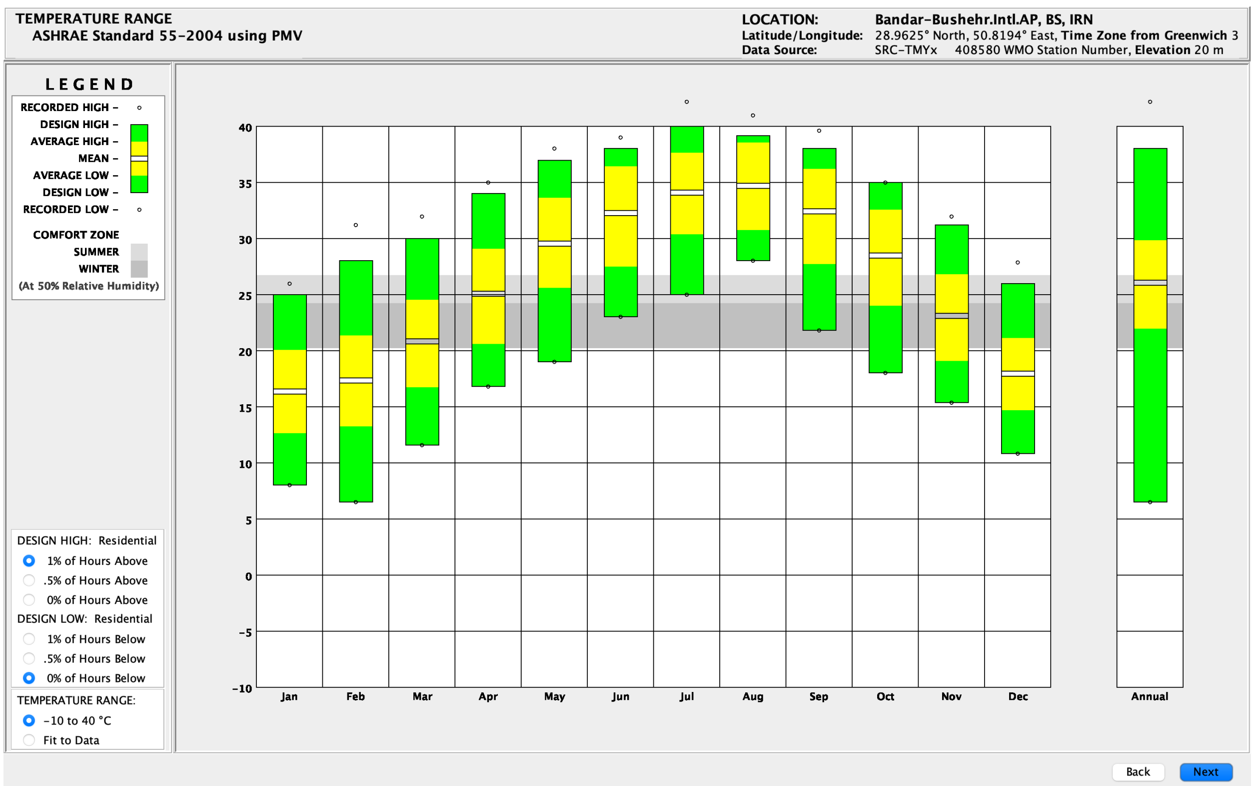
4.3.2 Bushehr – Hot Semi-Arid Climate (BSh)

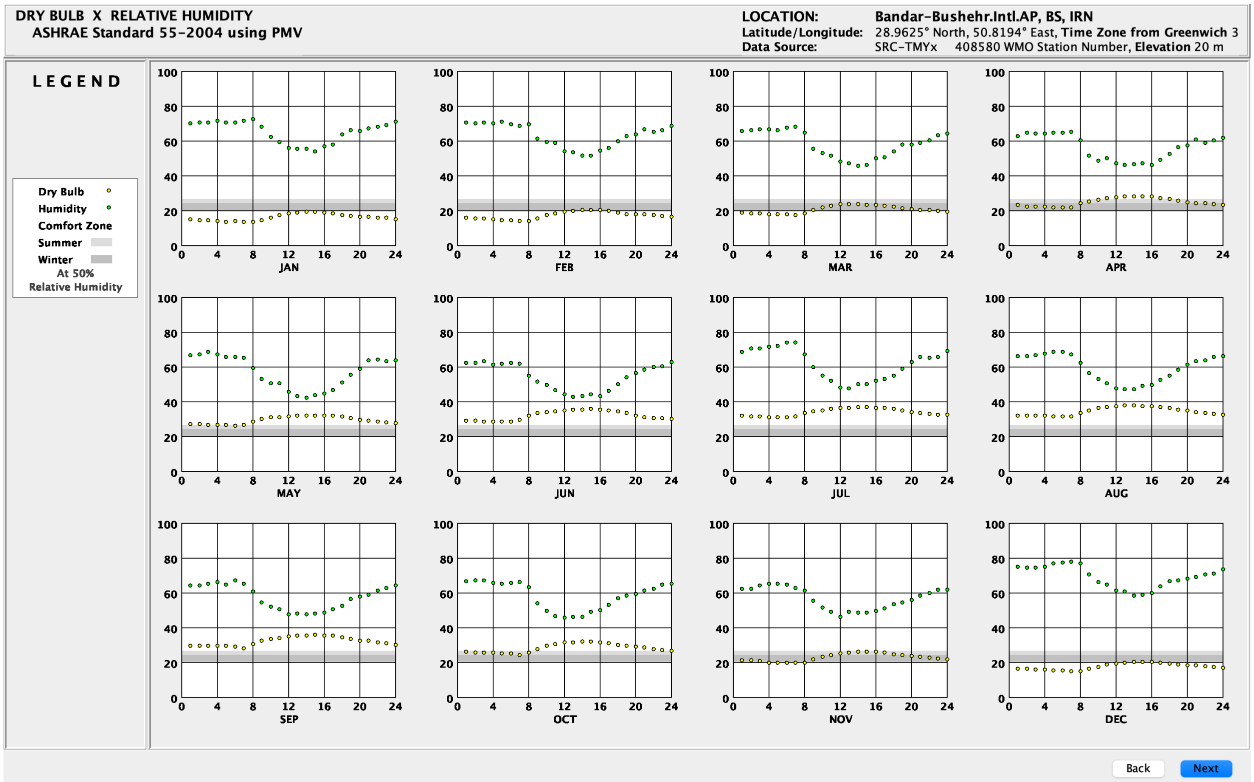
Geographic and Climatic Context

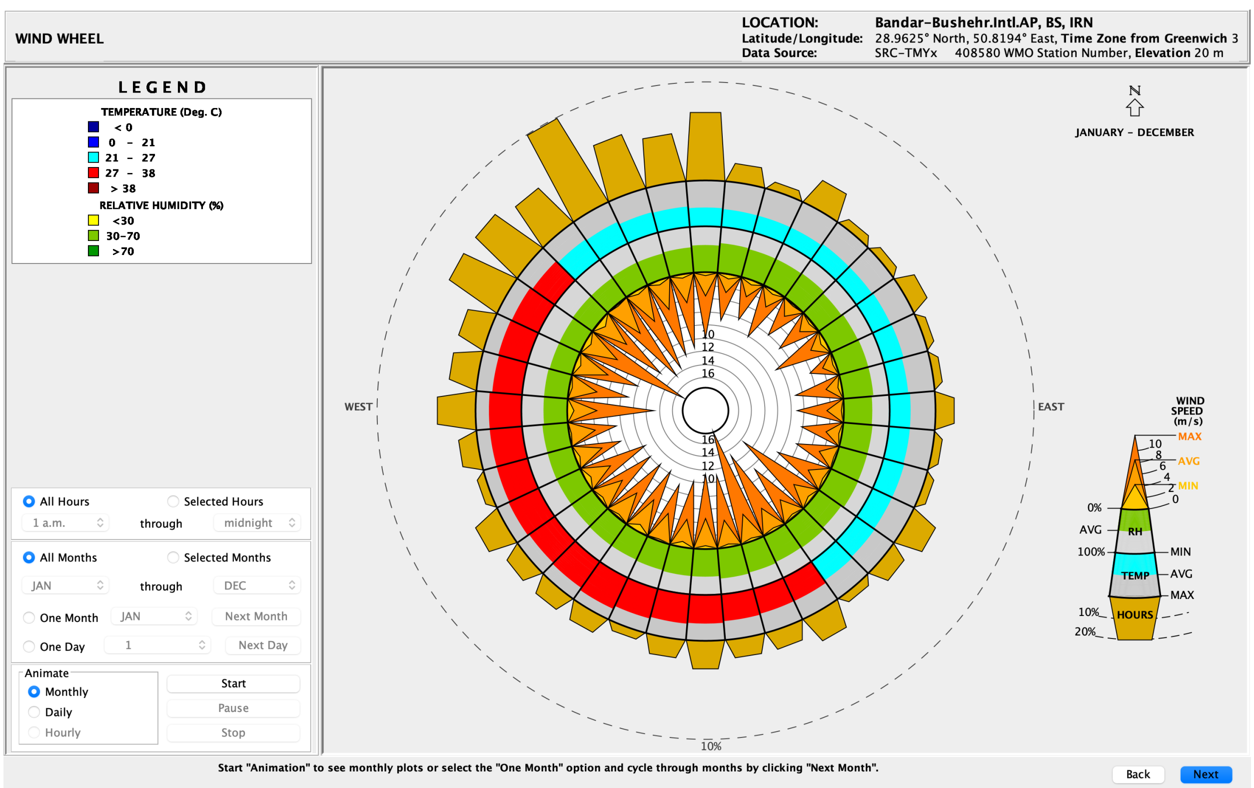
Bushehr, a coastal city and major port along the Persian Gulf, is located at near sea-level elevation and experiences a hot-humid climate strongly influenced by maritime air masses. The hourly distributions of dry-bulb temperature, relative humidity, wind patterns, and global horizontal and direct normal solar radiation for Bushehr are presented in Figures 12–15, based on Climate Consultant analyses.

Key Climatic Features

- **Temperature**: Persistent highs (25–45°C) with minimal diurnal variation (<7°C).
- **Humidity**: Elevated (70–80%), inhibiting latent cooling.
- **Wind**: Sea breezes (3–5 m/s) are warm and moist.
- **Solar Radiation**: Moderated by haze (~1,950 kWh/m²·year).




DRY BULB X RELATIVE HUMIDITY
ASHRAE Standard 55-2004 using PMV
LOCATION: Bandar-Bushehr.Intl.AP, BS, IRN
Latitude/Longitude: 28.9625° North, 50.8194° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408580 WMO Station Number, Elevation 20 m
LEGEND
Dry Bulb
Humidity
Comfort Zone
Summer
Winter
At 50%
Relative Humidity
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC
Back
Next


WIND WHEEL
LOCATION: Bandar-Bushehr.Intl.AP, BS, IRN
Latitude/Longitude: 28.9625° North, 50.8194° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408580 WMO Station Number, Elevation 20 m
LEGEND
TEMPERATURE (Deg. C)
< 0
0 - 21
21 - 27
27 - 38
> 38
RELATIVE HUMIDITY (%)
<30
30-70
>70
All Hours
Selected Hours
1 a.m.
through
midnight
All Months
Selected Months
JAN
through
DEC
One Month
JAN
Next Month
One Day
1
Next Day
Animate
Monthly
Daily
Hourly
Start
Pause
Stop
N
JANUARY - DECEMBER
WEST
EAST
10%
WIND SPEED (m/s)
MAX
AVG
MIN
RH
TEMP
HOURS
Start "Animation" to see monthly plots or select the "One Month" option and cycle through months by clicking "Next Month".
Back
Next

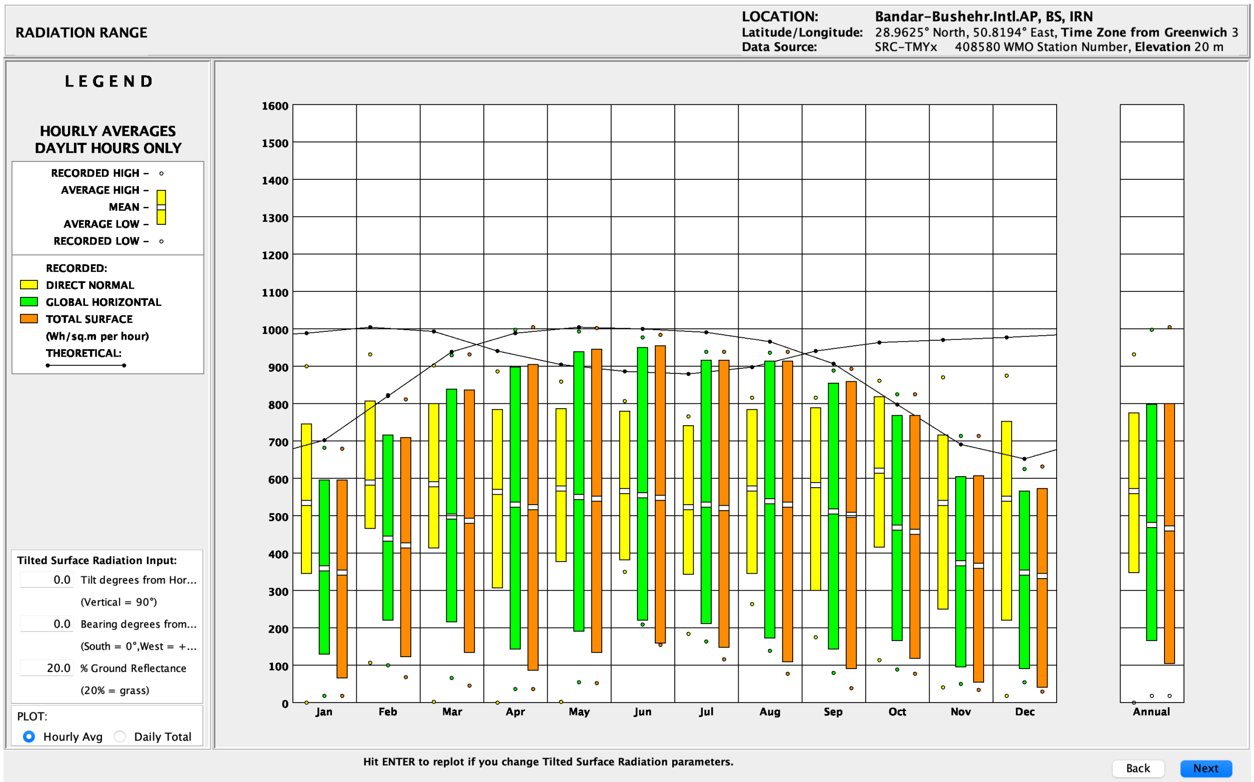


Figure 12-15: Hourly dry-bulb temperature, relative humidity, wind rose, and global horizontal/direct normal radiation profiles for Bushehr (generated via Climate Consultant).

Thermal Comfort and PCM Implications

The psychrometric analysis for Bushehr (Figure 16) indicates that only 17.6 % of annual hours fall within the comfort range, with the majority of conditions concentrated in the hot-humid region. The chart highlights that cooling with dehumidification (45.5 %) and sun shading (25.2 %) are the most critical passive and active strategies for achieving comfort. Due to the high relative humidity, evaporative cooling and night ventilation offer limited potential. In such conditions, Phase Change Materials (PCMs) with low melting points (21–23 °C) can provide modest thermal load reduction by storing daytime heat; however, their solidification at night is hindered by the persistently warm and humid air. Consequently, hybrid systems—combining PCMs with mechanical ventilation or dehumidification—are recommended to enhance latent heat cycling and maintain comfort in this coastal climate.

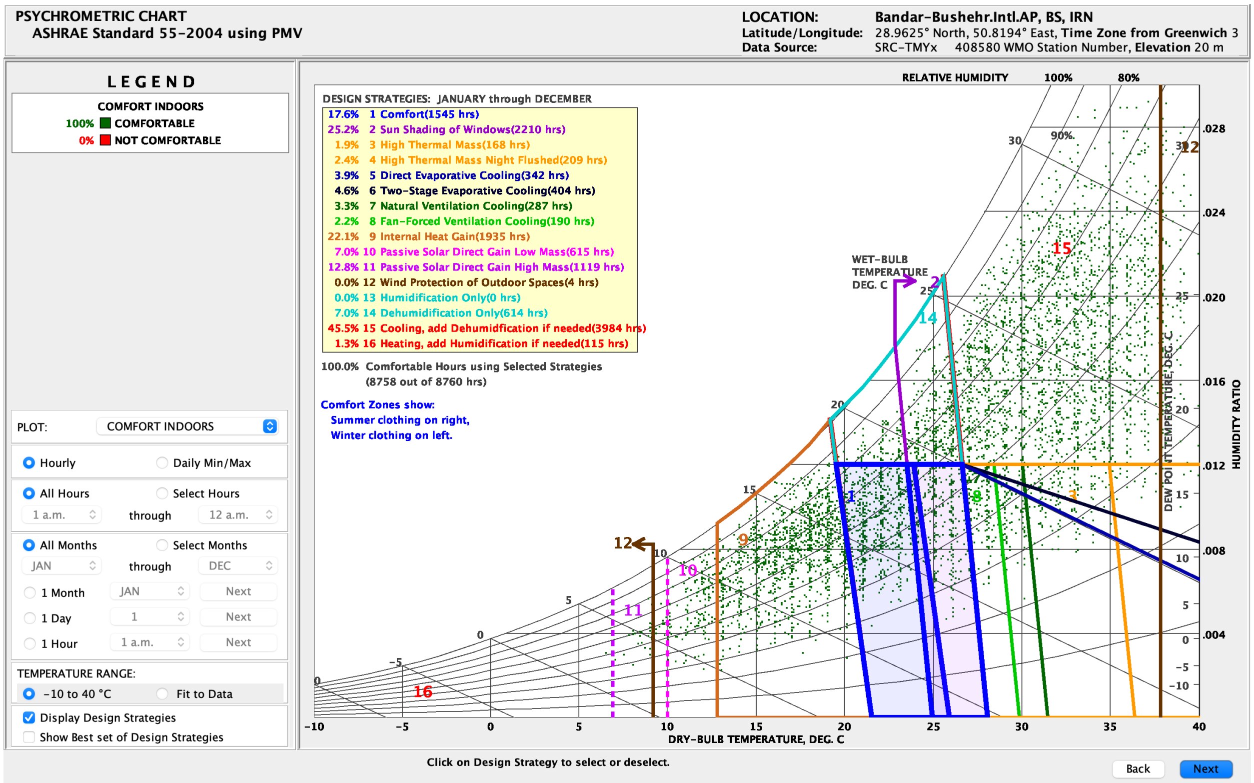


Figure 16: Psychrometric chart with passive strategies for Bushehr, generated using Climate Consultant software (UCLA Energy Design Tools Group, 2024).

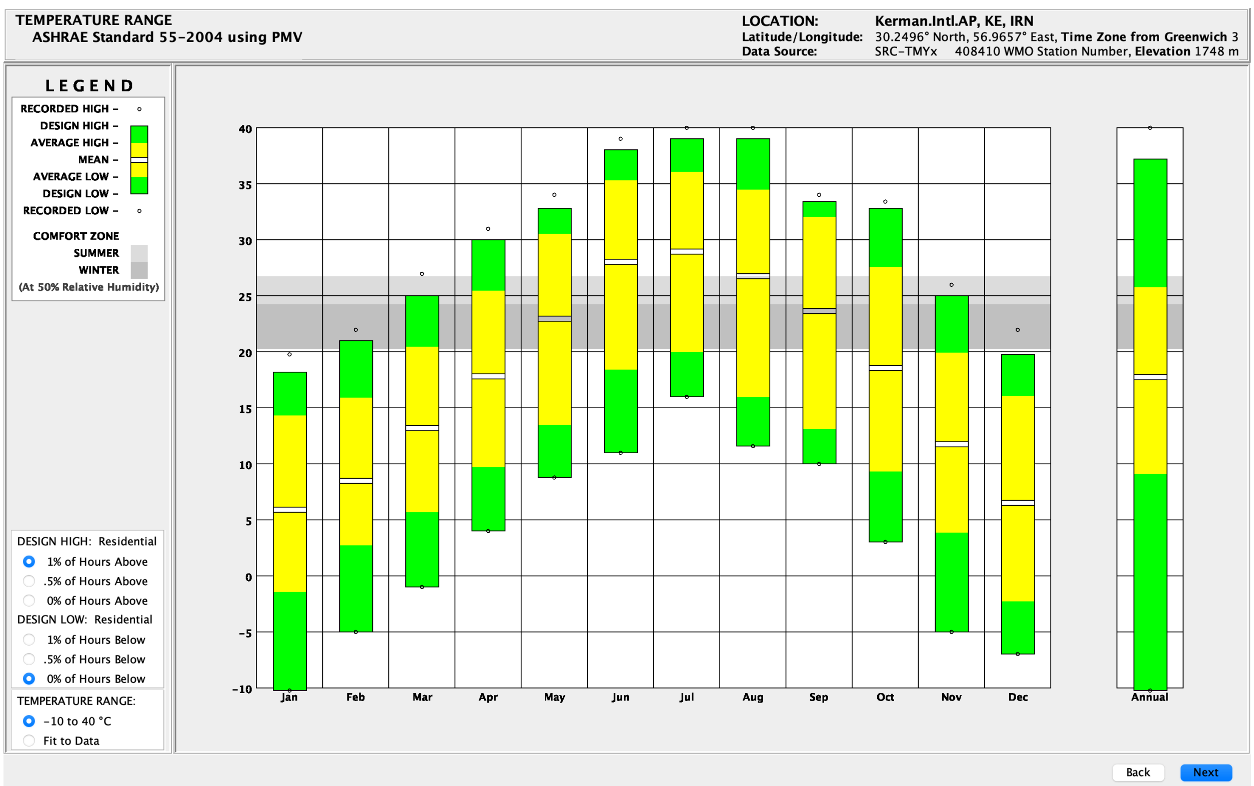
4.3.3 Kerman – Cold Desert Climate (BWk)

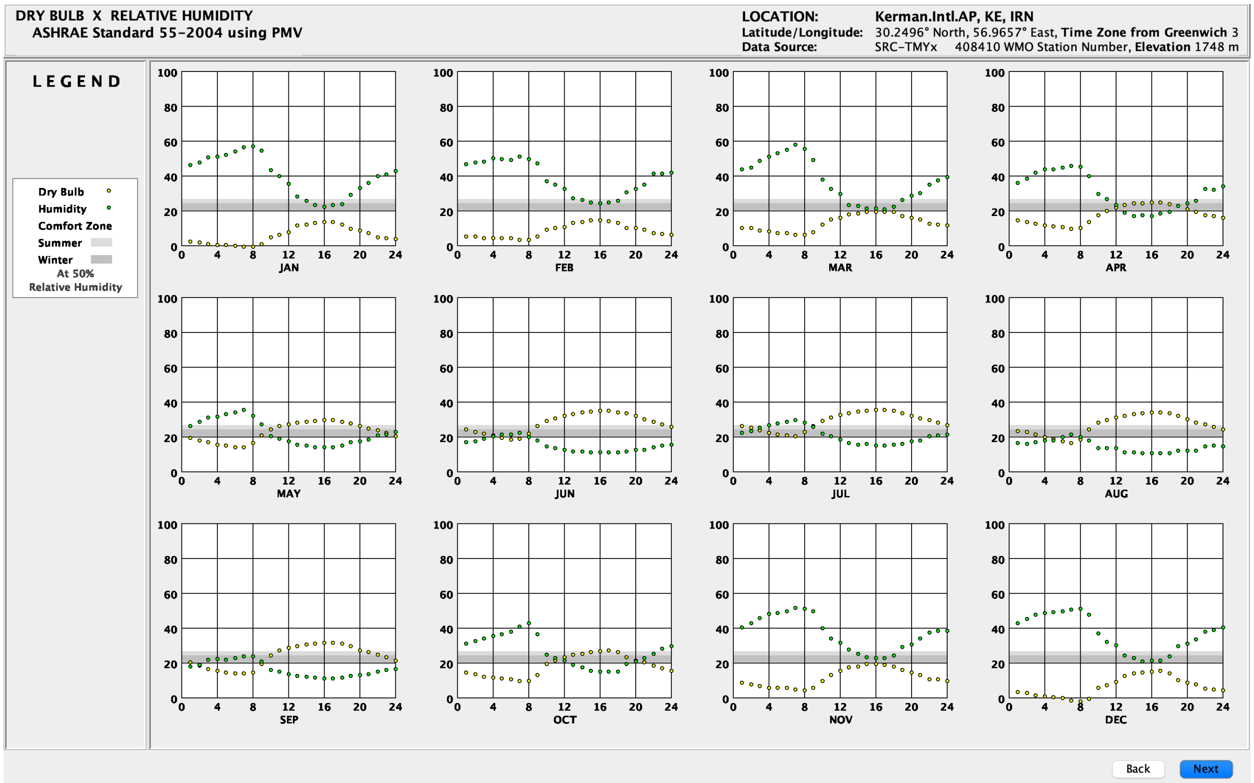
Geographic and Climatic Context

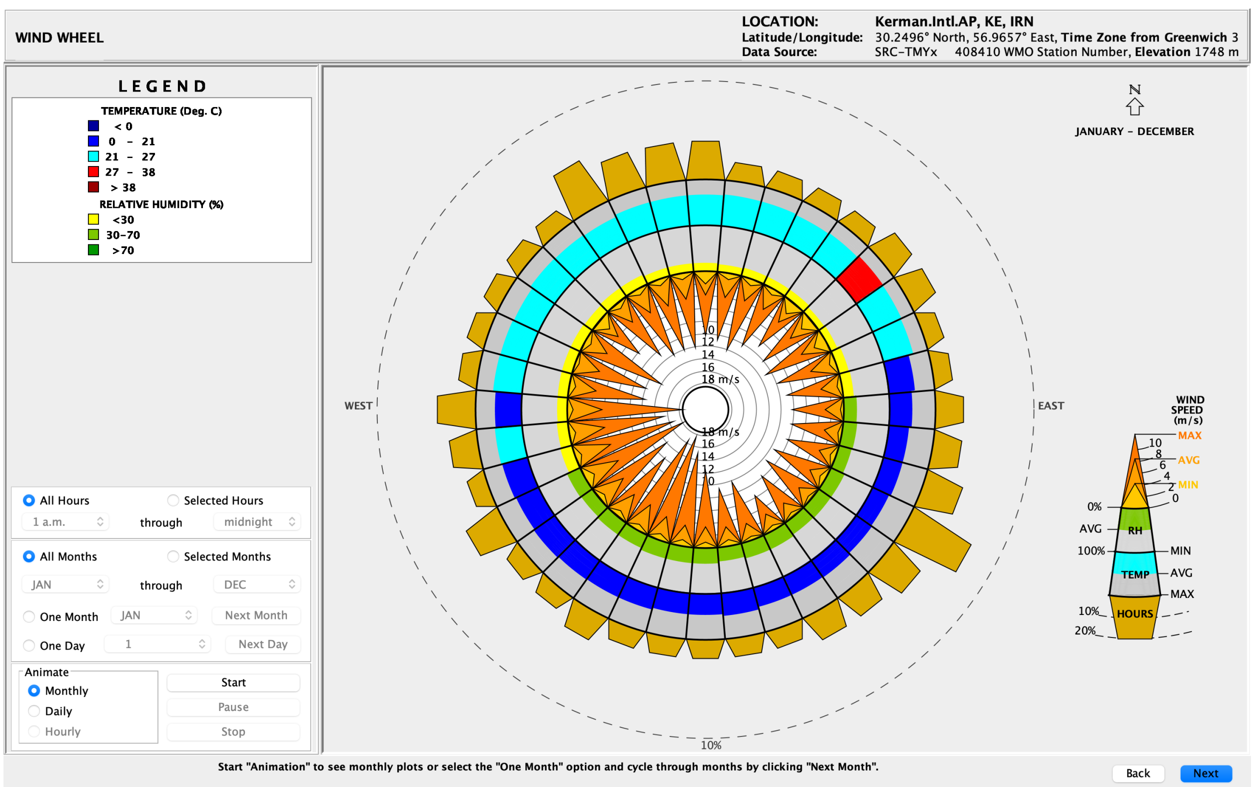
Kerman, located in southeastern Iran at an elevation of 1,755 m, exhibits a cold-arid climate characterized by pronounced seasonal temperature extremes. The hourly profiles of dry-bulb temperature, relative humidity, prevailing wind patterns, and global horizontal and direct normal solar radiation for Kerman are presented in Figures 17–20, as generated using Climate Consultant.

