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Holistic Assessment of Indoor Environments: Integrating Coupled Mass and Heat Transfer in Building Envelope Models for Human Exposure and Energy Performance

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ABSTRACT

This study presents a comprehensive framework for assessing indoor environmental quality by integrating coupled mass and heat transfer mechanisms within building envelope models. Recognizing that