Key Climatic Features

- **Temperature**: Hot summers (to 35°C) and cold winters (below 0°C); notable diurnal swings.
- **Humidity**: Low (30–40%).
- **Wind**: Variable, aiding seasonal ventilation.
- **Solar Radiation**: Abundant (~2,000 kWh/m²·year), dual heating/cooling asset.




DRY BULB X RELATIVE HUMIDITY
ASHRAE Standard 55-2004 using PMV
LOCATION: Kerman.Intl.AP, KE, IRN
Latitude/Longitude: 30.2496° North, 56.9657° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408410 WMO Station Number, Elevation 1748 m
LEGEND
Dry Bulb
Humidity
Comfort Zone
Summer
Winter
At 50% Relative Humidity
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC
Back
Next


WIND WHEEL
LOCATION: Kerman.Intl.AP, KE, IRN
Latitude/Longitude: 30.2496° North, 56.9657° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 408410 WMO Station Number, Elevation 1748 m
LEGEND
TEMPERATURE (Deg. C)
< 0
0 - 21
21 - 27
27 - 38
> 38
RELATIVE HUMIDITY (%)
<30
30-70
>70
All Hours
Selected Hours
1 a.m.
through
midnight
All Months
Selected Months
JAN
through
DEC
One Month
JAN
Next Month
One Day
1
Next Day
Animate
Monthly
Daily
Hourly
Start
Pause
Stop
N
JANUARY - DECEMBER
WEST
EAST
18 m/s
10%
WIND SPEED (m/s)
MAX
AVG
MIN
RH
TEMP
HOURS
Start "Animation" to see monthly plots or select the "One Month" option and cycle through months by clicking "Next Month".
Back
Next

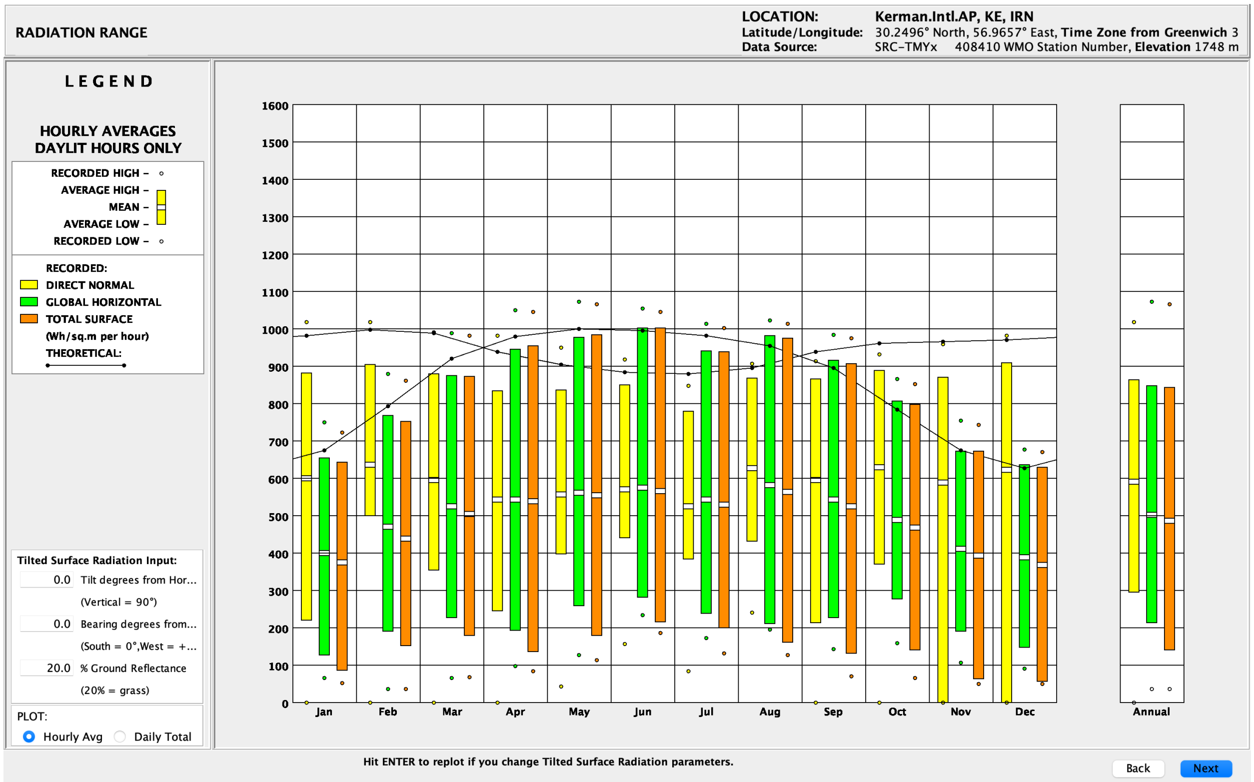


Figure 17-20: Hourly dry-bulb temperature, relative humidity, wind rose, and global horizontal/direct normal radiation profiles for Kerman (generated via Climate Consultant).

Thermal Comfort and PCM Implications

The psychrometric chart for Kerman (Figure 21) shows that only 18.2 % of the annual hours fall within the comfort zone, with conditions distributed between cold winters and hot-dry summers, confirming a bimodal climate pattern. The analysis indicates significant potential for both heating (15.8 %) and evaporative cooling (20–21 %) strategies, supported by high thermal mass and night flushing. This dual seasonal behavior makes Phase Change Materials (PCMs) highly suitable for Kerman. PCMs with melting points around 25–27 °C can effectively absorb excess heat during summer days and release it through night ventilation, while lower melting points (21–23 °C) help capture and store solar gains in winter. Multi-layer PCM applications integrated within walls and roofs can thus balance annual thermal loads, reducing both heating and cooling demands across seasons.

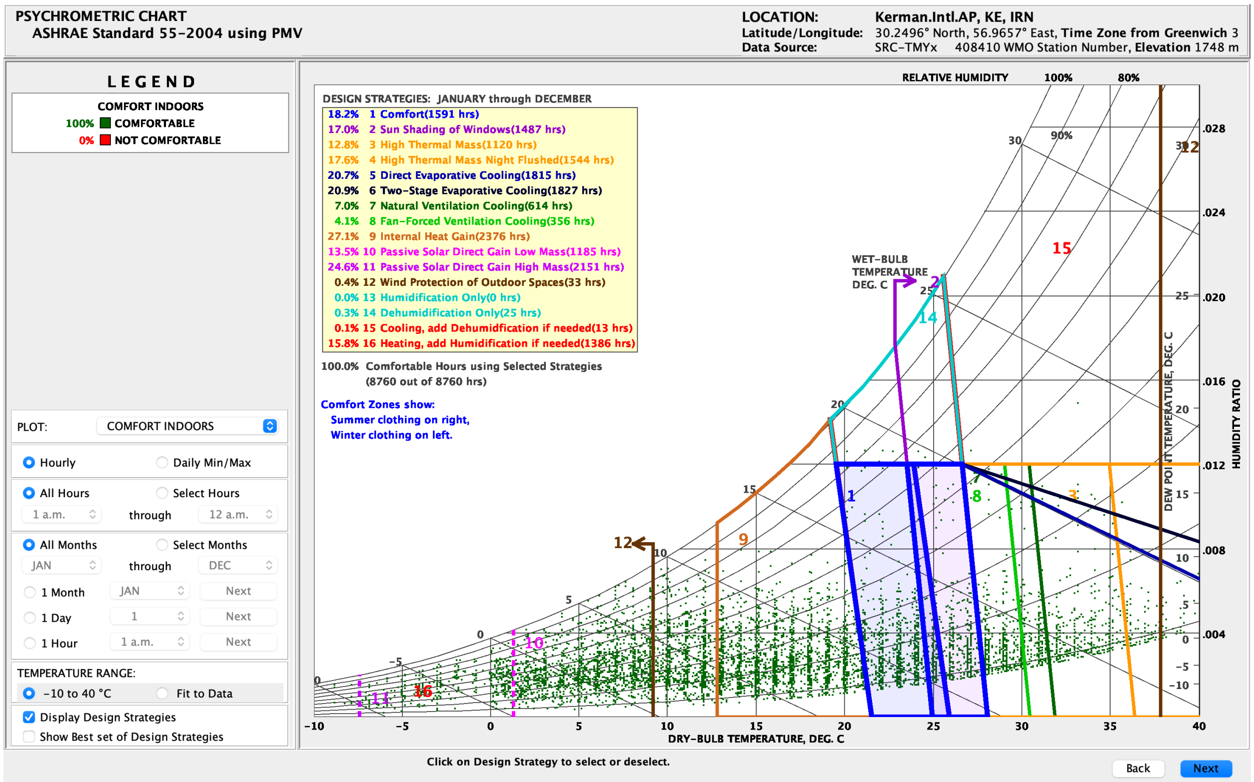


Figure 21: Psychrometric chart with passive strategies for Kerman, generated using Climate Consultant software (UCLA Energy Design Tools Group, 2024).

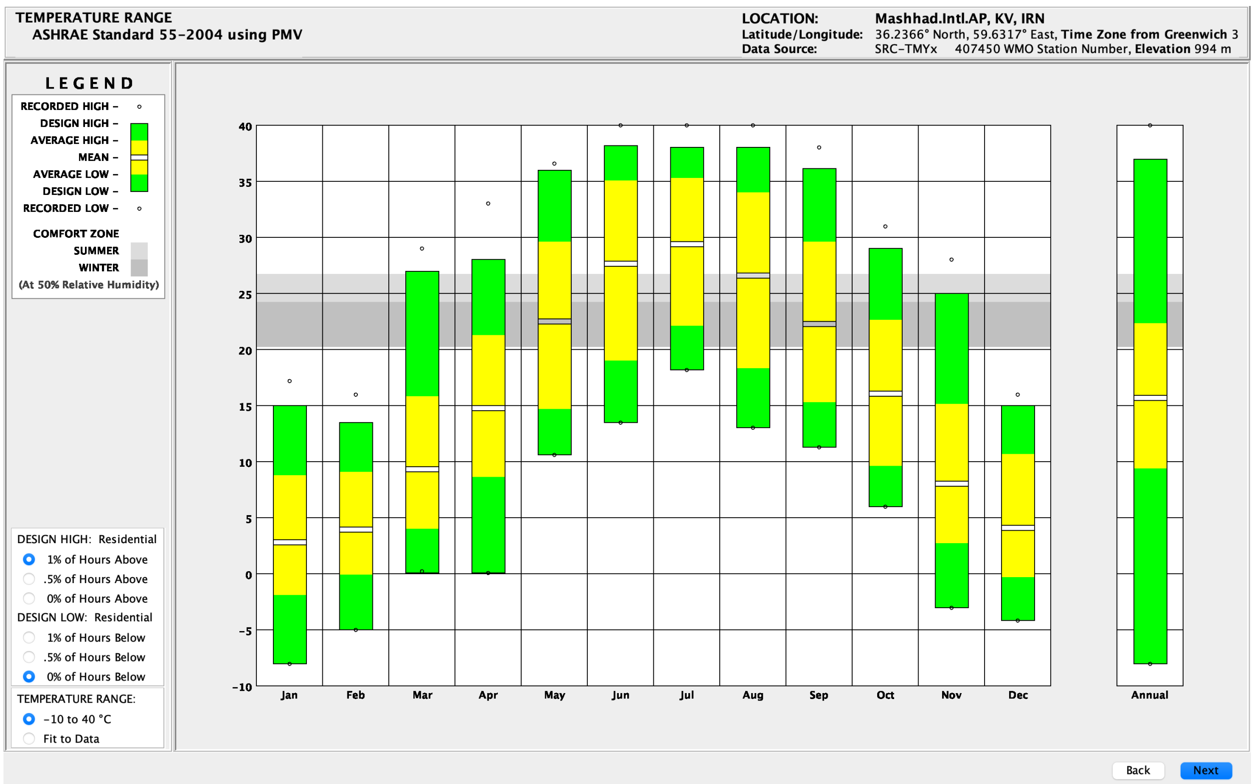
4.3.4 Mashhad – Cold Semi-Arid Climate (BSk)

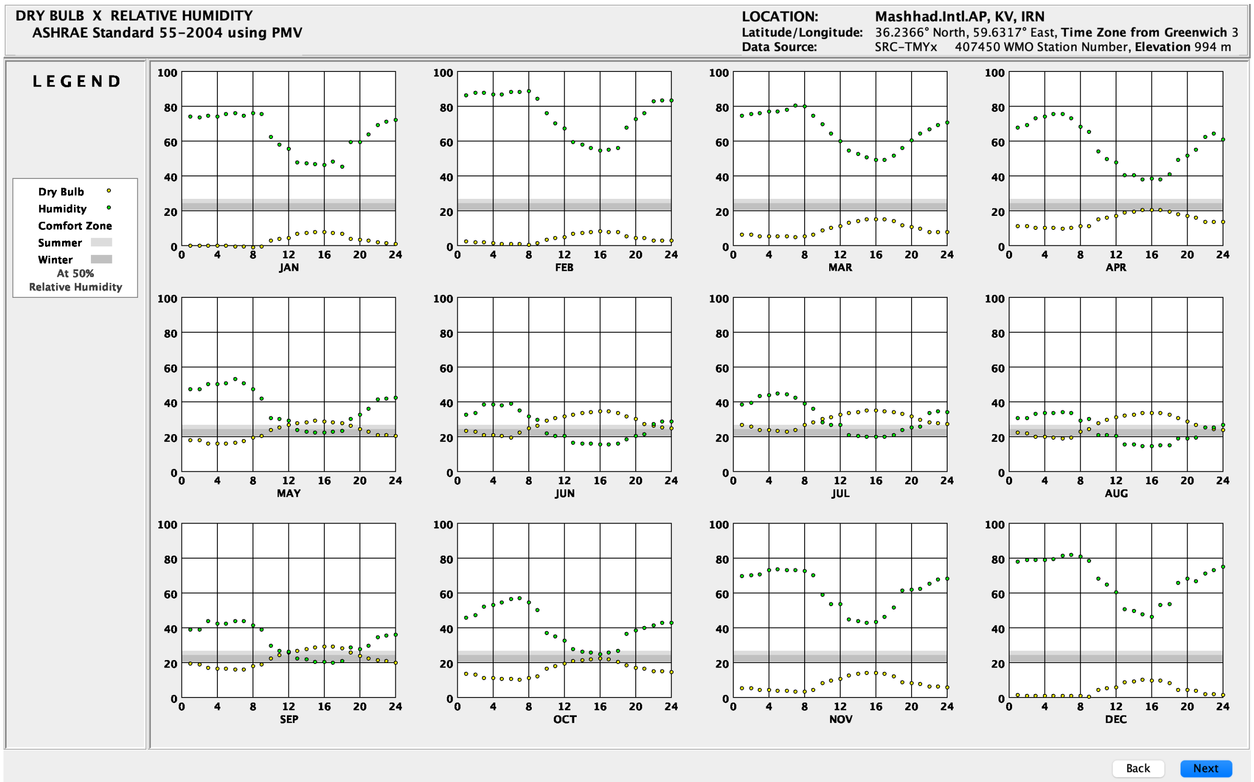
Geographic and Climatic Context

Mashhad, located in northeastern Iran at an elevation of 995 m within the Kashaf River valley, exhibits a climate influenced by continental conditions with a predominantly heating-dominated profile. The hourly distributions of dry-bulb temperature, relative humidity, prevailing wind patterns, and global horizontal and direct normal solar radiation for Mashhad are presented in Figures 22–25, as generated using Climate Consultant.

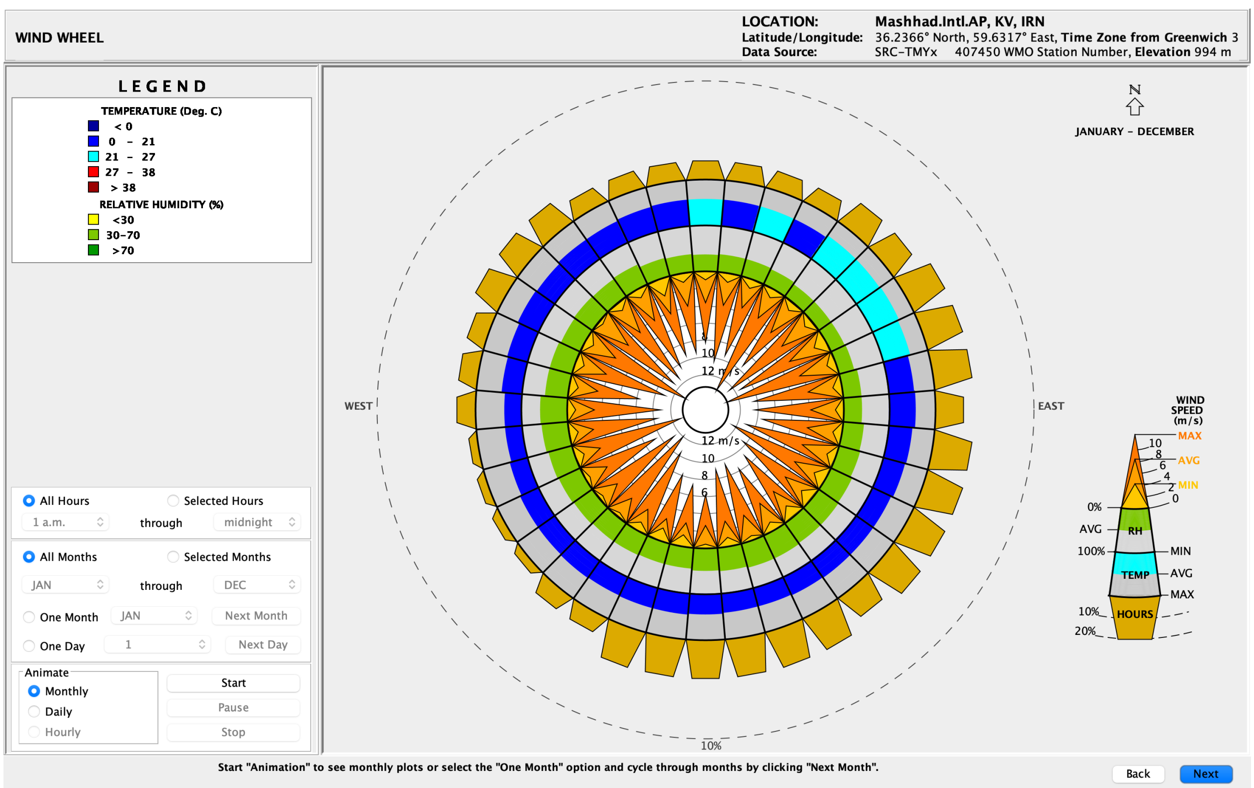
Key Climatic Features

- **Temperature:** Warm summers (to 35°C); severe winters (to -10°C or lower) with snowfall.
- **Humidity:** Moderate (40–50%).
- **Wind:** Seasonal, exacerbating winter chill.
- **Solar Radiation:** Reliable (~1,900 kWh/m²·year) for passive heating.





DRY BULB X RELATIVE HUMIDITY
ASHRAE Standard 55-2004 using PMV
LOCATION: Mashhad.Intl.AP, KV, IRN
Latitude/Longitude: 36.2366° North, 59.6317° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 407450 WMO Station Number, Elevation 994 m
LEGEND
Dry Bulb
Humidity
Comfort Zone
Summer
Winter
At 50%
Relative Humidity
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC
Back
Next



WIND WHEEL
LOCATION: Mashhad.Intl.AP, KV, IRN
Latitude/Longitude: 36.2366° North, 59.6317° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 407450 WMO Station Number, Elevation 994 m
LEGEND
TEMPERATURE (Deg. C)
< 0
0 - 21
21 - 27
27 - 38
> 38
RELATIVE HUMIDITY (%)
<30
30-70
>70
All Hours
Selected Hours
1 a.m.
through
midnight
All Months
Selected Months
JAN
through
DEC
One Month
JAN
Next Month
One Day
1
Next Day
Animate
Monthly
Daily
Hourly
Start
Pause
Stop
N
JANUARY - DECEMBER
WEST
EAST
12 m/s
10%
WIND SPEED (m/s)
MAX
AVG
MIN
RH
TEMP
HOURS
Start "Animation" to see monthly plots or select the "One Month" option and cycle through months by clicking "Next Month".
Back
Next

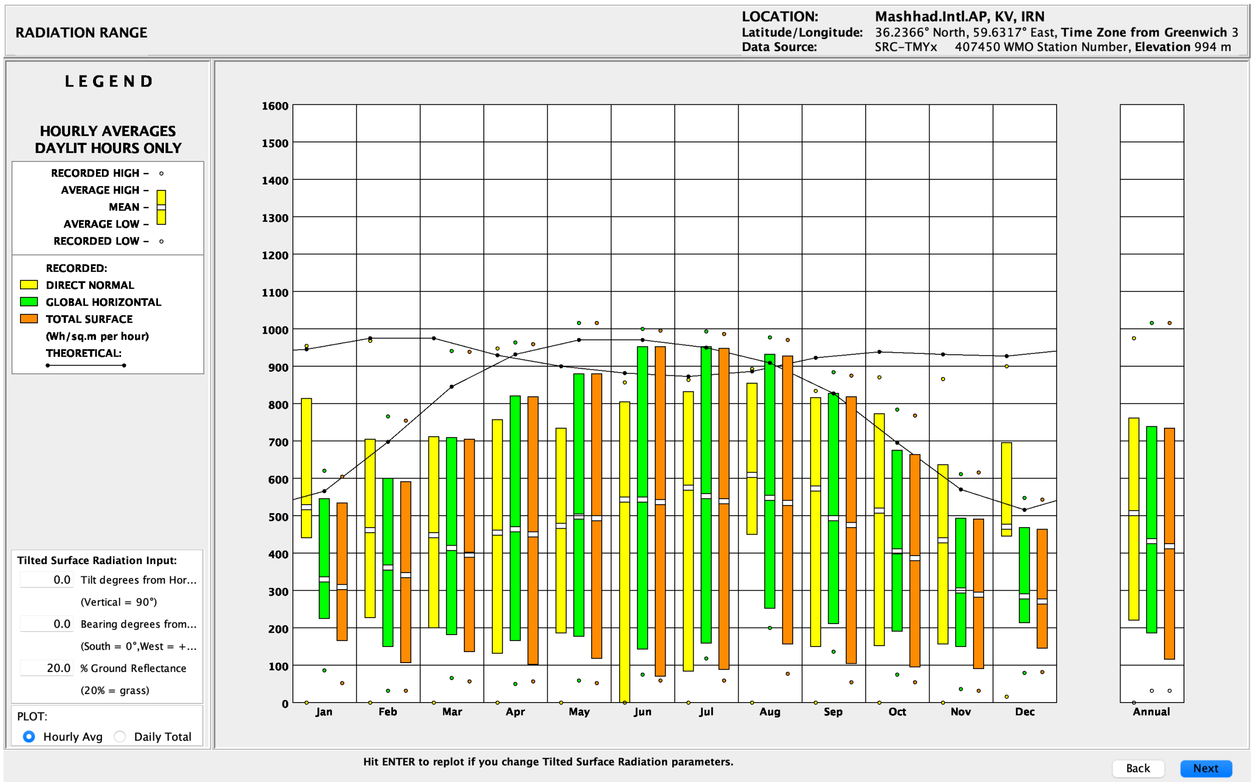


Figure 22-25: Hourly dry-bulb temperature, relative humidity, wind rose, and global horizontal/direct normal radiation profiles for Mashhad (generated via Climate Consultant).

Thermal Comfort and PCM Implications

The psychrometric analysis for Mashhad (Figure 26) shows that only 19.5 % of annual hours lie within the comfort zone, while a large portion of the year is dominated by cold conditions, with heating requirements accounting for 25.4 % of the total hours. The chart highlights that passive solar direct gain (20–21 %) and high thermal mass strategies play an important role in improving comfort during the heating season. This pattern emphasizes the need to prioritize heating demand reduction, especially during extended cold stress periods. Phase Change Materials (PCMs) with melting points between 21–23 °C are most effective for storing daytime solar gains and releasing them at night, particularly when applied to south-facing walls or interior surfaces. While summer benefits remain secondary, the integration of PCMs can contribute to smoother indoor temperature profiles and reduced heating energy demand in Mashhad's cold semi-arid climate.

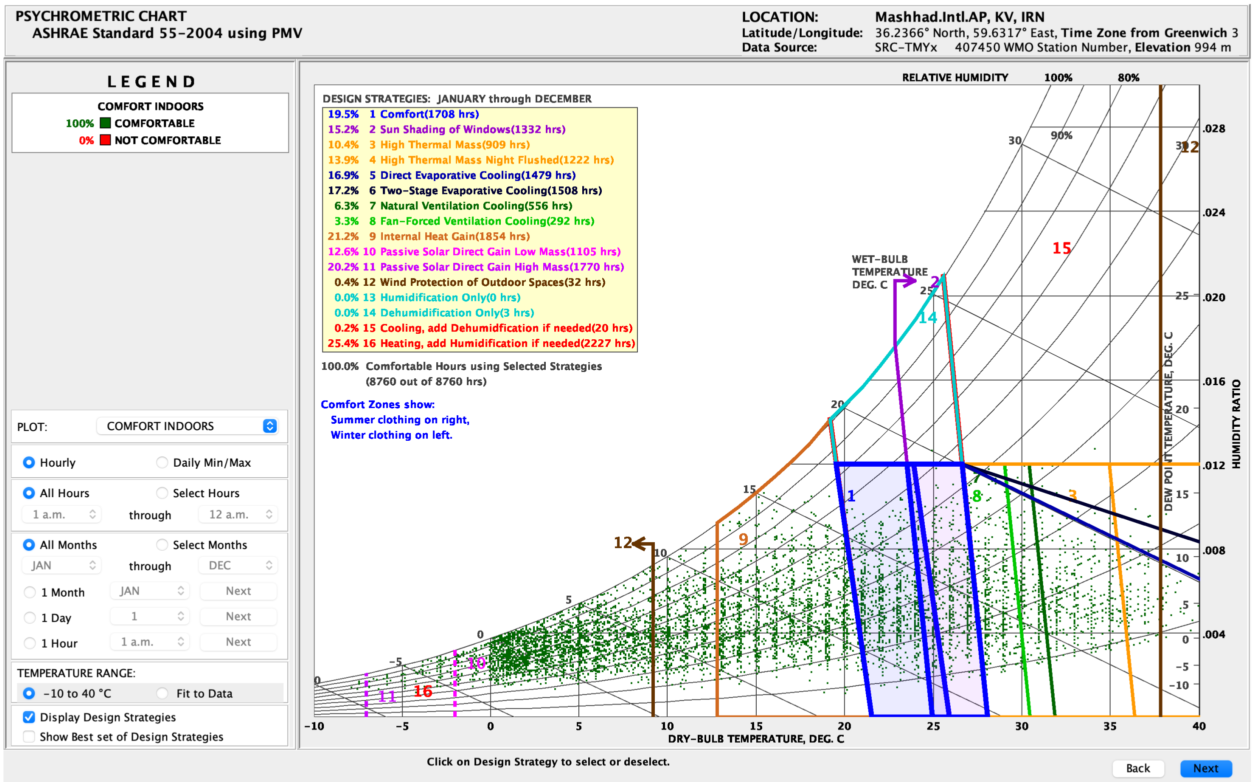


Figure 26: Psychrometric chart with passive strategies for Mashhad, generated using Climate Consultant software (UCLA Energy Design Tools Group, 2024).

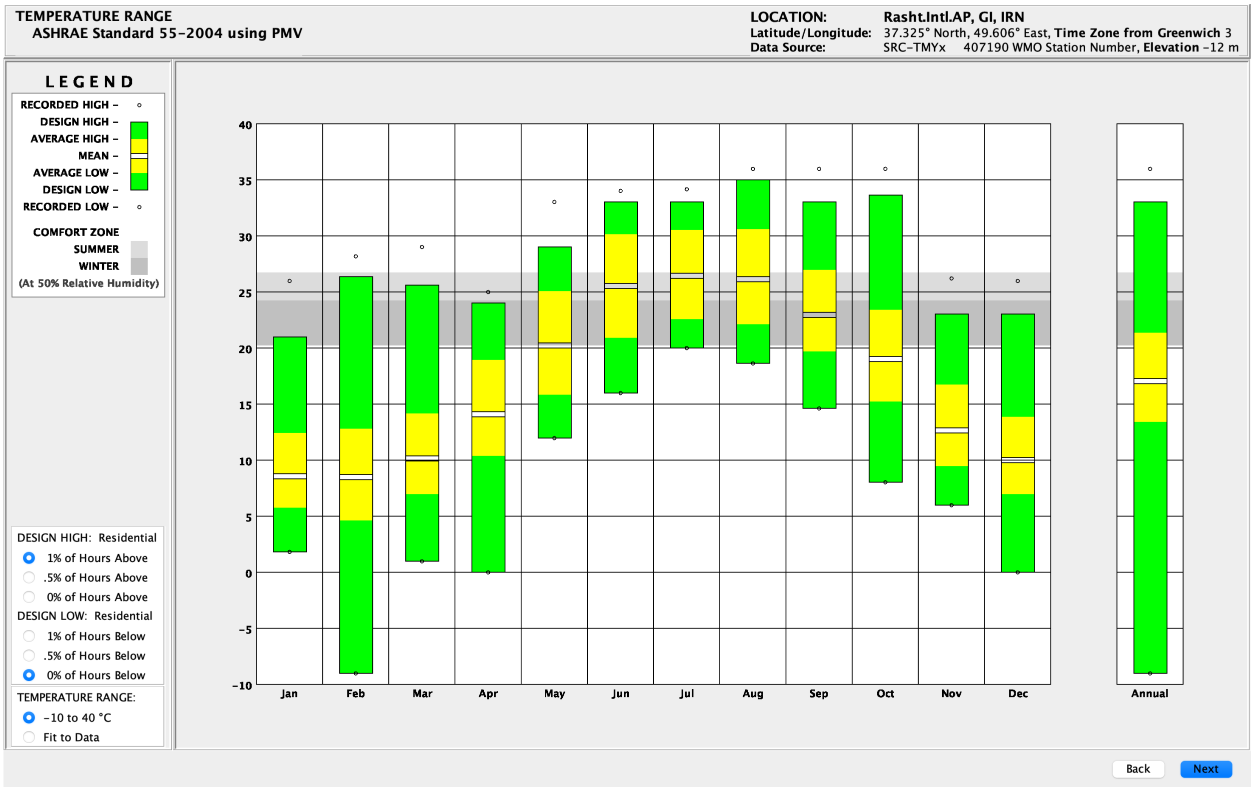
4.3.5 Rasht – Humid Subtropical Climate (Cfa)

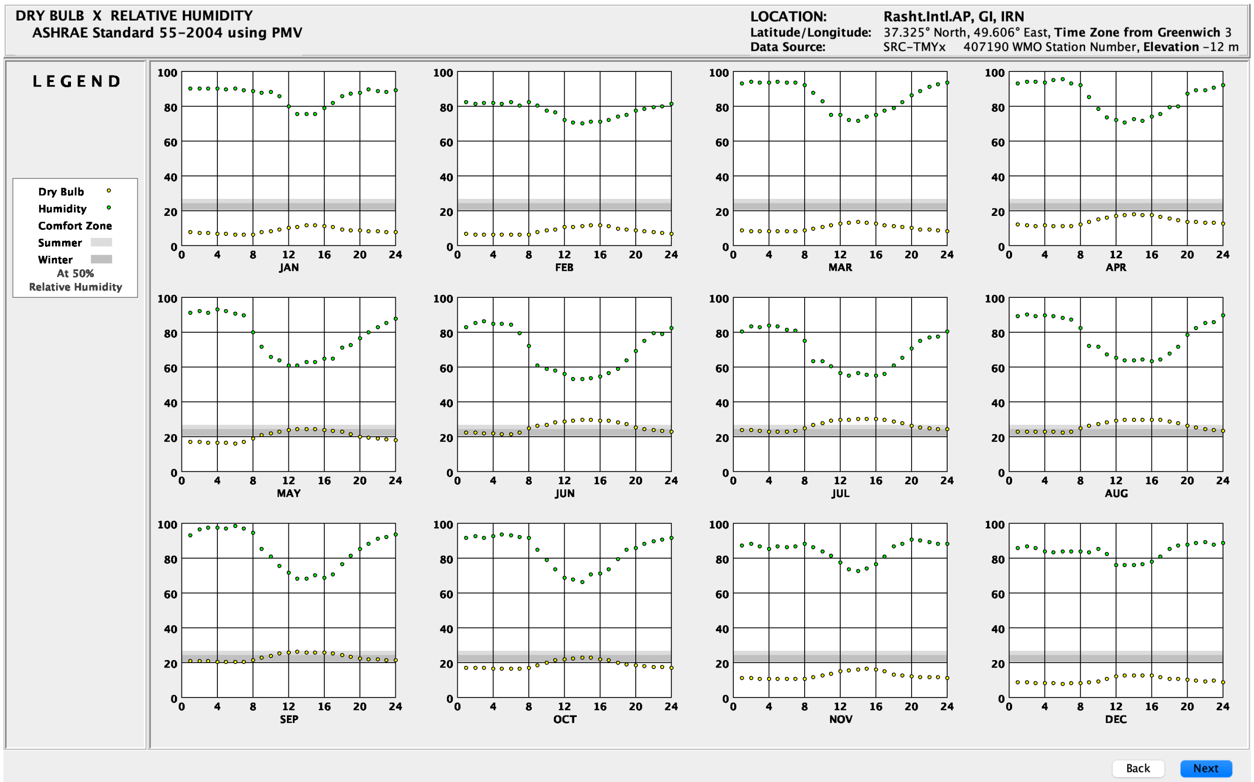
Geographic and Climatic Context

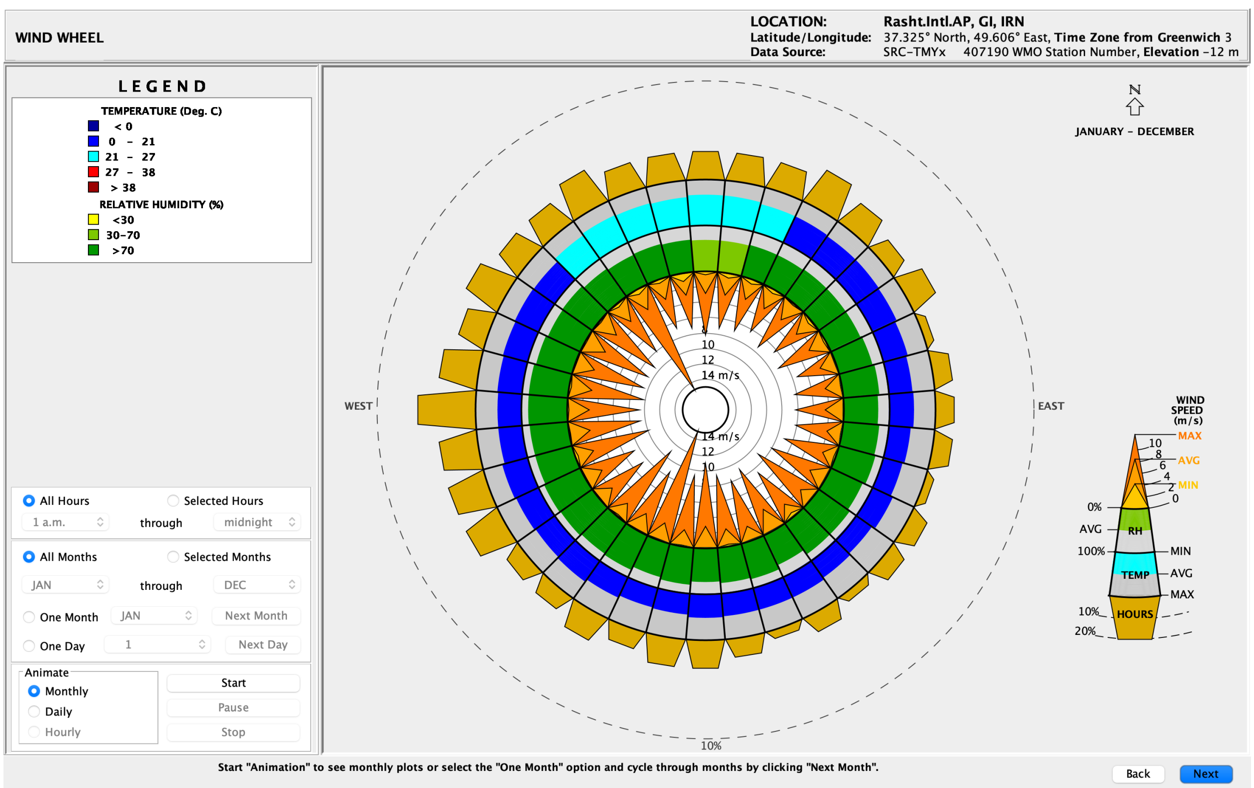
Rasht, a coastal city located between the Caspian Sea and the Alborz Mountains, experiences a mild and humid climate and is recognized as Iran's wettest major city. The hourly profiles of dry-bulb temperature, relative humidity, prevailing wind patterns, and global horizontal and direct normal solar radiation for Rasht are presented in Figures 27–30, as generated using Climate Consultant.

Key Climatic Features

- **Temperature:** Mild winters (>5°C); warm-humid summers (<35°C); small diurnal range.
- **Humidity:** High (80%+), with heavy precipitation.
- **Wind:** Moisture-laden breezes.
- **Solar Radiation:** Cloud-reduced (~1,600 kWh/m²·year).




DRY BULB X RELATIVE HUMIDITY
ASHRAE Standard 55-2004 using PMV
LOCATION: Rasht.Intl.AP, GI, IRN
Latitude/Longitude: 37.325° North, 49.606° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 407190 WMO Station Number, Elevation -12 m
LEGEND
Dry Bulb
Humidity
Comfort Zone
Summer
Winter
At 50%
Relative Humidity
JAN
FEB
MAR
APR
MAY
JUN
JUL
AUG
SEP
OCT
NOV
DEC
Back
Next


WIND WHEEL
LOCATION: Rasht.Intl.AP, GI, IRN
Latitude/Longitude: 37.325° North, 49.606° East, Time Zone from Greenwich 3
Data Source: SRC-TMYx 407190 WMO Station Number, Elevation -12 m
LEGEND
TEMPERATURE (Deg. C)
< 0
0 - 21
21 - 27
27 - 38
> 38
RELATIVE HUMIDITY (%)
<30
30-70
>70
N
JANUARY - DECEMBER
WEST
EAST
10%
WIND SPEED (m/s)
MAX
AVG
MIN
RH
TEMP
HOURS
All Hours
Selected Hours
1 a.m.
through
midnight
All Months
Selected Months
JAN
DEC
One Month
Next Month
One Day
Next Day
Animate
Monthly
Daily
Hourly
Start
Pause
Stop
Start "Animation" to see monthly plots or select the "One Month" option and cycle through months by clicking "Next Month".
Back
Next

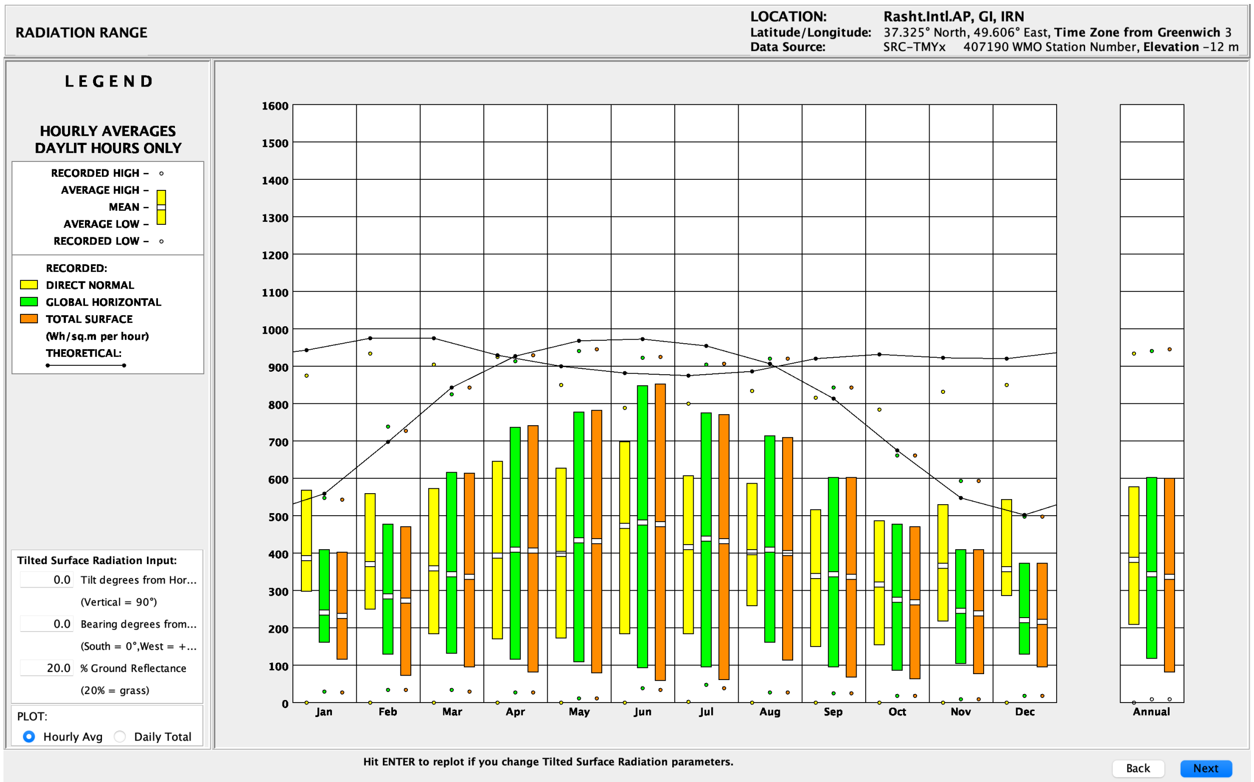


Figure 27-30: Hourly dry-bulb temperature, relative humidity, wind rose, and global horizontal/direct normal radiation profiles for Rasht (generated via Climate Consultant).

Thermal Comfort and PCM Implications

The psychrometric chart for Rasht (Figure 31) reveals that only 6.3 % of the annual hours fall within the comfort zone, while most conditions lie within the humid and cool regions, emphasizing persistent discomfort due to high relative humidity. The analysis shows that dehumidification (22.0 %) and heating (23.3 %) are the dominant strategies needed to achieve thermal comfort, as the high moisture content limits the effectiveness of natural ventilation and evaporative cooling. Under such conditions, thin Phase Change Material (PCM) layers with melting points around 21–23 °C can moderate short-term indoor temperature fluctuations but experience restricted charge–discharge cycles because of frequent cloud cover and limited solar radiation. Therefore, PCM systems should be coupled with controlled ventilation or dehumidification mechanisms to ensure effective latent heat exchange and maintain indoor comfort in Rasht's humid-temperate climate.

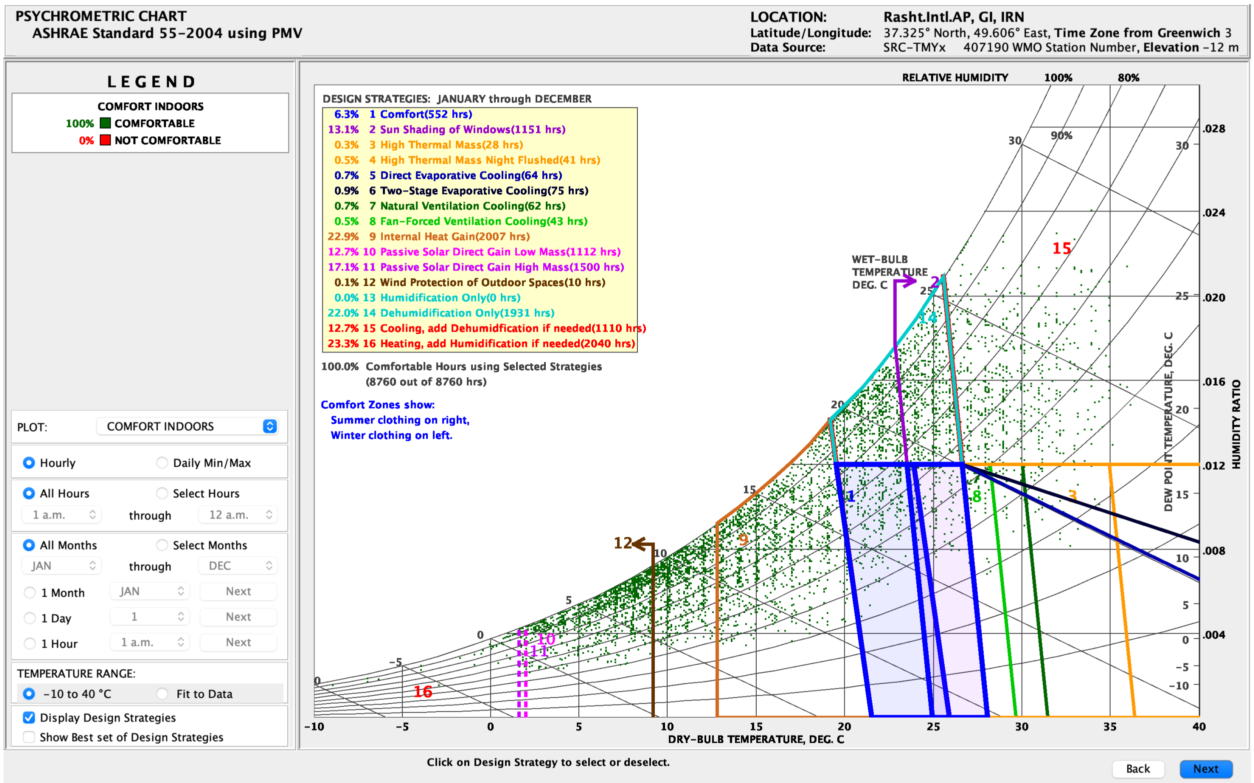


Figure 31: Psychrometric chart with passive strategies for Rasht, generated using Climate Consultant software (UCLA Energy Design Tools Group, 2024).

4.4 Comparative Analysis and PCM Optimization Insights

The climatic analyses presented in Section 4.3 demonstrate that the five selected cities pose fundamentally different thermal challenges, ranging from extreme cooling-dominance in Yazd to significant heating-dominance in Mashhad. These diverse boundary conditions directly influence the potential efficacy of passive PCM integration. The multi-objective optimization (MOO) framework, designed to minimize Energy Use Intensity (EUI) and maximize Thermal Comfort

Percentage (TCP), must navigate these varying conditions to identify optimal, climate-specific PCM configurations.

This section synthesizes the climatic implications from the case studies to provide a comparative analysis and anticipate the key optimization insights regarding PCM parameters.

4.4.1 Cross-Climatic Performance Potential

The most significant factor determining passive PCM effectiveness is the diurnal temperature swing—the difference between daytime highs and nighttime lows. A large swing, particularly one that crosses the PCM's melting/solidification points, is essential for a complete daily charge-discharge cycle.

- High Potential (Arid Climates: Yazd BWh, Kerman BWk): These hot-dry and cold-arid climates exhibit large diurnal temperature ranges (>15°C). This allows PCMs to fully charge (melt) by absorbing intense solar and internal gains during the day and, crucially, fully discharge (solidify) by releasing that heat into the cool night environment. This complete cycling maximizes latent heat storage potential, leading to significant expected reductions in both cooling loads (Yazd) and balanced seasonal loads (Kerman).
- Low Potential (Humid Climates: Bushehr BSh, Rasht Cfa): These hot-humid and humid-temperate climates are characterized by small diurnal temperature swings and high ambient humidity. Persistently high nighttime temperatures (often remaining above 25-27°C in Bushehr) prevent the PCM from adequately discharging. The material may remain in a liquid or partially-liquid state, becoming saturated after the first day and subsequently acting as a simple, low-R-value insulating layer. Consequently, the optimization is

expected to show marginal EUI and TCP improvements, highlighting the need for hybrid systems (e.g., active night ventilation) in these climates.

- Heating-Dominant Potential (Cold Climates: Mashhad BSk): As a cold semi-arid climate, Mashhad's primary challenge is heating. Here, the optimization goal for the PCM shifts. Instead of just mitigating summer heat, the PCM is optimized to absorb winter daytime solar gains (which are significant, as shown in Fig. 26) and internal heat gains, releasing this stored energy during the cold night. This process directly reduces heating EUI. The large diurnal range in this climate is also beneficial for summer cooling, making the PCM a viable year-round strategy.

4.5 Summary

This comparative analysis establishes PCM optimization as inherently localized and parameter driven. Yazd and Kerman exemplify high-potential autonomous regulation; Mashhad highlights year-round versatility; Bushehr and Rasht expose passive limitations, mandating hybrid approaches. These empirically grounded insights bridge simulation results to actionable guidelines in Chapter 6, advancing climate-responsive PCM deployment in Iranian office buildings. Detailed city-specific Pareto solutions are elaborated in Chapter 5.

5. Results and Discussion

5.1 Introduction

This chapter presents the outcomes of the multi-objective optimization framework, bridging the methodological foundations (Chapter 3) and case-study specifications (Chapter 4). It details simulation results, Pareto-optimal solutions, and cross-climatic insights for Phase Change Material (PCM) integration in office buildings across five Iranian climates (Yazd: hot-dry; Bushehr: hot-humid; Kerman: cold-arid; Mashhad: cold semi-arid; Rasht: humid-temperate). The primary objectives—minimizing Energy Use Intensity (EUI) and maximizing Thermal Comfort Percentage (TCP)—are evaluated against a non-PCM baseline model.

5.2 Optimization Framework and Objective Functions

5.2.1 Formal Definition of Objective Functions

Energy Use Intensity (EUI) is defined as annual primary energy consumption per unit floor area:

$$EUI = \frac{\sum(Eheating + Ecooling + Elighting + Eequipment)}{Afloor} \text{ (kWh/m}^2\text{/year)}$$

Thermal Comfort Percentage (TCP) is the fraction of occupied hours within the ASHRAE 55 adaptive comfort zone:

$$TCP = \frac{\sum h\ comfort}{\sum h\ occupied} \times 100\ (\%)$$

Trade-offs are visualized via Pareto fronts, with interpretation criteria emphasizing knee points for balanced solutions.

5.2.2 Parametric Workflow and Optimization Algorithm

The Rhino/Grasshopper environment integrates:

- **Ladybug/Honeybee:** Climate data processing and EnergyPlus simulation.
- **ChameleonPCM**: Custom plugin for dynamic PCM property injection (type, melting point, thickness, placement).
- **Octopus (NSGA-II)**: Multi-objective evolutionary algorithm for Pareto front generation.

Parametric variables are managed via data trees; workflow validation ensures convergence and output reliability (refer to Figures for schematic diagrams32- 39).

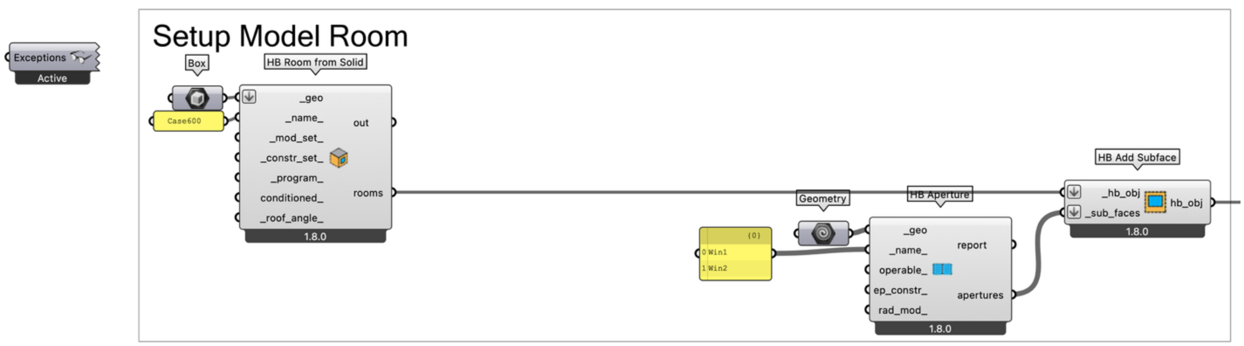


Figure 32: Setup of the baseline thermal zone in Grasshopper.

This part of the workflow defines the reference **Case 600** office model using the *HB Room from Solid* component. The geometry is generated from a simple box and converted into a conditioned Honeybee room with assigned construction and program sets. Two window geometries (*Win1* and *Win2*) are then created through the *HB Aperture* component and connected to the main room by *HB Add Subface*, forming the final thermal zone with its apertures. This setup establishes the base geometry for subsequent PCM parameterization and EnergyPlus simulations, ensuring that all optimization cases share identical boundary conditions and envelope configuration.

Figure 33: Definition of window construction in Grasshopper.

This section of the workflow defines the optical and thermal properties of the glazing system using the HB Window Material and HB Window Construction components. The window type "Double" is characterized by a U-factor of 2.72 $W/m^2 \cdot K$, solar heat gain coefficient (SHGC) of 0.76, and visible transmittance (VT) of 0.81, consistent with the baseline office model defined in Chapter 3. The resulting window construction object is then linked to the aperture geometry created in the previous step, ensuring accurate representation of solar gains, daylight transmission, and thermal behavior in the EnergyPlus simulations.

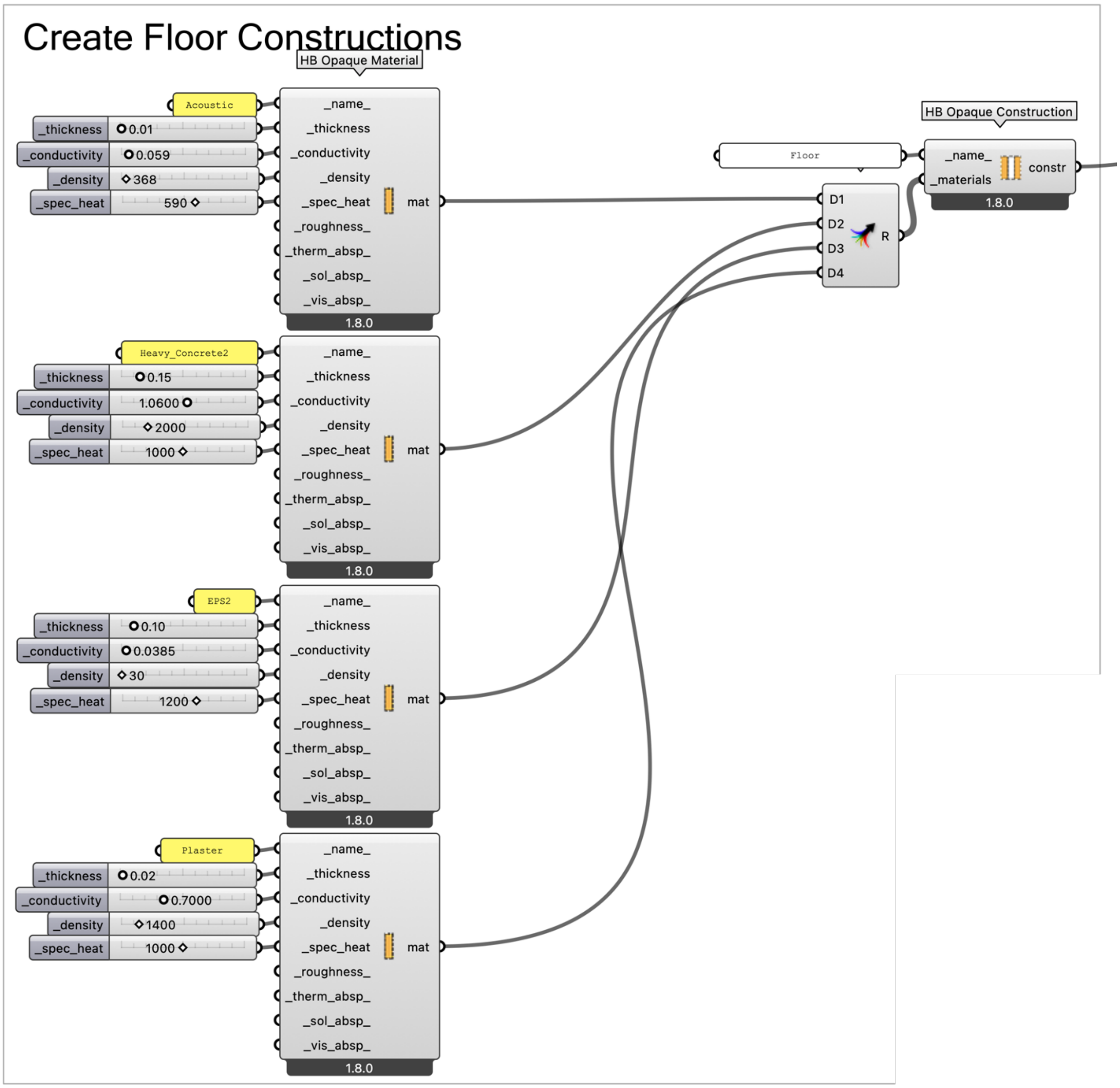


Figure 34: Definition of floor construction layers in Grasshopper.

This segment of the workflow establishes the multilayer composition of the floor assembly using the HB Opaque Material and HB Opaque Construction components. Each material layer is individually defined by its thermophysical properties—thickness, thermal conductivity, density, and specific heat—corresponding to Acoustic tile (0.01 m, 0.059 W/m·K), Heavy Concrete (0.15 m, 1.06 W/m·K), EPS insulation (0.10 m, 0.0385 W/m·K), and Plaster (0.02 m, 0.70 W/m·K). These parameters are consistent with the baseline envelope configuration described in Chapter 3. The layers are combined into a single floor construction object through HB Opaque Construction, forming the thermal mass and insulation base used in subsequent PCM integration and optimization analyses.

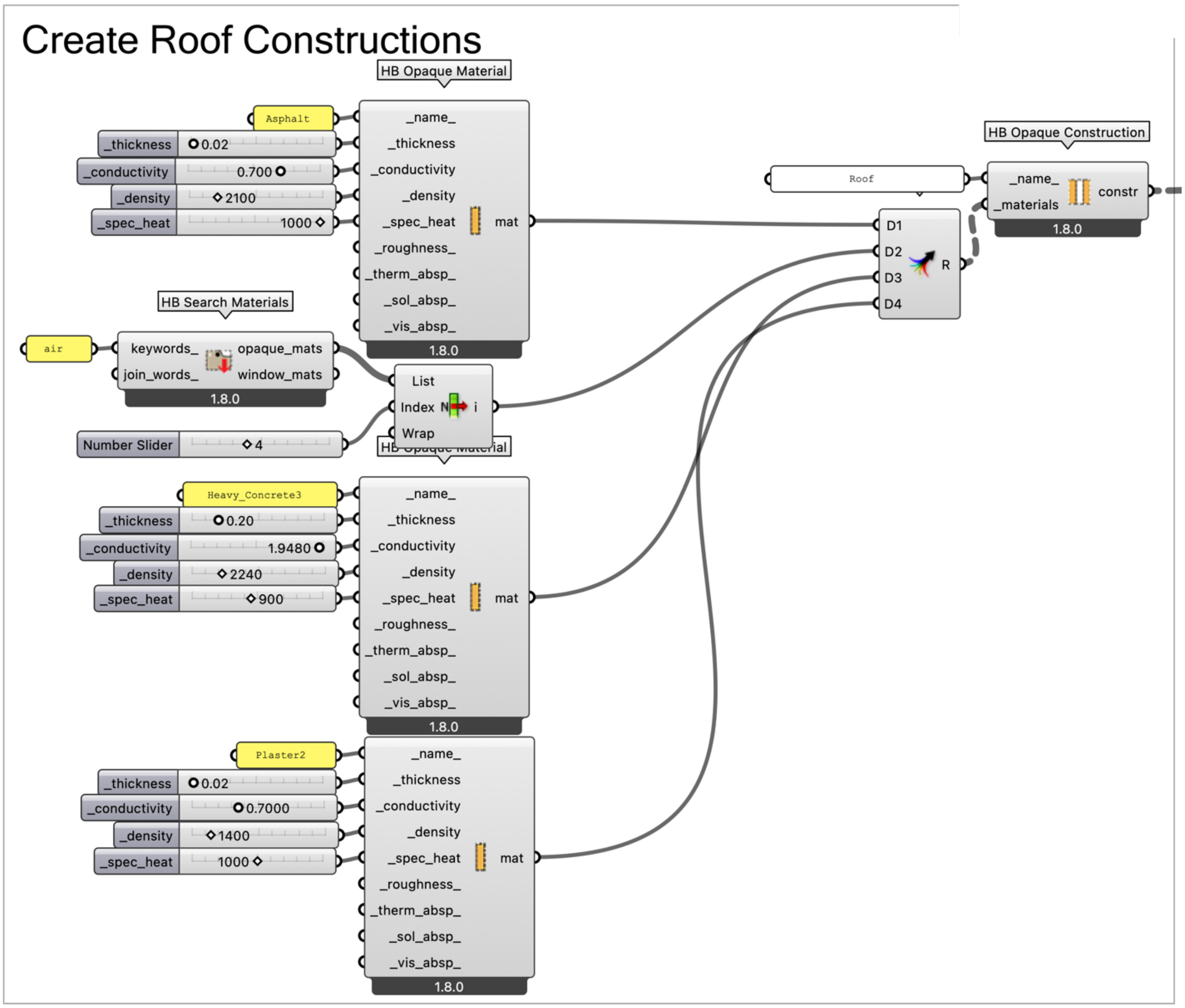


Figure 35: Definition of roof construction layers in Grasshopper.

This portion of the workflow defines the roof assembly through sequential layering of materials using the HB Opaque Material and HB Opaque Construction components. The roof is composed of Asphalt (0.02 m, 0.70 W/m·K), an Air gap (0.10 m), Heavy Concrete (0.20 m, 1.948 W/m·K), and Plaster (0.02 m, 0.70 W/m·K), forming a typical flat roof configuration aligned with the baseline model specifications. The HB Search Materials component retrieves the air-gap definition from the Honeybee library to ensure realistic thermal resistance between layers. The materials are combined into a unified roof construction object via HB Opaque Construction, representing the primary heat exchange interface for PCM integration in the subsequent parametric analyses.

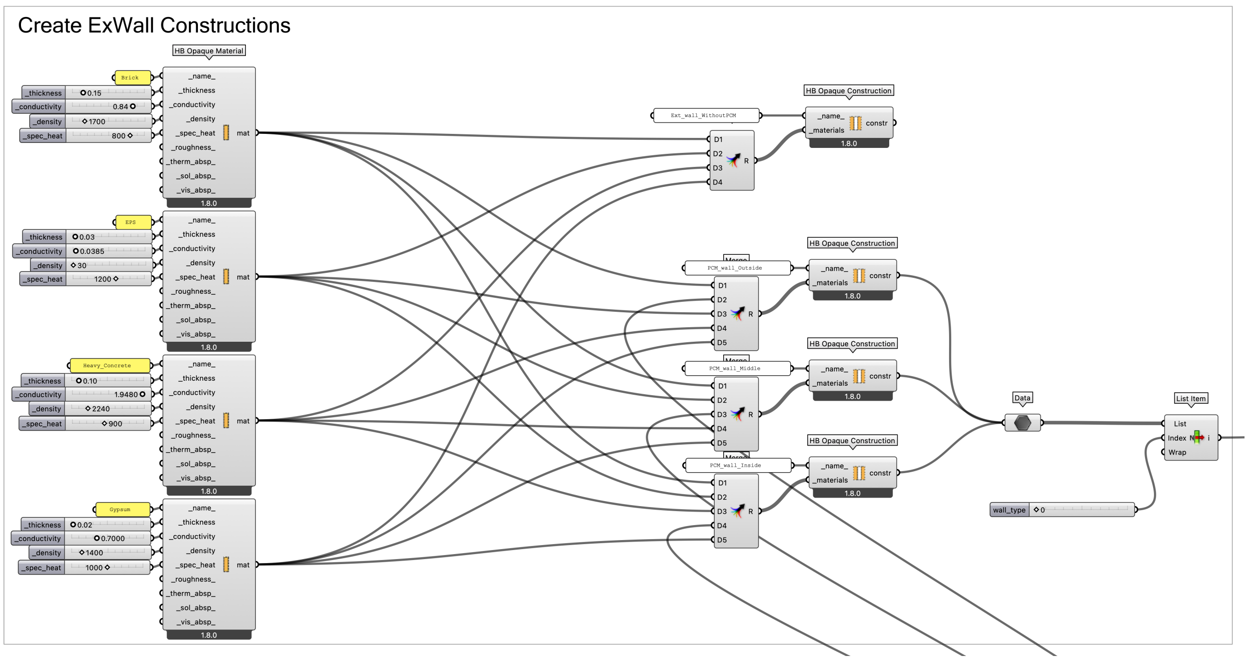


Figure 36: Definition of external wall constructions and PCM layer configurations.

This section of the Grasshopper workflow generates multiple external wall assemblies using the HB Opaque Material and HB Opaque Construction components. Each base wall is composed of Brick (0.15 m, 0.84 W/m·K), EPS insulation (0.03 m, 0.0385 W/m·K), Heavy Concrete (0.10 m, 1.948 W/m·K), and Gypsum plaster (0.02 m, 0.70 W/m·K), reproducing the baseline envelope defined in Chapter 3. Three PCM integration scenarios are then defined:

- **PCM_Wall_Outside:** PCM layer positioned externally, adjacent to the outer surface.
- **PCM_Wall_Middle:** PCM layer embedded within the wall's mid-layer.
- **PCM_Wall_Inside:** PCM layer located on the interior surface, facing the conditioned zone.

The workflow combines these configurations into a list structure to allow automated selection of the wall type during optimization. This modular approach enables the dynamic evaluation of PCM placement effects on energy and comfort performance within the same simulation framework.

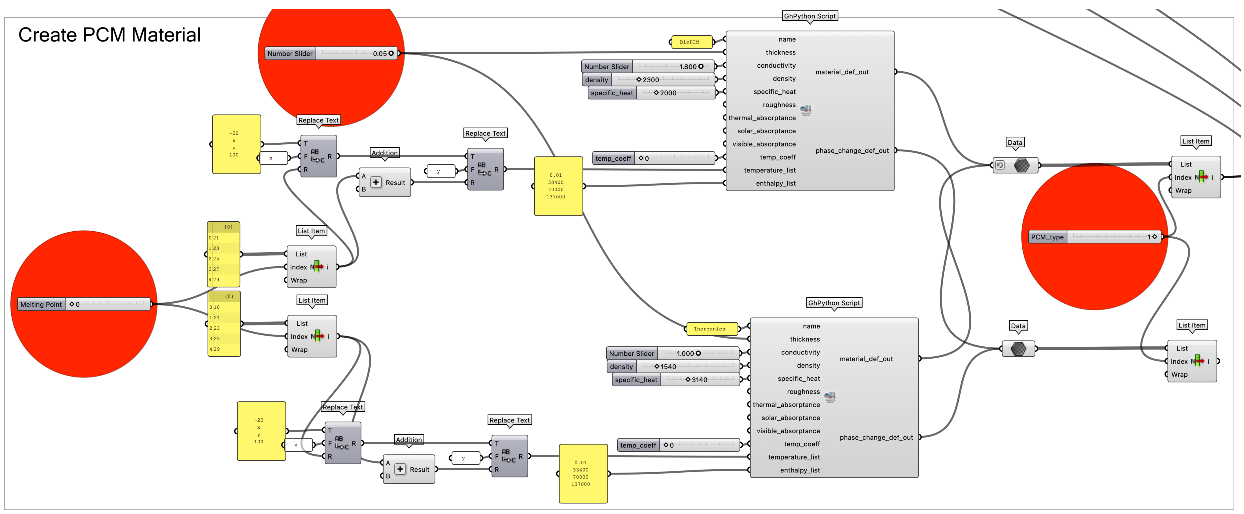


Figure 37: Definition of PCM material properties and parametric control in Grasshopper.

This part of the workflow generates the thermophysical properties of Phase Change Materials (PCMs) using customized GhPython Script components integrated within the ChameleonPCM framework. Two PCM categories are defined—organic (BioPCM) and inorganic (InfiniteR PCM)—each characterized by distinct density, thermal conductivity, and specific heat values. The Number Slider and List Item components allow the selection of melting points (18–29 °C) and thicknesses (0.01–0.05 m), which are dynamically assigned to the PCM layers. The Replace Text and Addition nodes manage the enthalpy–temperature curve definition, ensuring accurate modeling of the latent heat storage behavior across different phase transitions. This parametric structure enables automated generation of PCM variants for optimization, linking each configuration directly to the EnergyPlus material library for energy and comfort performance assessment.

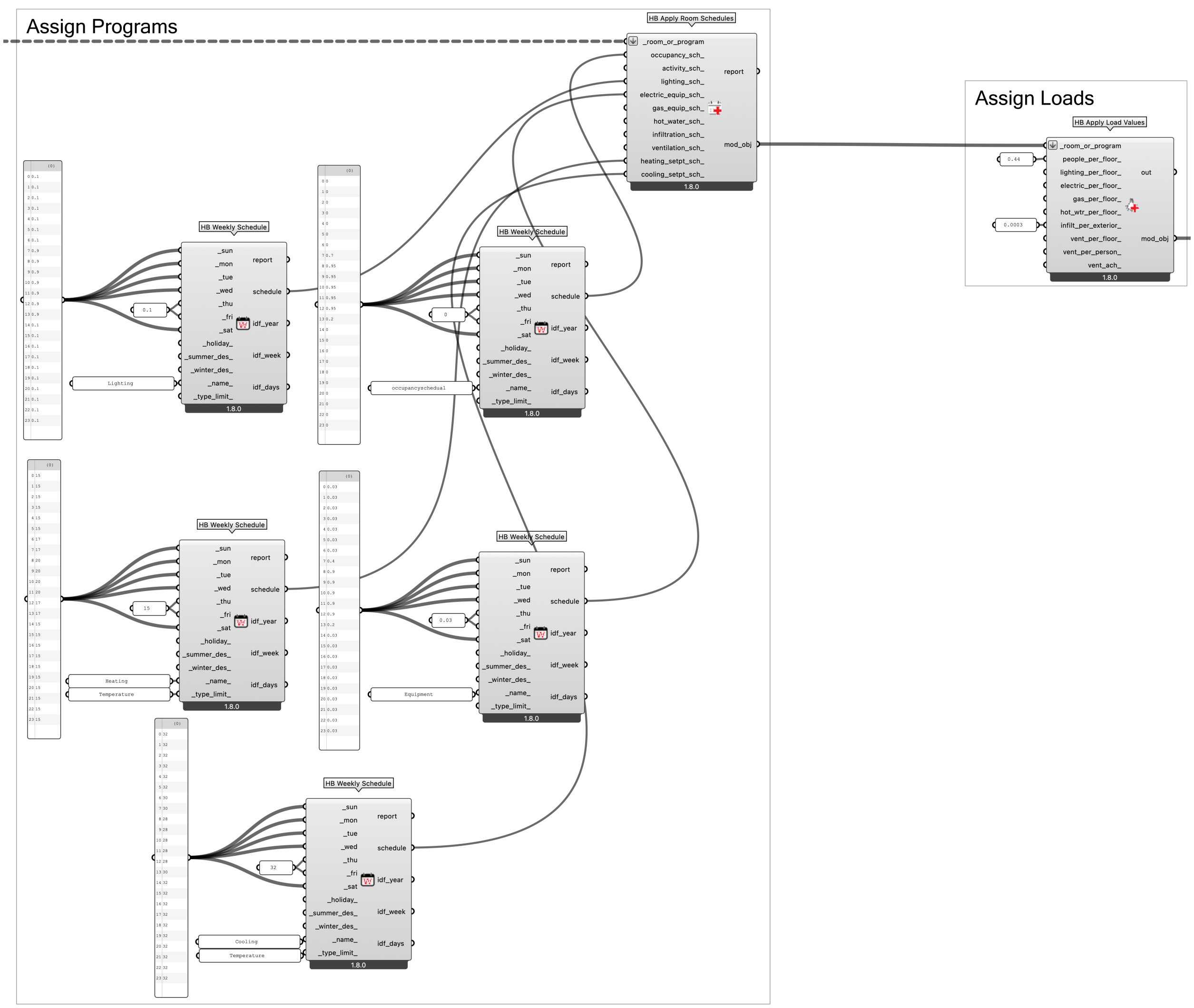


Figure 38: Assignment of internal loads and operational schedules in Grasshopper.

This portion of the workflow establishes the occupancy, lighting, equipment, and HVAC operation schedules for the reference classroom model. Using HB Weekly Schedule components, the daily and seasonal variations in internal gains are defined based on standardized school operation profiles. Each schedule specifies time-dependent patterns for occupancy density, plug loads, lighting usage, and setpoint temperatures for heating and cooling. These schedules are then compiled through the HB Apply Room Schedules component and linked to the thermal zone, ensuring accurate temporal representation of internal loads. Additionally, the HB Apply Load Values component assigns the magnitude of each internal gain source—expressed per unit floor area or per person—according to the base model parameters described in Chapter 3. This configuration guarantees that all optimization cases operate under consistent occupancy and HVAC conditions, isolating the effects of PCM parameters on overall performance.

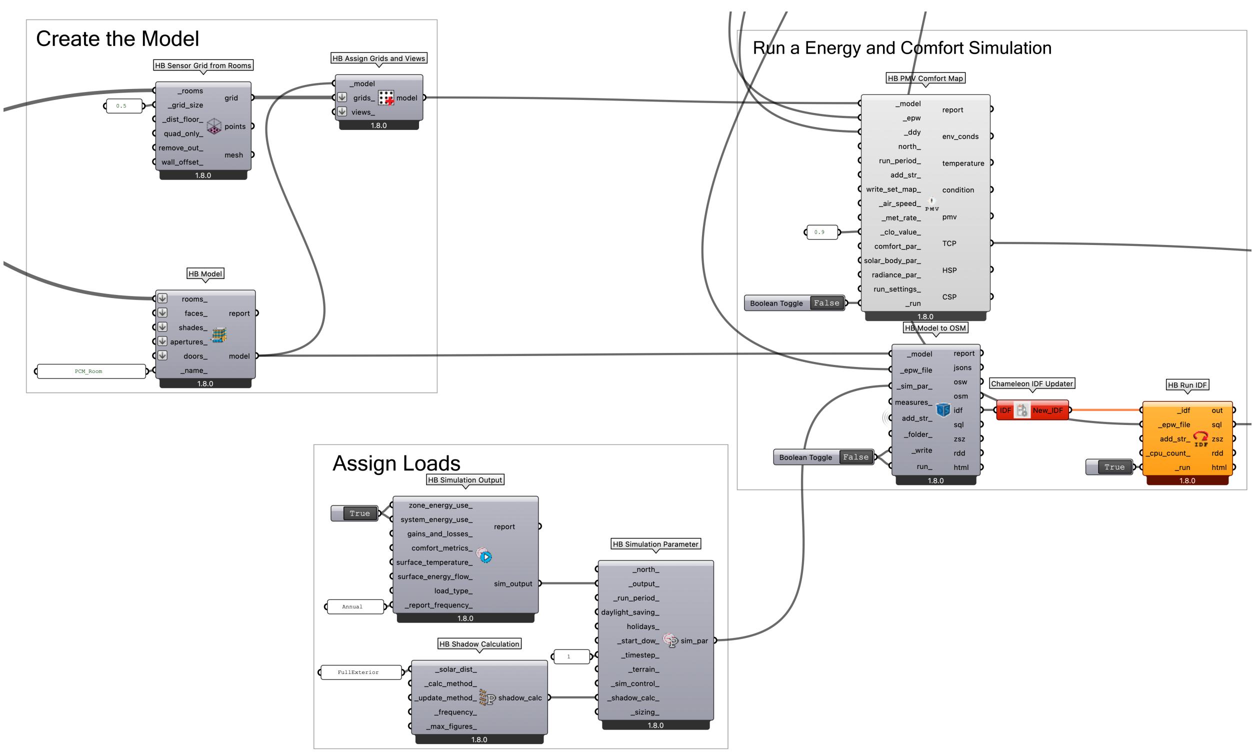


Figure 39: Model generation and simulation process in Grasshopper–EnergyPlus.

This stage of the workflow connects all previous components into a complete simulation-ready model. The HB Model component aggregates the thermal zones, constructions, apertures, and loads into a unified EnergyPlus model, while HB Sensor Grid from Rooms and HB Assign Grids and Views define analysis points for thermal comfort evaluation. The model is then exported through HB Model to OSM and dynamically updated via the ChameleonPCM IDF Updater, which assigns the PCM material definitions and configuration parameters before execution.

Energy and comfort simulations are run using HB Run IDF and HB PMV Comfort Map, generating hourly results for Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP). The simulation setup includes HB Shadow Calculation and HB Simulation Output components to control the reporting frequency, surface energy balance, and comfort metrics. This integrated parametric framework ensures that each PCM variation—defined by its melting point, thickness, and location—is automatically simulated, allowing direct extraction of objective values for the subsequent multi-objective optimization phase.

5.2.3 Overview of the Optimization Solution Space

For each climatic context, the optimization process evaluates the full parametric space defined in Chapter 3, generating a population of candidate PCM configurations. Rather than yielding a single optimal solution, the multi-objective framework produces a set of non-dominated solutions representing different trade-offs between Energy Use Intensity (EUI) reduction and Thermal Comfort Percentage (TCP) improvement. The following sections analyze this solution space to identify trends, sensitivities, and climate-specific design principles.

5.3 Baseline Model Performance

Figures 40 to 44 present the baseline simulation results of the reference classroom model without PCM integration for the five representative Iranian climates: **Bushehr** (hot-humid), **Kerman** (hot-arid), **Mashhad** (cold semi-arid), **Rasht** (humid-temperate), and **Yazd** (hot-dry). Each simulation was evaluated through the **Energy Use Intensity** (**EUI**, $kWh/m^2 \cdot year$) and the **Thermal Comfort Percentage** (**TCP**, %) indices. These values establish the performance benchmark for later PCM-based optimization.

The results show a clear dependency on climatic conditions.

- Bushehr (Figure 40) exhibits the highest energy consumption with an EUI of 192.5 kWh/m^2, primarily driven by cooling demand (151.7 kWh/m^2), while TCP remains extremely low (12.6 %). The persistent humidity and elevated outdoor temperatures significantly limit night-time cooling and natural heat rejection.

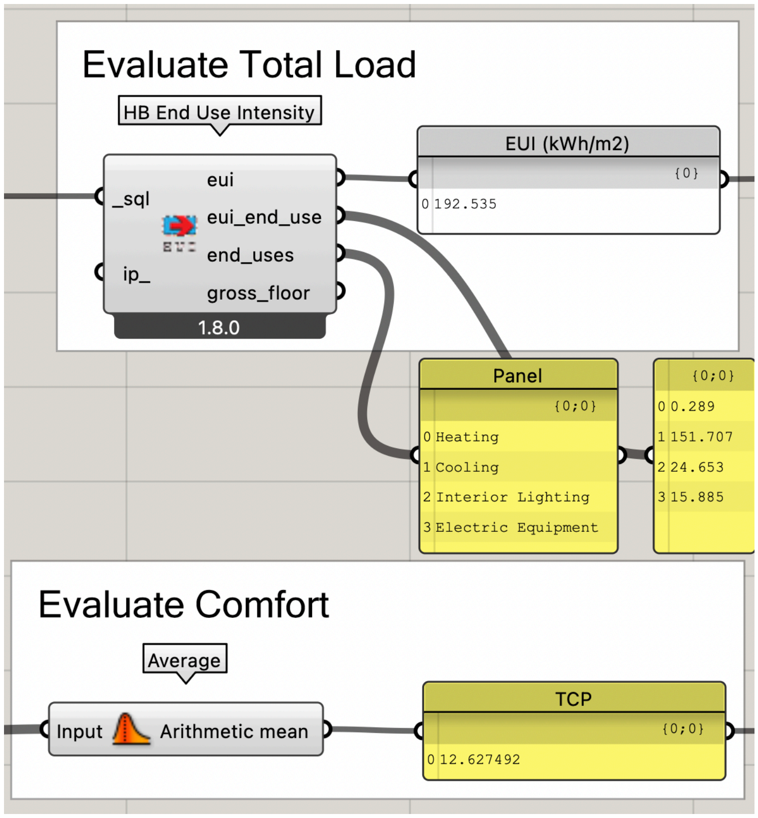


Figure 40: Baseline model performance in Bushehr (hot-humid climate).

- Kerman (Figure 41) demonstrates the lowest EUI among all cases (97.9 kWh/m²) and the highest TCP (58 %), indicating favorable conditions for passive strategies and effective building envelope performance under hot-arid conditions with large diurnal temperature swings.

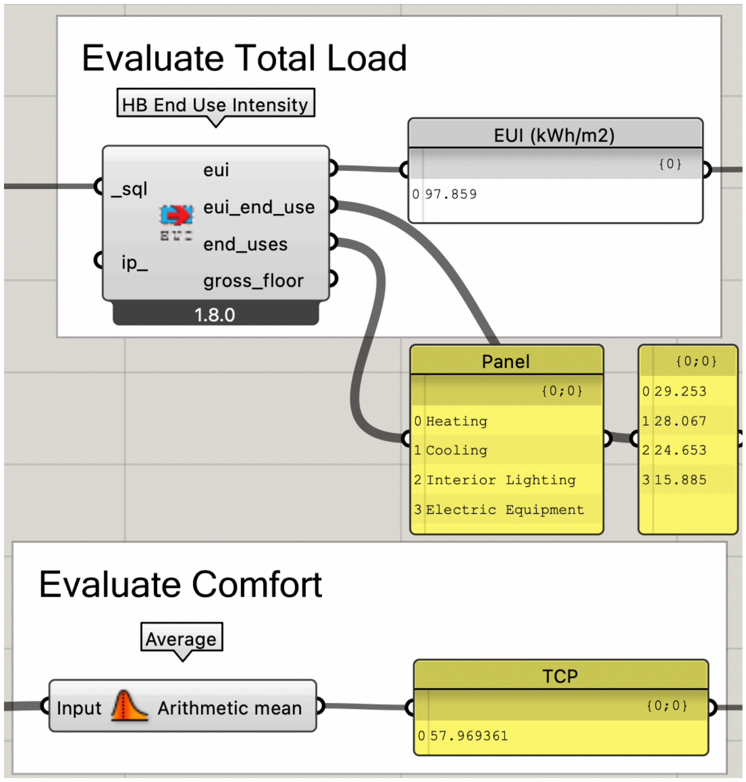


Figure 41: Baseline model performance in Kerman (hot-arid climate).

- Mashhad (Figure 42) presents a moderate EUI of 123.6 kWh/m², with heating loads (55 kWh/m²) dominating due to cold winters. TCP reaches 41.4 %, reflecting partial comfort during transitional and summer periods but discomfort during winter peaks.

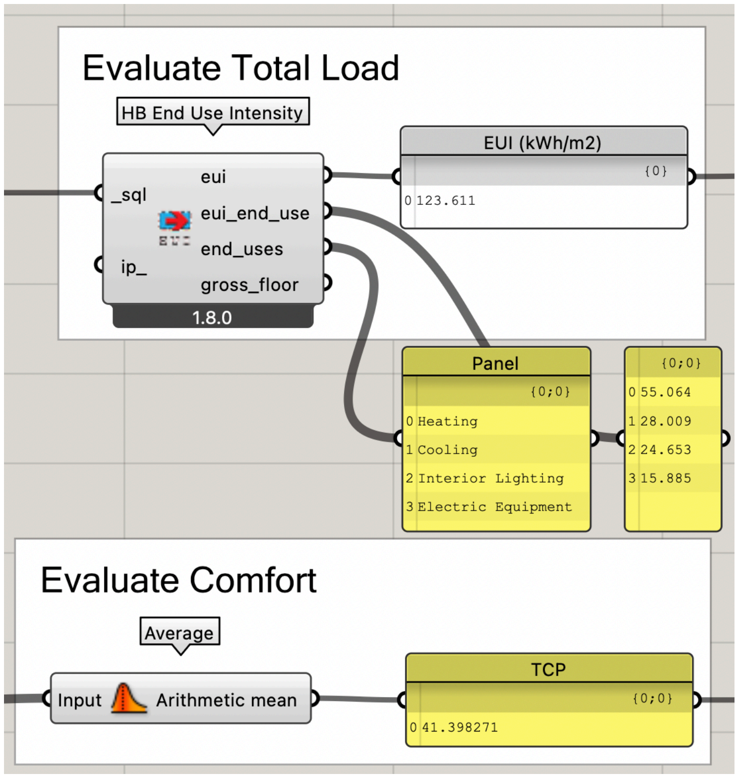


Figure 42: Baseline model performance in Mashhad (cold semi-arid climate).

- Rasht (Figure 43) records an EUI of 106.6 kWh/m², characterized by balanced heating (27.1 kWh/m²) and cooling (39 kWh/m²) loads. The TCP of 34.9 % reveals moderate thermal conditions but limited adaptive comfort potential because of persistent humidity.

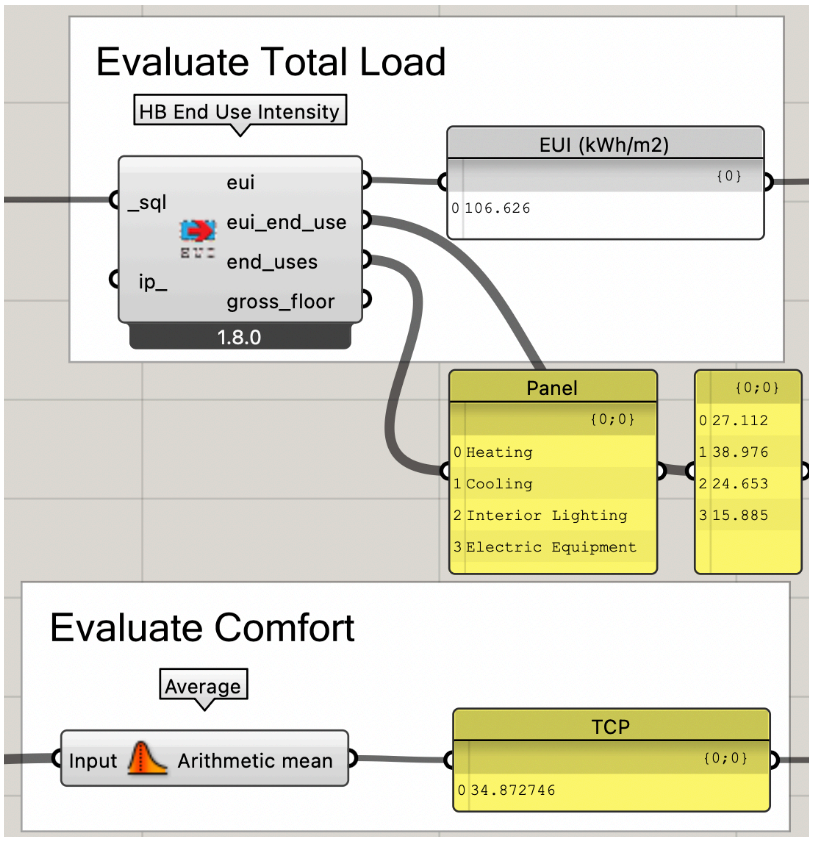


Figure 43: Baseline model performance in Rasht (humid-temperate climate).

- Yazd (Figure 44) yields an EUI of 115.7 kWh/m², largely due to cooling requirements (55.8 kWh/m²). TCP improves to 47.9 %, showing that despite high summer temperatures, the significant nocturnal temperature drop favors comfort recovery.

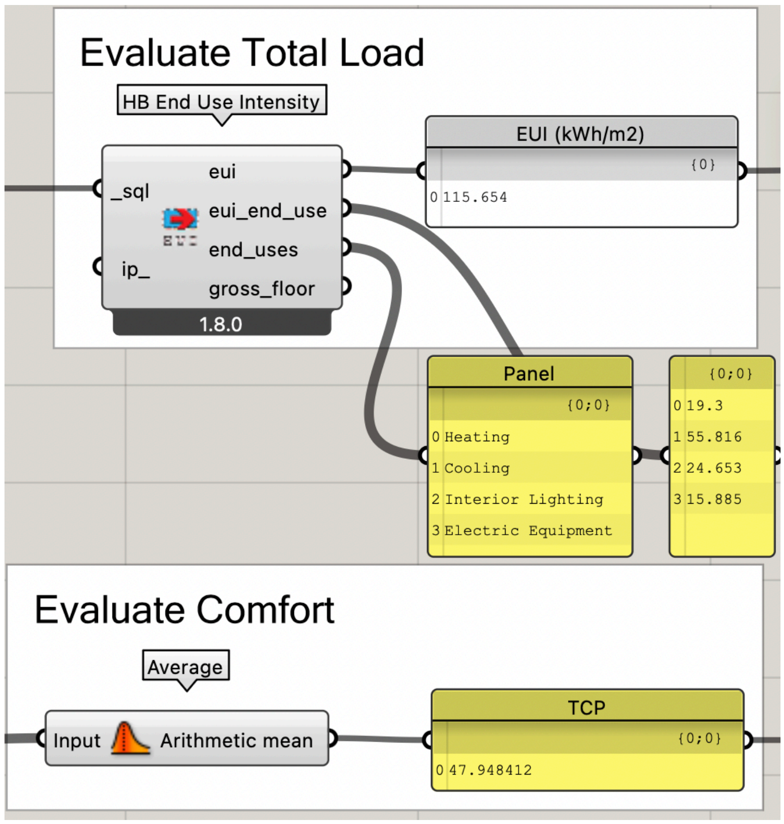


Figure 44: Baseline model performance in Yazd (hot-dry climate).

Table 8: Baseline model energy performance and comfort results across climates.

Climate (City)	**EUI (kWh/m²·yr)**	**Heating (kWh/m²)**	**Cooling (kWh/m²)**	**Interior Lighting (kWh/m²)**	**Electric Equipment (kWh/m²)**	**TCP (%)**	**Climate Type**
Bushehr	192.5	0.3	151.7	24.6	15.9	12.62	Hot-Humid (Csa)
Kerman	97.8	29.2	28	24.6	15.9	57.96	Hot-Arid (BWh)
Mashhad	123.6	55	28	24.6	15,9	41.39	Cold Semi-Arid (BSk)

Rasht	106.6	27.1	38.9	24.6	15.9	34.87	Humid-Temperate (Cfa)
Yazd	115.6	19.3	55.8	24.6	15.9	47.94	Hot-Dry (BWh)

To establish a reference point for evaluating the effectiveness of PCM integration, a baseline simulation was conducted for the reference office building across five representative Iranian climates: Bushehr, Kerman, Mashhad, Rasht, and Yazd. The baseline case represents the building without PCM layers in the envelope.

Figure 45 illustrates the annual Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP) for the baseline scenario. The results show significant climatic variation in building performance. Bushehr exhibits the highest energy demand due to its hot-humid climate, while Kerman shows the lowest EUI because of its cooler desert conditions. In contrast, TCP values vary considerably, reflecting the influence of outdoor climatic conditions on adaptive thermal comfort performance.

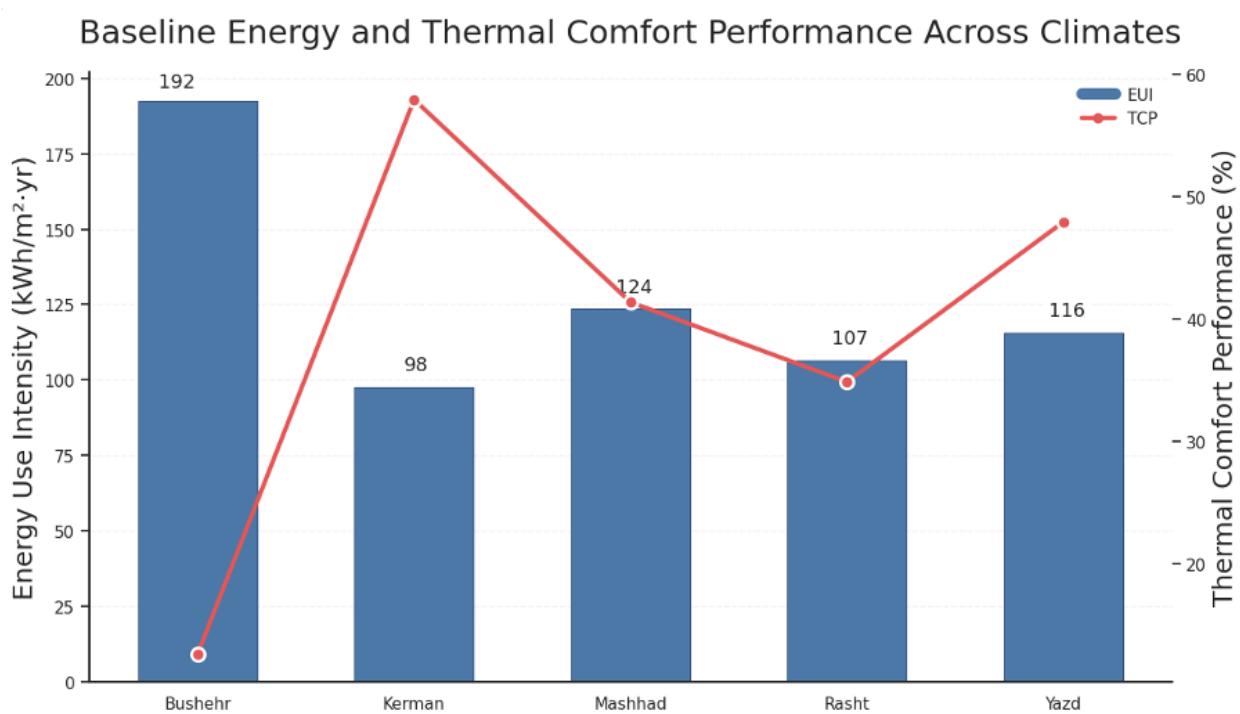


Figure 45: Baseline Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP) of the reference building across five representative Iranian climates.

Overall, these baseline simulations confirm that energy and comfort behaviors vary strongly with climatic context. Cooling dominates in hot regions (Bushehr, Yazd), while heating drives energy use in colder climates (Mashhad). The comfort index follows the opposite trend, being higher in dry climates with greater diurnal variations. These results from the reference benchmark against which PCM integration and optimization outcomes are compared in the following sections.

5.4 Multi-Objective Optimization Results by Climate

Pareto fronts (EUI vs. TCP) are presented for each climate, with optimal PCM configurations (type: BioPCM or InfiniteR; melting point; thickness; placement: inner/mid/outer-wall) selected at the knee point. Performance gains are reported relative to baseline.

5.4.1 Yazd (Hot-Dry Climate)

Figure 46 depicts the Pareto front and the total generation map for Yazd. The optimization shows a clear negative correlation between EUI and TCP, with an optimum cluster around EUI ≈ 105–107 kWh/m²·yr and TCP ≈ 47 %.

The highest-performing solution (Option #1, Table 9) corresponds to BioPCM (inner placement, 4 cm thick, melting point 27 °C), which achieved a 9 % reduction in EUI and nearly identical TCP to the baseline.

This outcome confirms that in Yazd's arid environment—with large diurnal temperature swings exceeding 15 °C—PCM layers complete full melt–freeze cycles, thereby stabilizing indoor temperatures. Low-melting PCMs (23–25 °C) performed slightly worse due to premature solidification, while InfiniteR materials with higher conductivity but lower latent heat yielded higher EUI.

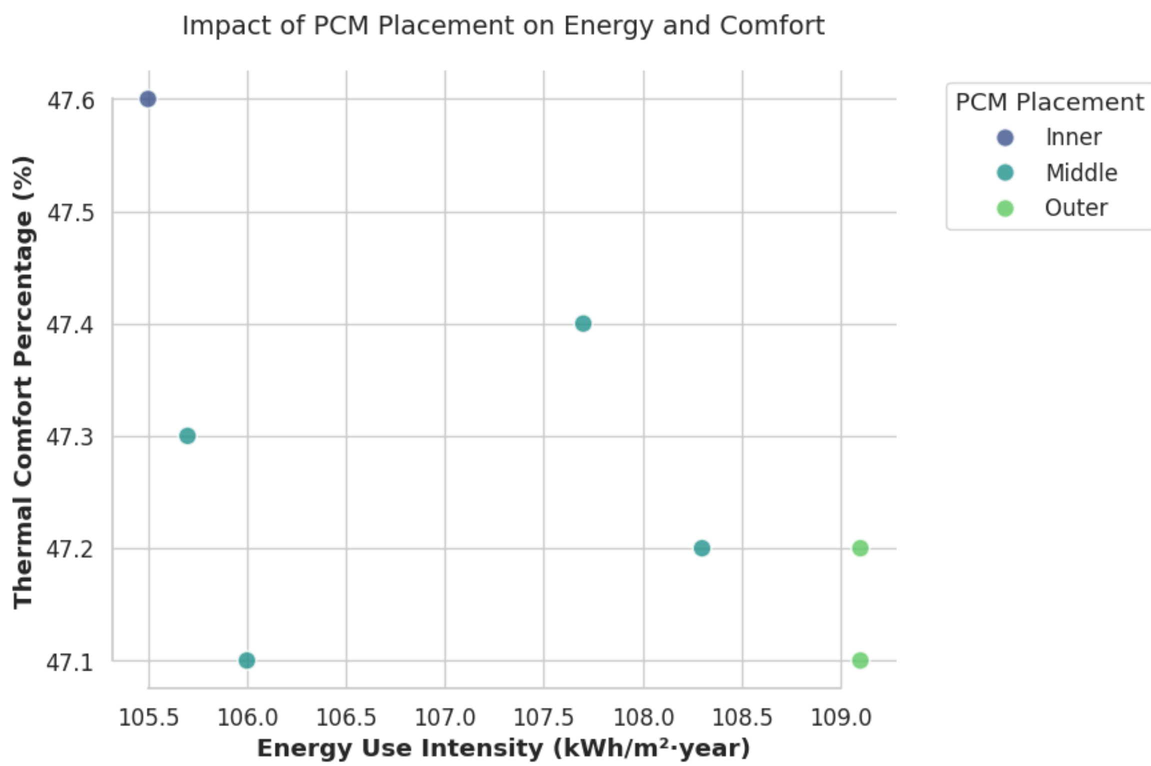


Figure 46: EUI–TCP scatter plot of Pareto front solutions PCM configurations for Yazd (hot-dry climate).

Table 9: Optimized PCM Configurations for Yazd.

Option	Placement	Type	Thickness (cm)	Melting point (°C)	EUI (kWh/m²·yr)	TCP (%)
#1	Inner	BioPCM	4	27	105.5	47.6
#2	Middle	BioPCM	5	27	105.7	47.3
#3	Middle	BioPCM	4	27	106	47.1
#4	Middle	InfiniteR	4	18	107.7	47.4
#5	Middle	InfiniteR	4	25	108.3	47.2
#6	Outer	BioPCM	5	25	109.1	47.1
#7	Outer	BioPCM	5	23	109.1	47.2

Mid-layer and inner placements consistently outperformed outer-layer installations, demonstrating the importance of coupling the PCM with interior air for nighttime discharge. The optimal melting point (≈ 27 °C) aligns with average indoor operative temperatures during cooling season peaks, confirming the expected thermal-lag benefits.

5.4.2 Bushehr (Hot-Humid Climate)

The Pareto front for Bushehr (Figure 47) exhibits a narrow spread, indicating limited sensitivity to PCM parameter variation. All Pareto solutions cluster around EUI ≈ 231–233 kWh/m²·yr and TCP ≈ 12 %, implying that PCM alone cannot overcome the high humidity and minimal diurnal variation (< 7 °C).

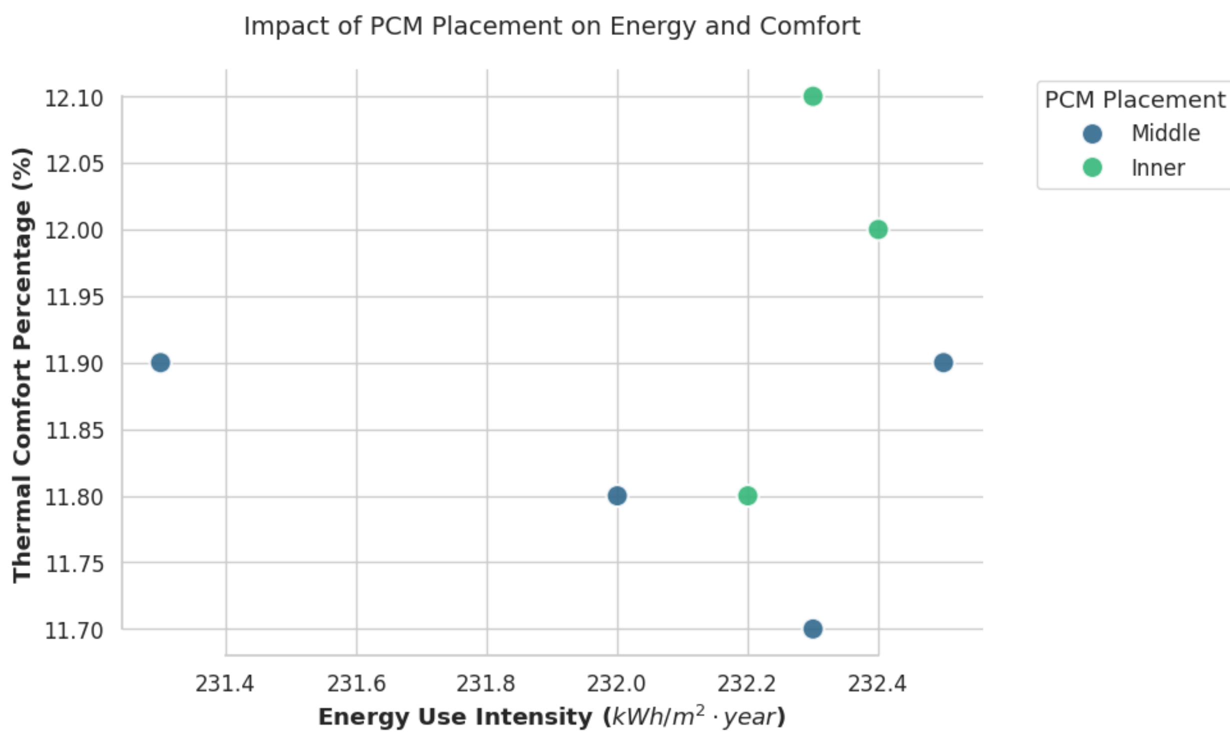


Figure 47: EUI–TCP scatter plot of Pareto front solutions PCM configurations for Bushehr (hot-humid climate).

Table 10: Optimized PCM Configurations for Bushehr.

Option	Placement	Type	Thickness (cm)	Melting point (°C)	EUI (kWh/m²·yr)	TCP (%)
#1	Middle	BioPCM	5	23	231.3	11.9
#2	Inner	InfiniteR	4	23	232.4	12
#3	Inner	InfiniteR	4	21	232.3	12.1

#4	Middle	InfiniteR	4	21	232.5	11.9
#5	Inner	InfiniteR	5	23	232.2	11.8
#6	Middle	InfiniteR	5	25	232.3	11.7
#7	Middle	InfiniteR	5	29	232	11.8

Minimal improvement (< 1 %) in EUI or TCP confirms that PCMs are ineffective when night temperatures remain above their freezing range. Even low-melting BioPCMs (21–23 °C) fail to solidify completely, losing their latent-storage capability. Hence, hybrid systems integrating dehumidification and mechanical night ventilation are essential for Bushehr to exploit any latent storage benefit.

5.4.3 Kerman (Cold-Arid Climate)

Kerman's optimization (Figure 48) yielded the lowest EUI and highest TCP of all climates. The Pareto front shows a steep gradient, demonstrating strong responsiveness to PCM parameters.

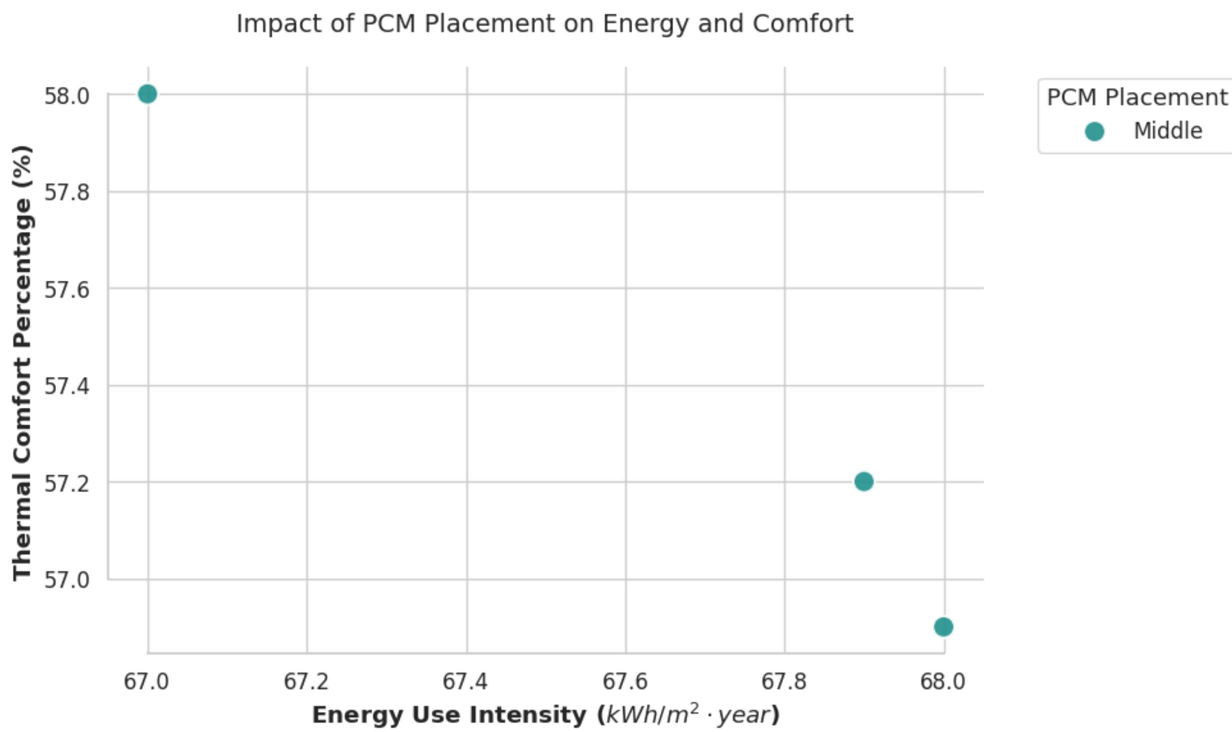


Figure 48: EUI–TCP scatter plot of Pareto front solutions PCM configurations for Yazd (hot-humid climate).

Table 11: Optimized PCM Configurations for Kerman.

Option	Placement	Type	Thickness (cm)	Melting point (°C)	EUI (kWh/m²·yr)	TCP (%)
#1	Middle	InfiniteR	5	23	67.9	57.2
#2	Middle	BioPCM	5	23	68	56.9
#3	Middle	BioPCM	1	27	67	58

The best case (Option #3) achieves ≈ 31 % EUI reduction and +0.8 percentage-point TCP gain relative to baseline. Both BioPCM and InfiniteR perform well, but the inorganic InfiniteR offers slightly better consistency across temperature swings. Mid-layer placement again proved optimal, as it moderates both summer cooling and winter heating demands by leveraging Kerman's pronounced diurnal variation (~18 °C).

5.4.4 Mashhad (Cold Semi-Arid Climate)

Figure 49 shows that the Pareto front for Mashhad has a gentle slope, highlighting moderate optimization potential.

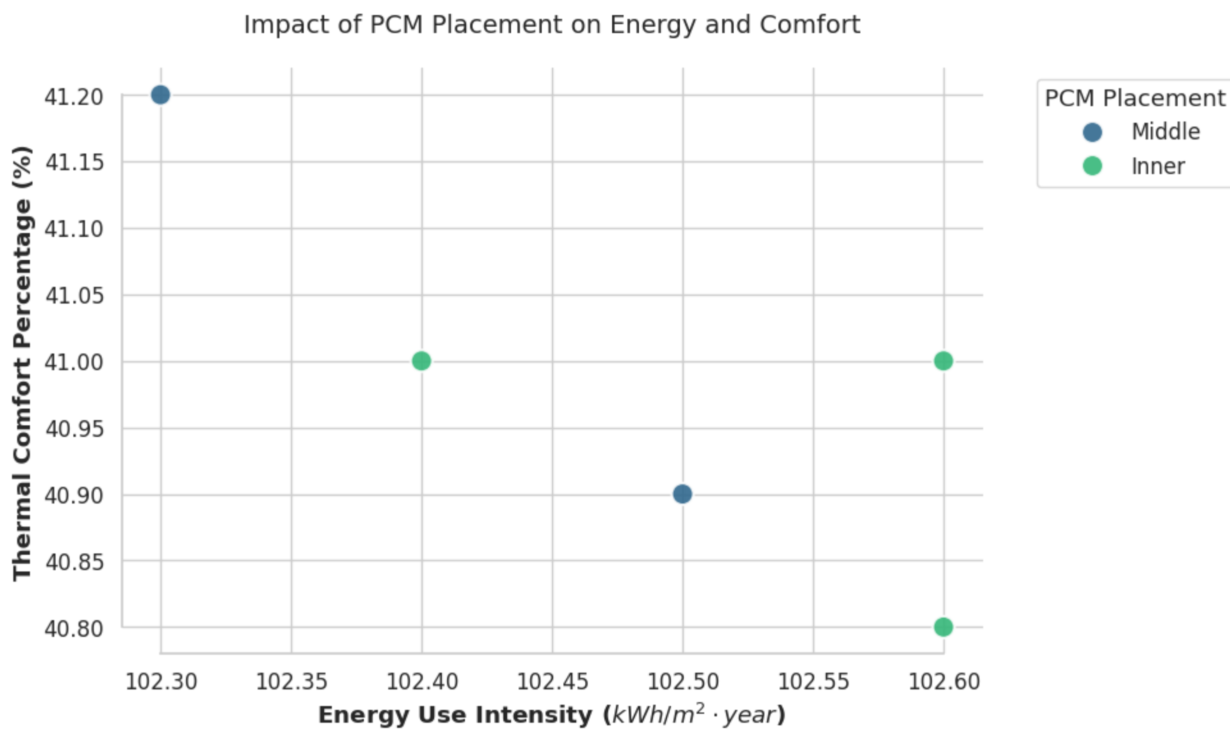


Figure 49: EUI–TCP scatter plot of Pareto front solutions PCM configurations for Mashhad (hot-humid climate).

Table 12: Optimized PCM Configurations for Mashhad.

Option	Placement	Type	Thickness (cm)	Melting point (°C)	EUI (kWh/m²·yr)	TCP (%)
#1	Middle	BioPCM	5	27	102.3	41.2
#2	Inner	BioPCM	4	27	102.4	41
#3	Middle	BioPCM	5	23	102.5	40.9
#4	Inner	BioPCM	3	27	102.6	41
#5	Inner	BioPCM	3	21	102.6	40.8

Mashhad's heating-dominated climate benefits from higher-melting BioPCMs (≈ 27 °C) that store daytime solar gains and release heat at night. Energy savings (~17 % vs. baseline) derive mainly from reduced heating load rather than cooling reduction. TCP improves slightly (≈ +0.2 pp), showing that thermal comfort stability is achieved by mitigating nighttime temperature drops. The mid-layer configuration again ensures balanced performance over the year.

5.4.5 Rasht (Humid-Temperate Climate)

Figure 50 illustrate the optimization outcomes for Rasht, representing Iran's humid-temperate coastal climate. The Pareto front exhibits a narrow and nearly horizontal distribution, indicating very limited sensitivity of performance to PCM parameter variation. All solutions converge around EUI ≈ 91–94 kWh/m²·year and TCP ≈ 35 %, implying that PCM integration in this context yields minimal thermal or energy benefits.

Table 13 lists the top Pareto-optimal configurations. The best case (Option #1) corresponds to InfiniteR, mid-layer placement, 5 cm thickness, melting point 27 °C, achieving an EUI of 91.8 kWh/m²·yr and TCP of 35.24 %. These values represent only a ≈ 1.5 % EUI reduction and negligible comfort improvement relative to the non-PCM baseline (EUI ≈ 93 kWh/m²·yr, TCP ≈ 34.9 %).

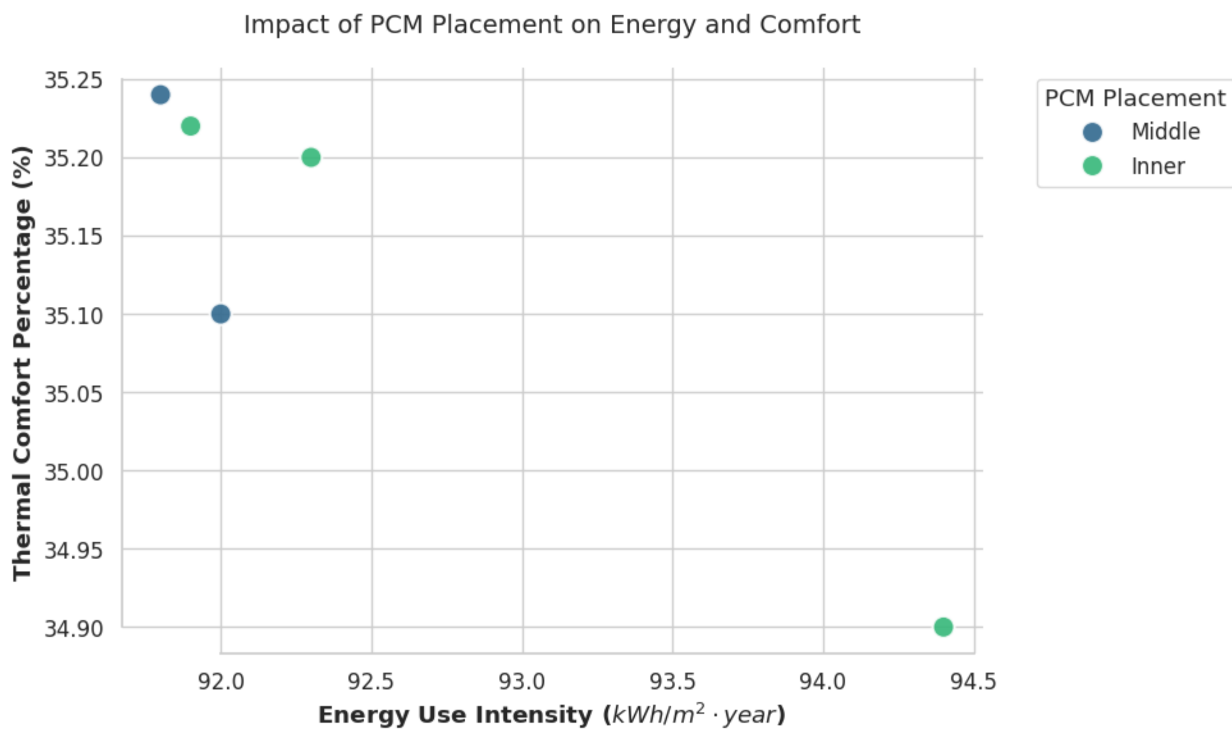


Figure 50: EUI–TCP scatter plot of Pareto front solutions PCM configurations for Rasht (hot-humid climate).

Table 13: Optimized PCM Configurations for Rasht.

Option	Placement	Type	Thickness (cm)	Melting point (°C)	EUI (kWh/m²·yr)	TCP (%)
#1	Middle	InfiniteR	5	27	91.8	35.24
#2	Inner	InfiniteR	4	27	91.9	35.22
#3	Middle	InfiniteR	5	23	92	35.1
#4	Inner	InfiniteR	3	27	92.3	35.2
#5	Inner	InfiniteR	3	21	94.4	34.9

The marginal improvement in energy performance arises from Rasht's narrow diurnal temperature range (typically < 5 °C) and persistent high humidity (≈ 80 %), which prevent complete phase reversal of the PCM. Even low-melting InfiniteR (21–23 °C) remain partially liquid throughout the cooling season, resulting in diminished latent-heat storage and acting instead as low-conductivity layers with limited thermal benefit.

Mid-layer or inner-surface configurations exhibited slightly better results than outer placements, primarily because these positions allow the PCM to interact more directly with conditioned air, moderating short-term indoor fluctuations during brief sunny periods. However, the lack of significant solar radiation and the absence of strong nighttime cooling hinder effective charging and discharging cycles.

To provide a clearer comparison between the baseline and optimized scenarios, Figure 51 summarizes the impact of PCM optimization on Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP) in the arid and semi-arid climates of Kerman, Mashhad, and Yazd. The results demonstrate that the optimized PCM configurations significantly reduce energy consumption while maintaining or slightly improving thermal comfort levels.

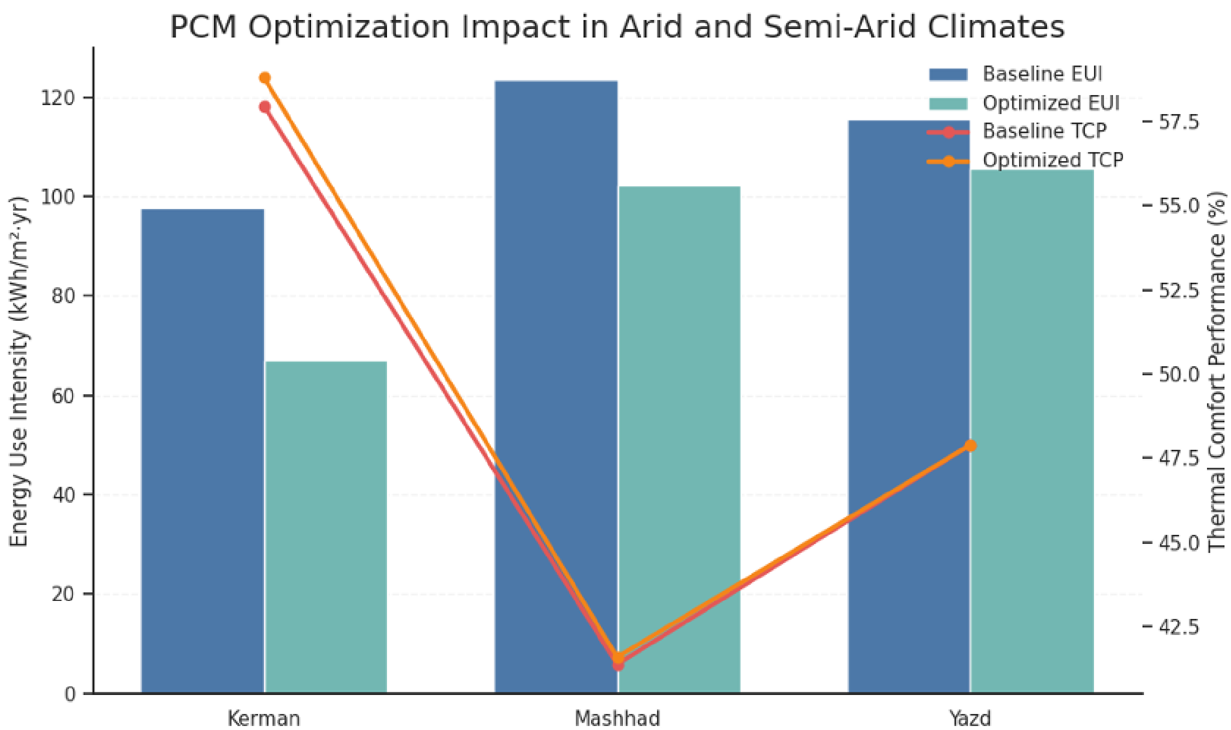


Figure 51: Comparison of baseline and optimized Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP) for PCM-optimized solutions in Kerman, Mashhad, and Yazd.

To further examine the influence of PCM optimization in humid climates, Figure 52 compares the baseline and optimized scenarios for Bushehr and Rasht. The results highlight the different responses of energy performance and thermal comfort to PCM integration under humid climatic conditions. While the optimization significantly improves thermal comfort levels, the impact on energy consumption varies between the two climates due to differences in temperature patterns, humidity levels, and cooling demand.

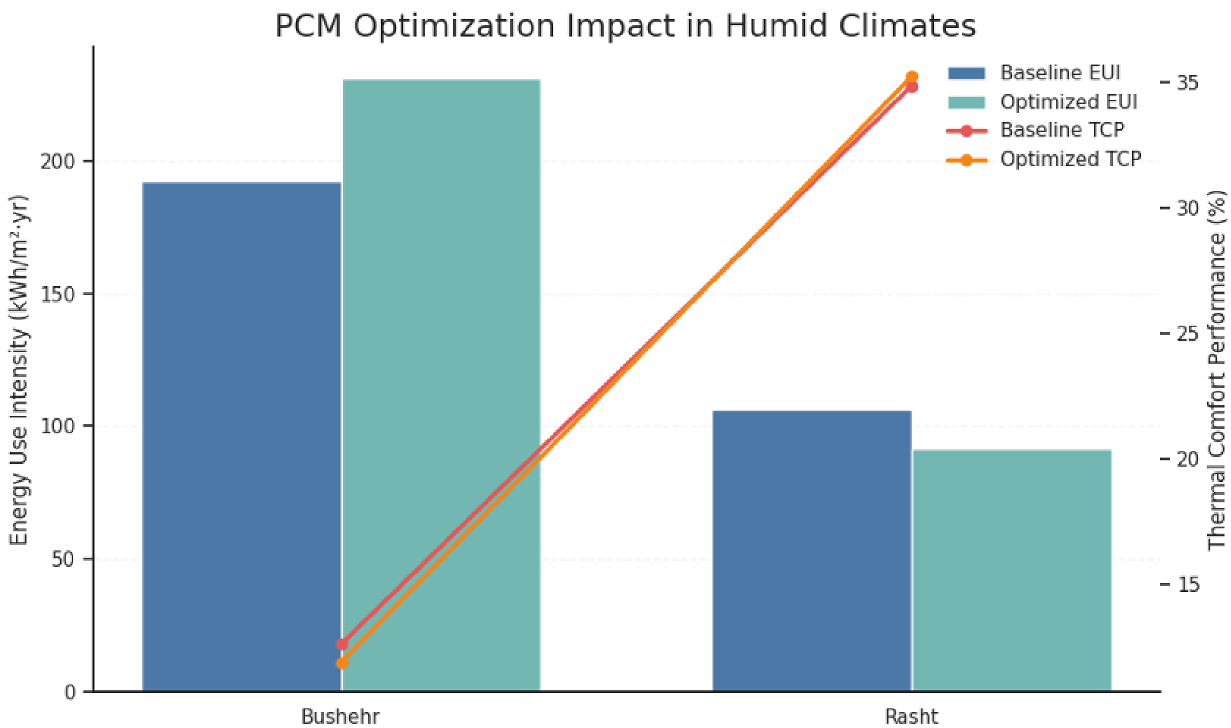


Figure 52: Comparison of baseline and optimized Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP) in humid climates (Bushehr and Rasht).

5.5 Optimized Results Across Future

Future climate projections were generated using Meteonorm v8.2, adopting the RCP 8.5 scenario for the year 2080, which represents a high-emission trajectory with significant global temperature rise. The generated weather files were used as inputs for parametric optimization runs in Grasshopper–Honeybee, maintaining the same building geometry, schedules, and boundary conditions as the baseline model. The only variation was the use of future weather data, allowing evaluation of the long-term effectiveness of PCM optimization under warmer climatic conditions.

The performance indicators—Energy Use Intensity (EUI) and Thermal Comfort Percentage (TCP)—were recalculated for each city. Figures 53 to 57 illustrate the optimized results based on future climate conditions, while Table 14 summarizes the numerical outcomes.

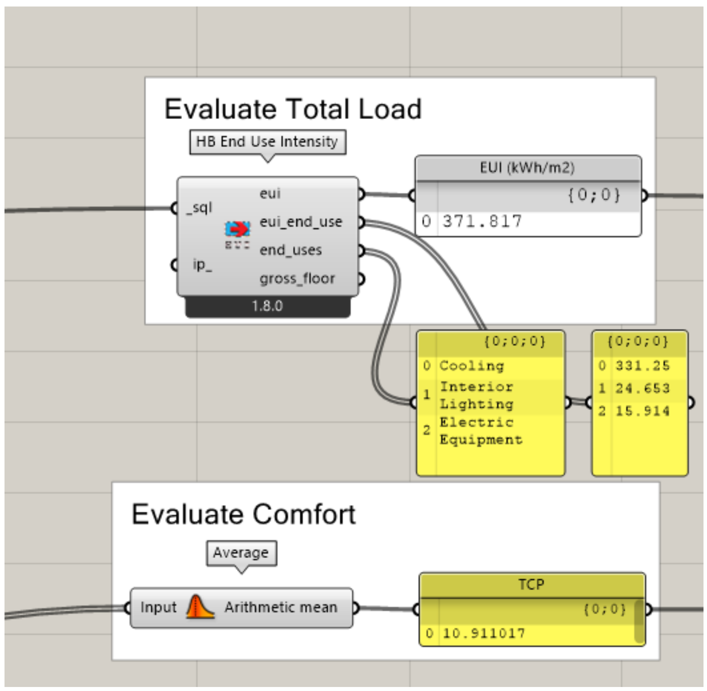


Figure 53: Optimized model performance in Bushehr (RCP 8.5 – 2080).

The simulation yields an EUI of 371.8 kWh/m² and a TCP of 10.9%, indicating a significant increase in cooling energy demand (331.3 kWh/m²) due to elevated ambient temperatures and humidity.

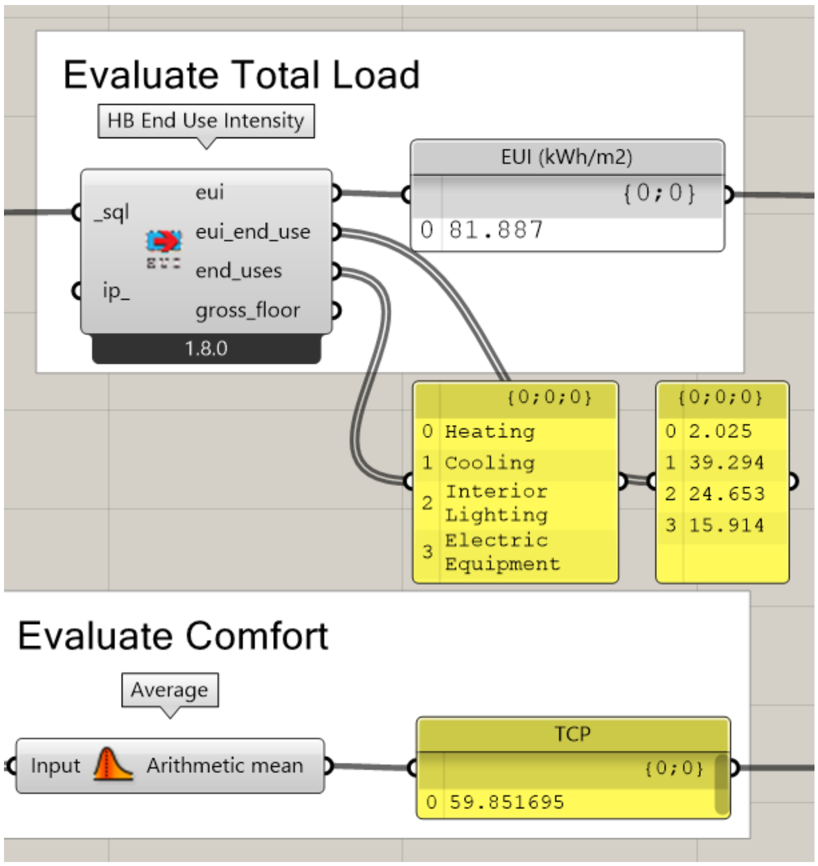


Figure 54: Optimized model performance in Kerman (RCP 8.5 – 2080).

Under future conditions, EUI drops to 81.9 kWh/m², with a TCP of 59.9%, suggesting stable performance of optimized PCM configurations and the persistence of effective passive cooling potential in hot-arid climates.

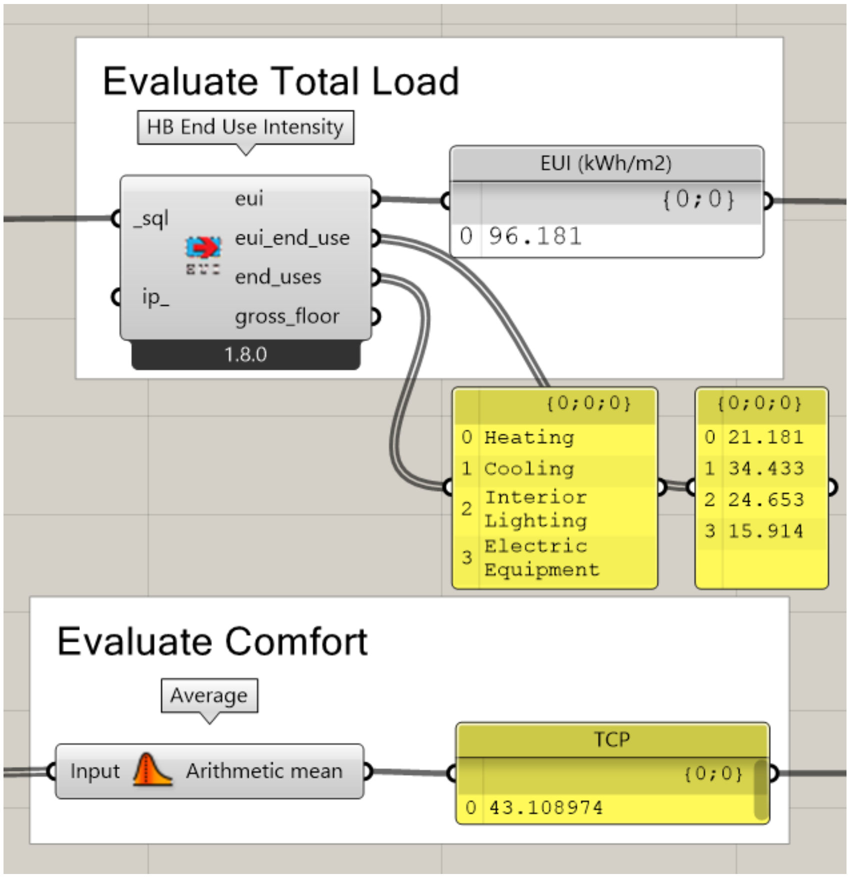


Figure 55: Optimized model performance in Mashhad (RCP 8.5 – 2080).

The model shows EUI = 96.2 kWh/m² and TCP = 43.1%, with cooling energy becoming the dominant load (34.4 kWh/m²) as winters become milder and heating demand decreases.

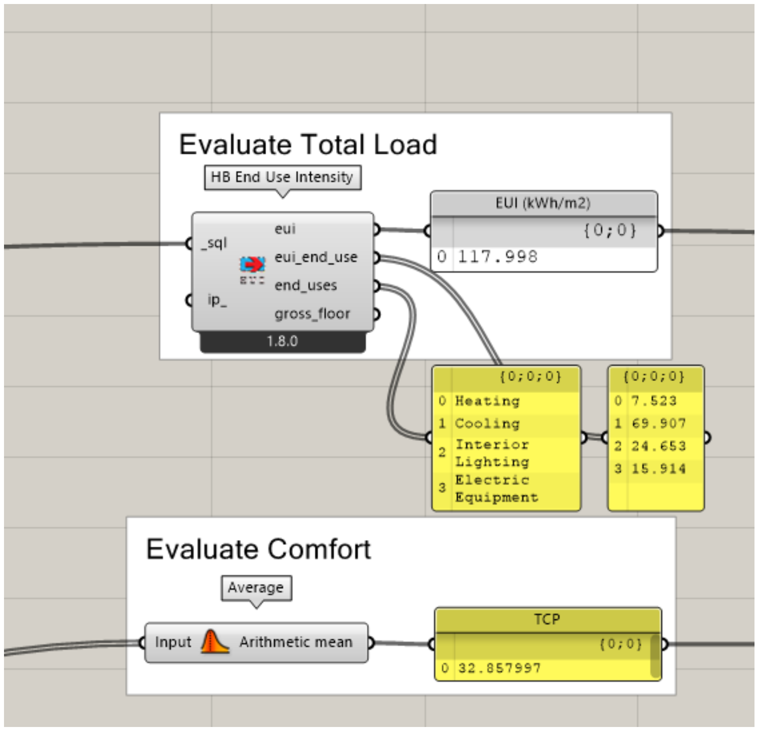


Figure 56: Optimized model performance in Rasht (RCP 8.5 – 2080).

The EUI of 110.4 kWh/m² and TCP of 45.1% indicate moderate energy use but reduced comfort compared to Kerman, mainly due to high humidity that limits PCM phase transition cycles.

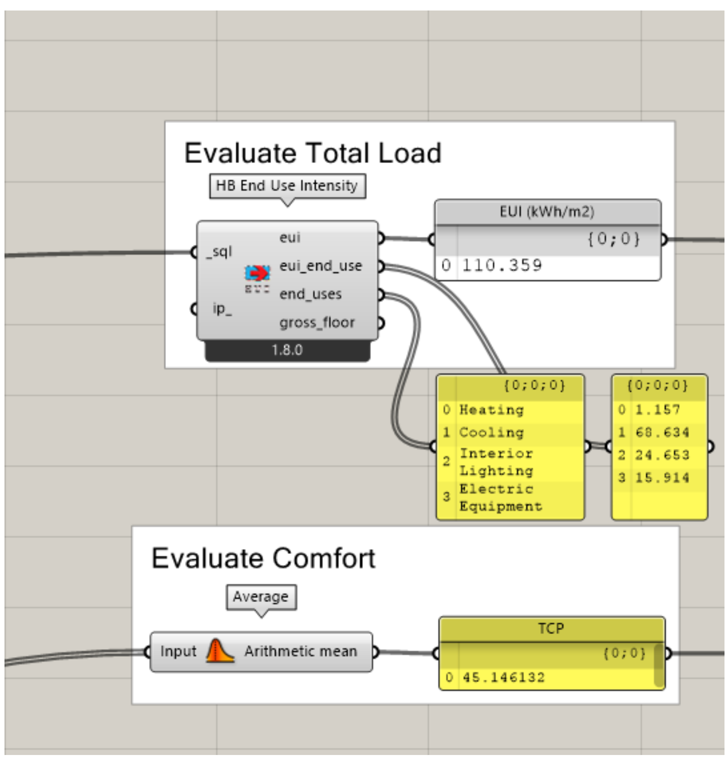


Figure 57: Optimized model performance in Yazd (RCP 8.5 – 2080).

The optimized case achieves **EUI = 118.0 kWh/m²** and **TCP = 32.9%**, where cooling remains the major end use (**69.9 kWh/m²**), highlighting the increasing difficulty of achieving comfort under extreme heat.

Table 14: Energy and comfort results for future optimized cases (RCP 8.5, 2080).

Climate (City)	**EUI (kWh/m²·yr)**	**Heating (kWh/m²)**	**Cooling (kWh/m²)**	**Interior Lighting (kWh/m²)**	**Electric Equipment (kWh/m²)**	**TCP (%)**	**Climate Type**
Bushehr	371	-	331.2	24.6	15.9	10.91	Hot-Humid (Csa)
Kerman	81.1	2.1	39.3	24.6	15.9	59.85	Hot-Arid (BWh)
Mashhad	96.1	21.2	34.4	24.6	15,9	43.10	Cold Semi-Arid (BSk)
Rasht	117.9	7.5	69.9	24.6	15.9	32.85	Humid-Temperate (Cfa)
Yazd	110.3	1.15	68.63	24.6	15.9	45.16	Hot-Dry (BWh)

Compared to the baseline (current climate), future simulations under RCP 8.5 project a substantial increase in cooling energy demand and a reduction in overall comfort, particularly in coastal and humid areas such as Bushehr and Rasht. Conversely, Kerman maintains superior performance, with both low EUI and high TCP, emphasizing the continued benefit of PCM use in climates with large diurnal temperature variation.

To provide a climate-level overview of building energy performance and thermal comfort, Figures 58–60 summarize the simulation results using aggregated indicators for the selected cities. These figures present the total Energy Use Intensity (EUI), the breakdown of energy consumption by end-use, and the resulting Thermal Comfort Percentage (TCP), allowing a direct comparison of climatic influence on energy demand and comfort conditions prior to detailed optimization analysis.

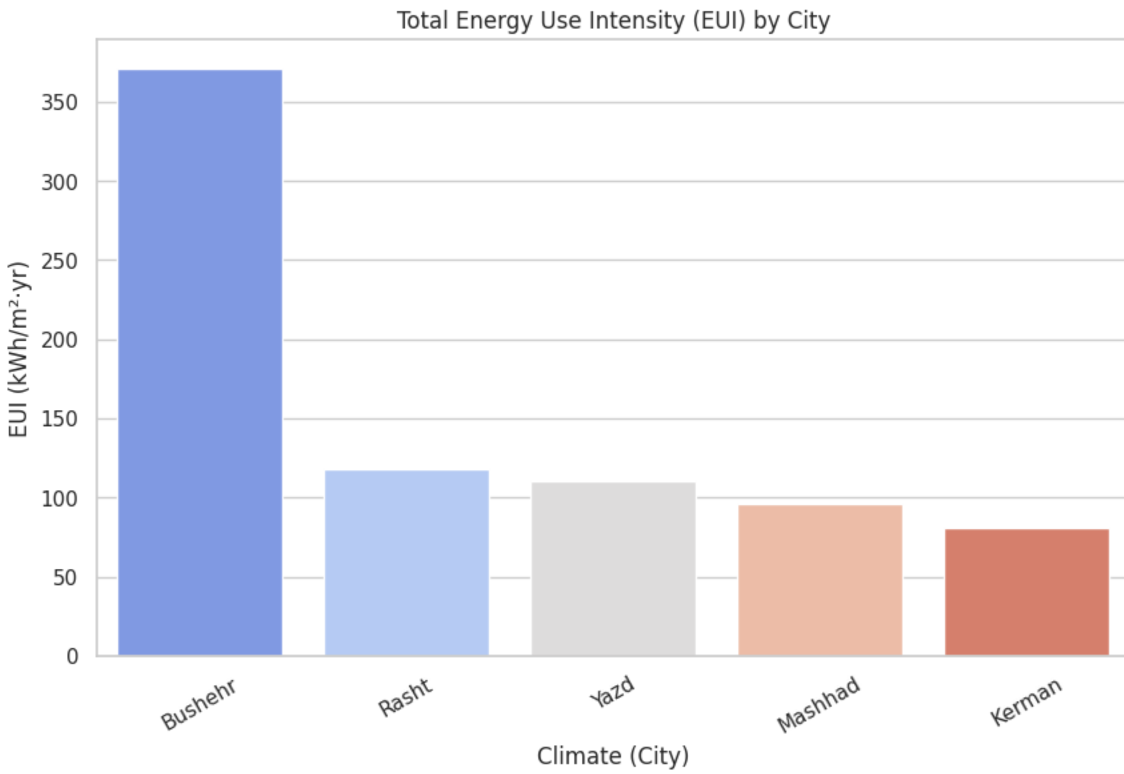


Figure 58: Comparison of Total Energy Use Intensity (EUI) for the selected climatic locations.

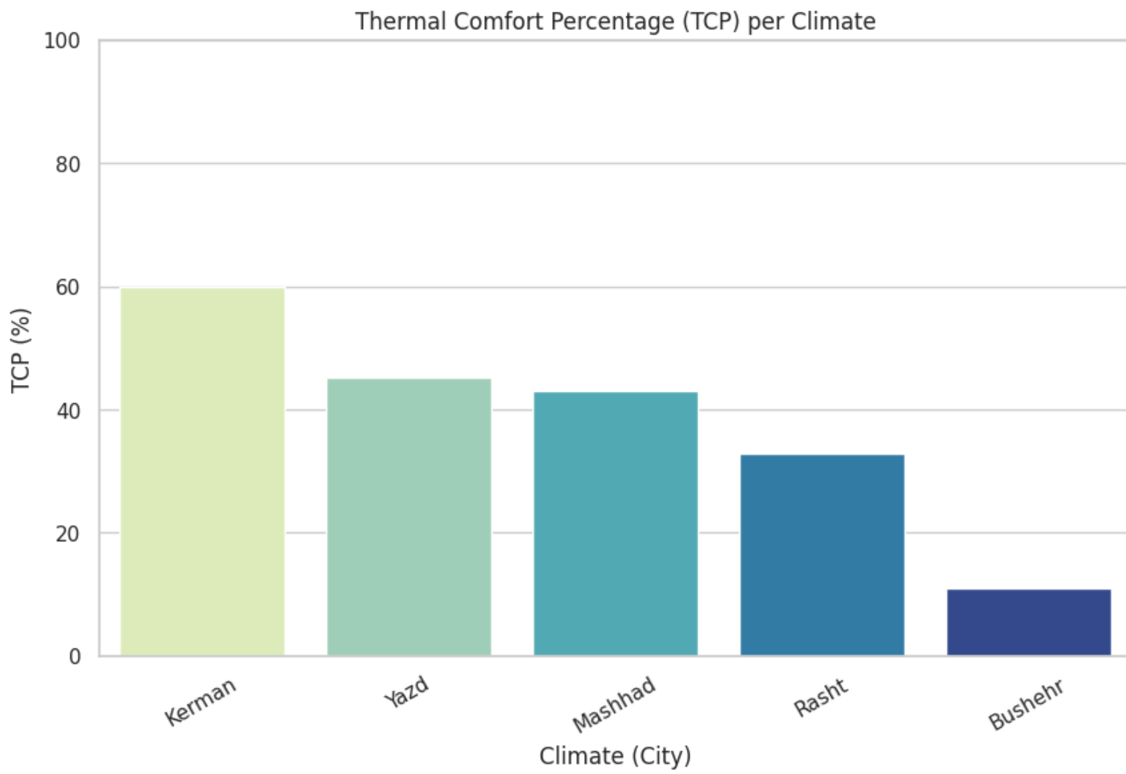


Figure 59: Breakdown of annual energy consumption by end-use across the selected climates.

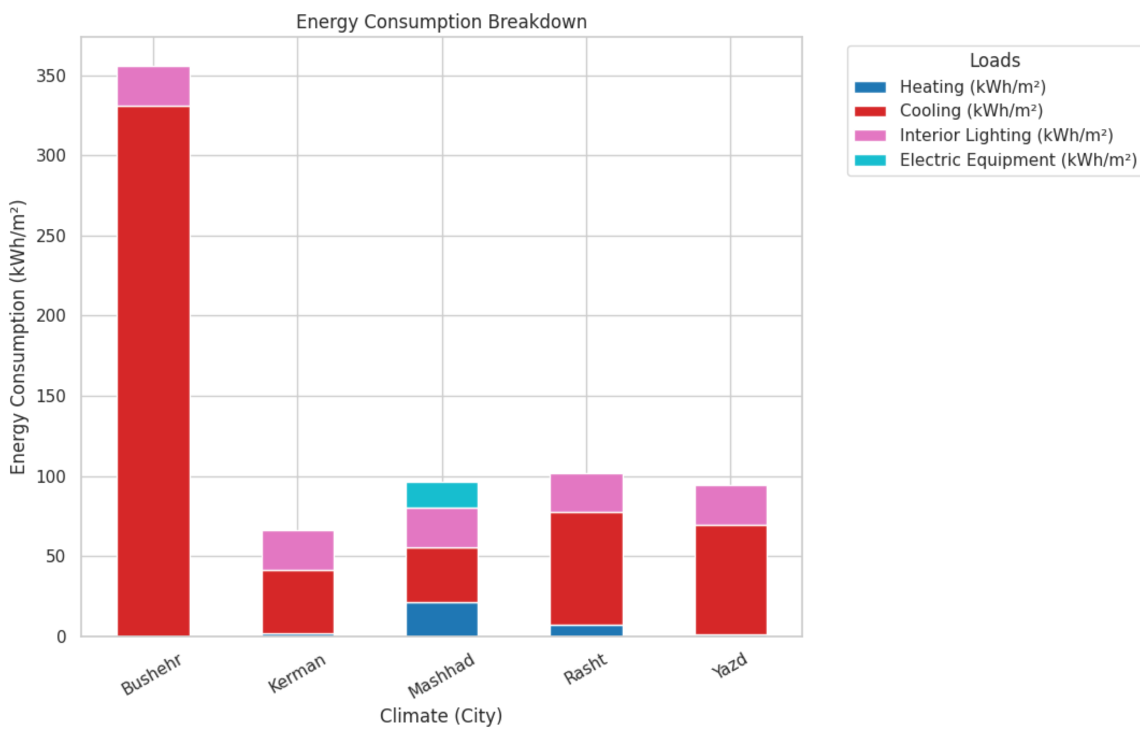


Figure 60: Thermal Comfort Percentage (TCP) for the selected climatic locations.

Heating energy demand decreases across all cities, confirming the warming trend projected for 2080. The results highlight that climate-responsive PCM optimization remains effective in arid regions, while its performance deteriorates in humid and coastal climates due to limited solidification cycles. This emphasizes the need for hybrid strategies combining PCMs with active cooling or dehumidification systems to ensure resilience under future climatic stress.

5.6 Summary of Results

This study developed and applied a multi-objective optimization (MOO) framework, powered by the NSGA-II algorithm and the ChameleonPCM plugin, to evaluate the integration of phase-change materials (PCMs) in office buildings across five representative Iranian climates. The framework simultaneously minimized Energy Use Intensity (EUI) and maximized Thermal Comfort Percentage (TCP), generating Pareto fronts that quantified the inherent trade-offs between energy efficiency and occupant comfort. The results underscore the profound influence of local climatic parameters—particularly diurnal temperature amplitude, humidity, and seasonal load dominance—on PCM performance, validating the need for climate-tailored design strategies.

Baseline simulations (Section 5.4) established reference performance without PCMs, revealing stark regional disparities. Hot-humid Bushehr exhibited the highest EUI (192.5 kWh/m^2·yr) and lowest TCP (12.6%), driven by dominant cooling demands. In contrast, cold-arid Kerman displayed the most balanced profile (EUI 97.8 kWh/m^2·yr; TCP 58.0%), while hot-dry Yazd (EUI

115.6 kWh/m²·yr), cold semi-arid Mashhad (EUI 123.6 kWh/m²·yr), and humid-temperate Rasht showed intermediate challenges shaped by their respective heating or cooling biases.

Under current climate conditions (Section 5.5), optimization outcomes highlighted a clear hierarchy of PCM efficacy tied to diurnal temperature swings:

- **High-Impact Arid Zones (Yazd and Kerman; >15 °C swings)**: Complete melt–freeze cycles maximized latent-heat utilization. In Yazd (hot-dry), the optimal configuration—BioPCM, inner-layer placement, 4 cm thickness, 27 °C melting point—reduced EUI by ~9% with negligible TCP impact. Kerman (cold-arid) delivered the study's most compelling gains: ~31% EUI reduction and +0.8 percentage points in TCP using InfiniteR PCM (mid-layer, 5 cm, 23 °C), stabilizing both summer cooling and winter heating loads.
- **Moderate-Impact Semi-Arid Zone (Mashhad; ~12 °C swings)**: PCMs primarily mitigated heating demands by capturing daytime solar and internal gains for nocturnal release. The optimized setup (BioPCM, mid-layer, 5 cm, 27 °C) achieved ~17% EUI savings and modest TCP improvements.
- **Low-Impact Humid Zones (Bushehr and Rasht; <7 °C swings)**: Persistent high humidity and minimal diurnal variation impeded full solidification, limiting PCMs to passive insulation effects. Improvements were marginal (<1% EUI reduction in Bushehr; ~1.5% in Rasht) with no meaningful TCP gains, underscoring the inadequacy of standalone passive PCMs in these environments.

Across viable climates, optimal designs converged on key principles: mid- or inner-layer placements to facilitate direct indoor heat exchange; melting points within ±2 °C of mean operative temperature (typically 25–27 °C); and thicknesses of 4–5 cm, beyond which diminishing returns arose from incomplete phase transitions.

Future climate projections under RCP 8.5 (2080 horizon; Section 5.5) amplified cooling loads and eroded comfort universally, yet PCM resilience varied markedly. Arid regions (Yazd and Kerman) retained substantial benefits, with Kerman's optimized EUI at 81.1 kWh/m²·yr and TCP at 59.9%. Humid coastal areas (Bushehr and Rasht) suffered acute degradation—e.g., Bushehr's EUI surged to 371.8 kWh/m²·yr with TCP dropping to 10.9%—highlighting vulnerability to overheating. These findings advocate for hybrid augmentation (e.g., mechanical night ventilation or dehumidification) in humid zones to sustain charge–discharge cycles amid warmings.

In conclusion, passive PCM integration emerges as a potent, resilient strategy for arid and semi-arid Iranian climates (BWh, BWk, BSk classifications), yielding EUI reductions of 9–31% while preserving or enhancing comfort. It proves marginally effective or unsuitable in humid regimes (BSh, Cfa) lacking adequate nocturnal cooling for thermal discharge. The MOO framework robustly quantifies these climate contingencies, furnishing empirical evidence for the actionable, region-specific PCM guidelines elaborated in Chapter 6. These insights advance sustainable building design by aligning material selection, placement, and sizing with environmental contexts, thereby promoting energy-efficient and thermally comfortable office environments in Iran.

6. Conclusion

6.1 Summary of Research Objectives and Methodology

Buildings account for a substantial share of global energy consumption, with heating and cooling demands posing acute environmental and economic challenges in climatically diverse regions such as Iran. This thesis addressed this issue by developing a systematic, simulation-based framework to optimize the integration of Phase Change Materials (PCMs) in office building envelopes, aiming to minimize Energy Use Intensity (EUI) while maximizing Thermal Comfort Percentage (TCP). The study focused on five representative Iranian cities spanning distinct Köppen classifications: Yazd (BWh, hot-dry), Kerman (BWk, cold-arid), Mashhad (BSk, cold semi-arid), Rasht (Cfa, humid-temperate), and Bushehr (BSh, hot-humid).

A robust multi-objective optimization (MOO) workflow was implemented using EnergyPlus for energy and comfort simulations, interfaced via the Honeybee/Ladybug tools in Rhino/Grasshopper. The custom ChameleonPCM plugin enabled seamless definition and injection of PCM properties into EnergyPlus models. The NSGA-II genetic algorithm facilitated exploration of a parametric design space encompassing PCM type (BioPCM, InfiniteR), melting temperature (18–29 °C), thickness (1–5 cm), and placement (inner, mid-layer, outer). A standardized single-zone reference office model (adapted from ASHRAE Standard 140 Case 600) ensured consistency, with evaluations conducted under both current Typical Meteorological Year (TMY) conditions and future projections (RCP 8.5, 2080 horizon). Pareto fronts quantified trade-offs between EUI and TCP, yielding climate-specific optimal configurations.

6.2 Key Findings

PCM efficacy is inherently climate-contingent, governed primarily by diurnal temperature amplitude and humidity levels, which determine the completeness of daily melt–freeze cycles.

High Performance in Arid and Semi-Arid Climates (BWh, BWk, BSk):

Regions with pronounced day–night temperature swings (>15 °C) enabled full utilization of latent heat storage.

- In Kerman, the optimal configuration (InfiniteR, mid-layer, 5 cm, 23 °C melting point) achieved a ~31% EUI reduction (to ~62 kWh/m²·yr) with a +0.8 percentage-point TCP improvement, balancing summer cooling and winter heating mitigation.
- In Yazd, BioPCM (inner-layer, 4 cm, 27 °C) delivered ~9% EUI savings while preserving TCP.
- In Mashhad, BioPCM (mid-layer, 5 cm, 27 °C) reduced heating-dominant loads by ~17%. Convergent design patterns included mid- or inner-layer placement to enhance coupling with indoor air, melting points within ±2 °C of mean operative temperature (typically 25–27 °C), and thicknesses of 4–5 cm, beyond which incomplete cycling yielded diminishing returns.

Limited Efficacy in Humid Climates (BSh, Cfa):

Narrow diurnal ranges (<7 °C), warm nights, and high relative humidity impeded PCM solidification, resulting in marginal EUI reductions (≤1.5%) and negligible TCP gains in Bushehr and Rasht. PCMs effectively functioned as low-R-value insulation after initial saturation, underscoring the inadequacy of standalone passive strategies in these zones.

Future Climate Resilience (RCP 8.5, 2080):

Warming exacerbated cooling loads and degraded comfort universally, but arid/semi-arid regions retained PCM benefits (e.g., Kerman: EUI ≈ 81 kWh/m²·yr, TCP ≈ 60%). Humid cities faced severe stress (e.g., Bushehr: EUI ≈ 372 kWh/m²·yr, TCP ≈ 11%), highlighting vulnerability and the imperative for hybrid interventions, such as mechanical night ventilation or dehumidification, to restore charge–discharge cycles.

6.3 Methodological and Practical Contributions

This work advances PCM application in building design through:

- A comprehensive MOO pipeline tailored to PCM variables, rendering the energy–comfort trade-space explicit and enabling large-scale, cross-climate exploration.
- The ChameleonPCM plugin, which automates PCM integration into EnergyPlus, promoting reproducibility and scalability.
- Actionable heuristics: Initiate with melting point ≈ operative temperature (±2 °C), 4–5 cm thickness, and mid/inner placement; refine via local weather data and MOO.
- Climate-specific guidance: Prioritize PCMs in arid/semi-arid contexts for 9–31% EUI reductions without comfort penalties; augment with active systems in humid zones.

These outputs provide architects, engineers, and policymakers with a decision-making toolkit for low-energy, comfortable offices, resilient under climate change.

6.4 Limitations

The analysis relied on a simplified single-zone model with deterministic schedules, TMY data, and fixed infiltration/controls, limiting direct extrapolation to complex geometries, variable operations, or stochastic conditions. Humidity buffering and advanced HVAC interactions (e.g., model predictive control, hybrid PCM-HVAC) were not co-optimized, potentially underestimating benefits in humid climates. Embodied carbon, life-cycle costs, and PCM durability were excluded, focusing solely on operational performance. Field validation remains essential for real-world generalization.

6.5 Directions for Future Research

- Extend to multi-zone models incorporating occupancy variability, geometric diversity, and uncertainty in climate/aging.
- Investigate hybrid PCM systems (e.g., with night ventilation, dehumidification, or demand-controlled strategies) to enhance viability in humid regions.
- Integrate life-cycle assessment (LCA), techno-economic analysis, and embodied impacts for triple-bottom-line (energy, carbon, cost) optimization.
- Pursue in-situ pilots across Köppen classes, generating open datasets to support machine learning surrogates and broader benchmarking.

6.6 Closing Statement

This thesis establishes that optimized PCM integration offers substantial, resilient operational gains in Iran's arid and semi-arid climates through targeted matching of material properties to local diurnal dynamics, as revealed by rigorous Pareto analysis. Conversely, it delineates the inherent limitations of passive PCMs in humid environments, necessitating hybrid approaches amid escalating warmings. The proffered MOO framework and ChameleonPCM tool empower designers to navigate these nuances efficiently, fostering sustainable, comfortable built environments tailored to Iran's climatic mosaic. Ultimately, as global temperatures rise, strategic PCM deployment—where intrinsically effective and augmented where required—will be pivotal in achieving low-carbon, adaptive workplaces.

The analysis relied on a simplified single-zone model with deterministic schedules, TMY data, and fixed infiltration/controls, limiting direct extrapolation to complex geometries, variable operations, or stochastic conditions. Humidity buffering and advanced HVAC interactions (e.g., model predictive control, hybrid PCM-HVAC) were not co-optimized, potentially underestimating benefits in humid climates. Embodied carbon, life-cycle costs, and PCM durability were excluded, focusing solely on operational performance. Field validation remains essential for real-world generalization.

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Appendix A — Manufacturer Datasheets of PCM Materials Used in the Study

A.1 Introduction

To ensure full transparency, traceability, and reproducibility of the simulation methodology, the Phase Change Materials (PCMs) implemented in this research were selected based on commercially available products with documented thermophysical properties. The PCM materials used in the simulations correspond to real manufacturer products from two established suppliers:

- **BioPCM®**, manufactured by Phase Change Energy Solutions Inc. (USA), representing organic, bio-based PCM materials.
- **InfiniteR PCM**, manufactured by Infinite R Technologies (USA), representing inorganic, salt-hydrate-based PCM materials.

Each PCM melting temperature evaluated in the parametric and optimization analyses corresponds to a specific commercial PCM product with a clearly defined phase transition temperature range, as specified in the respective manufacturer technical datasheets.

The thermophysical properties adopted in the EnergyPlus and ChameleonPCM simulations—including phase transition temperature, latent heat capacity, density, and thermal conductivity—were derived from these manufacturer datasheets. This ensures that the simulation inputs represent realistic and physically achievable material performance.

The datasheets included in this appendix provide full documentation of the PCM products used in this study, enabling independent verification and ensuring methodological rigor.

A.2 BioPCM® (Organic PCM) Products

The organic PCM materials used in this study correspond to BioPCM® products developed by Phase Change Energy Solutions Inc. These materials are bio-based, paraffin-derived PCMs specifically designed for building envelope thermal energy storage applications.

The following BioPCM products were used to represent the organic PCM melting temperatures investigated in this research:

Simulation Melting Temperature (°C)	Corresponding Product	Manufacturer
21 °C	BioPCM® Q21	Phase Change Energy Solutions
23 °C	BioPCM® Q23	Phase Change Energy Solutions
25 °C	BioPCM® Q25	Phase Change Energy Solutions
27 °C	BioPCM® Q27	Phase Change Energy Solutions
29 °C	BioPCM® Q29	Phase Change Energy Solutions

These products are specifically designed for integration within building envelope systems, including wallboards, ceilings, and insulation layers.

The corresponding manufacturer technical datasheets are included in the following sections:

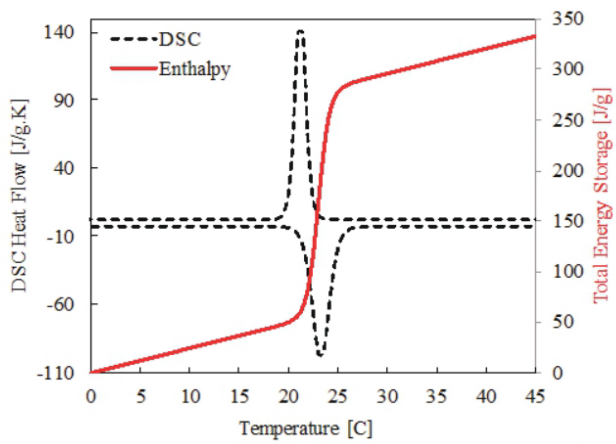
- Appendix A.2.1 — BioPCM® Q21 Datasheet

BioPCM® Technical Data **Q21**

- Environmentally-friendly, derived from naturally occuring, food grade substances
- Non-toxic and biodegradable
- Tunable energy storage capacity; more BTUs per pound of PCM
- Tunable density; more BTUs in the same volume
- Tunable thermal conductivity, for improved reaction with subtle changes in temperature
- Non-corrosive
- Chemically stable
- Long lifetime of performance, no degredation in melting temperature or thermal energy storage after thousands of freeze/ melt cycles (100+ years)
- Small volume changes during phase transitions

BioPCM Q23 Tunable Physical and Chemical Properties

Property	Value (SI)	Value (Imperial)
Melting Point	21°C	71.4° F
Latent Heat	210 – 250 J/g	90 – 110 BTU/lb
Energy Storage Capacity	400 – 1250 kJ/m²	35 – 110 BTU/sq ft
Specific Heat	2.2 – 4.5 J/gK	0.6 – 1.1 BTU/lb°F
Thermal Conductivity	0.15 – 2.5 W/mK	0.09 – 1.45 BTU/ft hr °F
Relative density	0.85 – 1.4 g/mL	53 – 87 lb/ft³
Viscosity	Liquid, viscous gel, solid-solid gel	



NOTE: Tunable material, physical/chemical properties vary depending on the presence and the concentration of gelling agents

Phase Change Energy Solutions is a global leader in the development and deployment of next generation energy efficiency and thermal storage solutions that harness the power of BioPCM®, the company's proprietary phase change material. Phase Change Energy Solution's BioPCM® products are used to improve whole-building energy efficiency in retail, commercial, hospitality and industrial applications; enable safe transport of sensitive food and pharmaceutical products; and provide enhanced thermal storage capabilities for industrial processes. Fortune 100 banking, telecom, hospitality and technology companies, as well as the U.S. government, have installed millions of square feet of BioPCM® products to reduce operating expenses and environmental impact.

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PHASECHANGE ENERGY SOLUTIONS

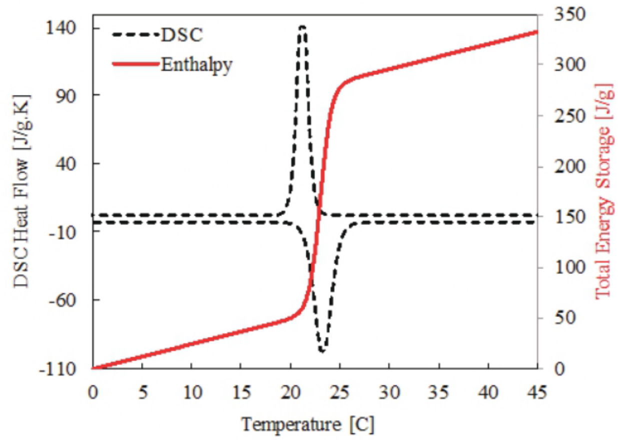
- Appendix A.2.2 — BioPCM® Q23 Datasheet

BioPCM® Technical Data Q23

- Environmentally-friendly, derived from naturally occuring, food grade substances
- Non-toxic and biodegradable
- Tunable energy storage capacity; more BTUs per pound of PCM
- Tunable density; more BTUs in the same volume
- Tunable thermal conductivity, for improved reaction with subtle changes in temperature
- Non-corrosive
- Chemically stable
- Long lifetime of performance, no degradation in melting temperature or thermal energy storage after thousands of freeze/melt cycles (100+ years)
- Small volume changes during phase transitions

BioPCM Q23 Tunable Physical and Chemical Properties

Property	Value (SI)	Value (Imperial)
Melting Point	23°C	73.4° F
Latent Heat	210 – 250 J/g	90 – 110 BTU/lb
Energy Storage Capacity	400 – 1250 kJ/m²	35 – 110 BTU/sq ft
Specific Heat	2.2 – 4.5 J/gK	0.6 – 1.1 BTU/lb°F
Thermal Conductivity	0.15 – 2.5 W/mK	0.09 – 1.45 BTU/ft hr °F
Relative density	0.85 – 1.4 g/mL	53 – 87 lb/ft³
Viscosity	Liquid, viscous gel, solid-solid gel	



NOTE: Tunable material, physical/chemical properties vary depending on the presence and the concentration of gelling agents

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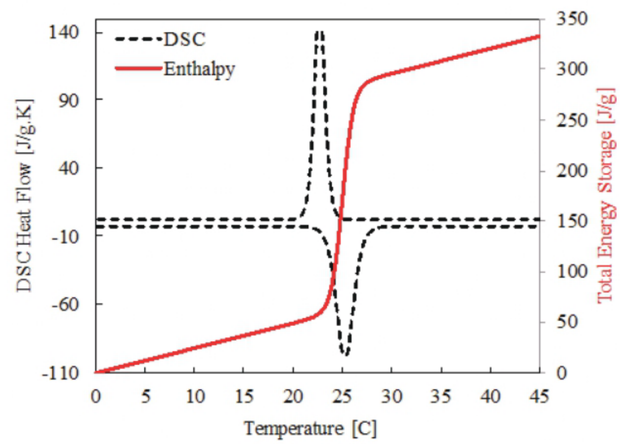
- Appendix A.2.3 — BioPCM® Q25 Datasheet

BioPCM® Technical Data Q25

- Environmentally-friendly, derived from naturally occuring, food grade substances
- Non-toxic and biodegradable
- Tunable energy storage capacity; more BTUs per pound of PCM
- Tunable density; more BTUs in the same volume
- Tunable thermal conductivity, for improved reaction with subtle changes in temperature
- Non-corrosive
- Chemically stable
- Long lifetime of performance, no degradation in melting temperature or thermal energy storage after thousands of freeze/melt cycles (85+ years)
- Small volume changes during phase transitions

BioPCM Q25 Physical and Chemical Properties

Property	Value (SI)	Value (Imperial)
Melting Point	25°C	77° F
Latent Heat	210 – 250 J/g	90 – 110 BTU/lb
Energy Storage Capacity	400 – 1250 kJ/m²	35 – 110 BTU/sqft
Specific Heat	2.5 J/g.K	0.6 BTU/lb.°F
Thermal Conductivity	0.15 – 0.25 W/m.K	0.09 – 0.14 BTU/ft.hr.°F
Relative density	0.85 – 0.95 g/cm³	53 – 59 lb/ft³
Viscosity	Liquid, viscous gel, solid-solid gel	



NOTE: Physical/Chemical properties vary depending on the presence and the concentration of gelling agent

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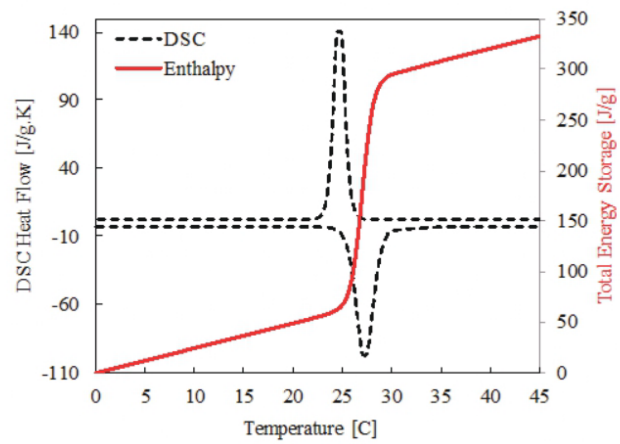
- Appendix A.2.4 — BioPCM® Q27 Datasheet

BioPCM® Technical Data Q27

- Environmentally-friendly, derived from naturally occuring, food grade substances
- Non-toxic and biodegradable
- Tunable energy storage capacity; more BTUs per pound of PCM
- Tunable density; more BTUs in the same volume
- Tunable thermal conductivity, for improved reaction with subtle changes in temperature
- Non-corrosive
- Chemically stable
- Long lifetime of performance, no degradation in melting temperature or thermal energy storage after thousands of freeze/melt cycles (85+ years)
- Small volume changes during phase transitions

BioPCM Q27 Physical and Chemical Properties

Property	Value (SI)	Value (Imperial)
Melting Point	27°C	80.6° F
Latent Heat	210 – 250 J/g	90 – 110 BTU/lb
Energy Storage Capacity	400 – 1250 kJ/m²	35 – 110 BTU/sqft
Specific Heat	2.5 J/g.K	0.6 BTU/lb.°F
Thermal Conductivity	0.15 – 0.25 W/m.K	0.09 – 0.14 BTU/ft.hr.°F
Relative density	0.85 – 0.95 g/cm³	53 – 59 lb/ft³
Viscosity	Liquid, viscous gel, solid-solid gel	



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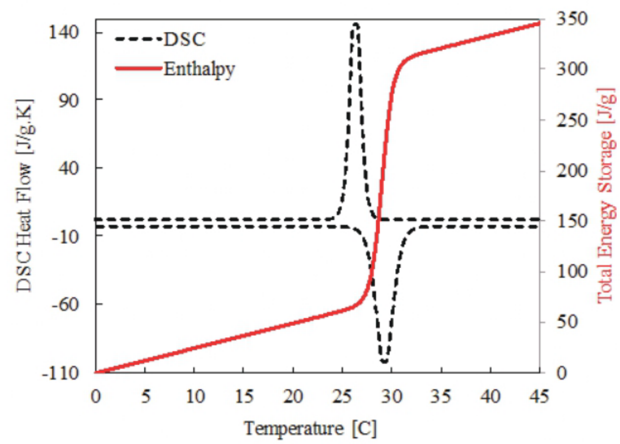
- Appendix A.2.5 — BioPCM® Q29 Datasheet

BioPCM® Technical Data Q29

- Environmentally-friendly, derived from naturally occuring, food grade substances
- Non-toxic and biodegradable
- Tunable energy storage capacity; more BTUs per pound of PCM
- Tunable density; more BTUs in the same volume
- Tunable thermal conductivity, for improved reaction with subtle changes in temperature
- Non-corrosive
- Chemically stable
- Long lifetime of performance, no degradation in melting temperature or thermal energy storage after thousands of freeze/melt cycles (100+ years)
- Small volume changes during phase transitions

BioPCM Q29 Tunable Physical and Chemical Properties

Property	Value (SI)	Value (Imperial)
Melting Point	29°C	84.2° F
Latent Heat	210 – 250 J/g	90 – 110 BTU/lb
Energy Storage Capacity	400 – 1250 kJ/m^2	35 – 110 BTU/sq ft
Specific Heat	2.2 – 4.5 J/gK	0.6 – 1.1 BTU/lb°F
Thermal Conductivity	0.15 – 2.5 W/mK	0.09 – 1.45 BTU/ft hr °F
Relative density	0.85 – 1.4 g/mL	53 – 87 lb/ft^3
Viscosity	Liquid, viscous gel, solid-solid gel	



NOTE: Tunable material, physical/chemical properties vary depending on the presence and the concentration of gelling agents

Phase Change Energy Solutions is a global leader in the development and deployment of next generation energy efficiency and thermal storage solutions that harness the power of BioPCM®, the company's proprietary phase change material. Phase Change Energy Solution's BioPCM® products are used to improve whole-building energy efficiency in retail, commercial, hospitality and industrial applications; enable safe transport of sensitive food and pharmaceutical products; and provide enhanced thermal storage capabilities for industrial processes. Fortune 100 banking, telecom, hospitality and technology companies, as well as the U.S. government, have installed millions of square feet of BioPCM® products to reduce operating expenses and environmental impact.

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Manufacturer:
Phase Change Energy Solutions Inc.
https://phasechange.com

A.3 InfiniteR PCM (Inorganic PCM) Products

The inorganic PCM materials used in this study correspond to InfiniteR PCM products developed by Infinite R Technologies. These materials are based on advanced salt-hydrate formulations designed for thermal energy storage in building applications.

The following InfiniteR PCM products were used to represent the inorganic PCM melting temperatures investigated in this research:

Simulation Melting Temperature (°C)	Corresponding Product	Manufacturer
18 °C	InfiniteR PCM 18	Infinite R Technologies
21 °C	InfiniteR PCM 21	Infinite R Technologies
23 °C	InfiniteR PCM 23	Infinite R Technologies
25 °C	InfiniteR PCM 25	Infinite R Technologies
29 °C	InfiniteR PCM 29	Infinite R Technologies

These materials are engineered for building thermal storage applications and are characterized by high latent heat capacity, good thermal conductivity, and stable phase transition behavior.

The corresponding manufacturer technical datasheets are included in the following sections:

Appendix A.3.1 — InfiniteR PCM 18, 21, 23, 25 and 29 Datasheet

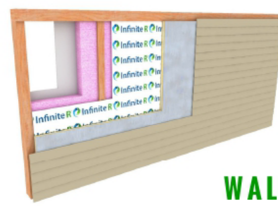
Infinite R™

Contact Us 1-800-509-2199
www.insolcorp.com

PHASE CHANGE MATERIAL

Infinite R™ is a building product using phase change materials to store and release heat during winter, and to reduce heat buildup, air conditioning costs and peak loads in summer.

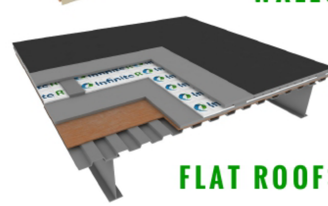
InfiniteR™ phase change material products are built around a fundamental property of Nature: The natural tendency of materials to absorb heat when they melt (phase change from solid to liquid/gel) and to release heat when they solidify (phase change from liquid/gel to solid). When these phase change materials are placed in quantity into the structure of a building, they will naturally absorb heat or air condition the building during the day and release heat at night. Working to provide year round comfort with heating and cooling savings.



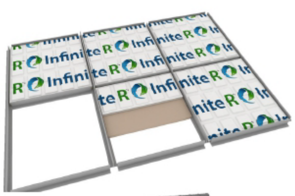
WALLS

SPECIFICATIONS

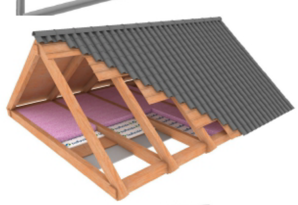
THERMAL CAPACITY 100btu/sf
PHASE CHANGE MATERIAL Mineral Based/Inorganic
TEMPERATURES 65F(18), 69F(21C), 73F(23C), 78F(25C), 84F(29C)
DIMENSIONS Standard 16" & 24" wide x 24", 48" & 96" long
LATENT HEAT 86 btu/lb
SPECIFIC HEAT 1.35 btu/lb
THERMAL CONDUCTIVITY ~0.16 W/ft/K Liquid, ~0.33 W/ft/K Solid
THICKNESS & WEIGHT 0.25" thick; 1.1 lbs/sf (+/-)
FLAME SPREAD ASTM E84|UL723 - Flame 5, Smoke 10
PERMEABILITY ASTM E96 - 0.08 (grains/hr*ft2inHg)



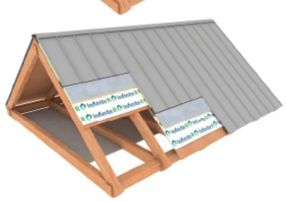
FLAT ROOFS



CEILINGS



ATTICS



PITCHED ROOFS

RESIDENTIAL

Infinite-R™ MORE THAN pays for itself by reducing HVAC system sizing, insulation and wall framing depths WITHOUT adding the weight of conventional mass. **Infinite-R™ is essential to any NetZero or Passive House design.**

COMMERCIAL/INDUSTRIAL

Installed during roof replacements (flat roof or pitched roof), Infinite-R™ has been shown to substantially reduce heat flux of the roof. With Class A fire rating, it can also be installed in suspended ceilings, interior and exterior walls and remain exposed in high internal gain spaces.

AGRICULTURE

Perhaps the most ideal application for phase change materials - stabilize crop temperatures in greenhouses, reduce risk in crop storage, maintain animal comfort in nurseries and barns, save huge energy costs & reduce product loss & fatalities.

INSOLCORP
INNOVATIVE SOLUTIONS CORPORATION

A.4 Traceability and Simulation Consistency

Each PCM melting temperature evaluated in the simulation and optimization framework corresponds directly to one specific commercial PCM product listed above. This establishes a one-to-one correspondence between:

- Simulation PCM definition
- Manufacturer product
- Technical datasheet
- Thermophysical material properties

This ensures that the simulation results reflect realistic material performance and that the study can be independently verified and reproduced using commercially available PCM products.

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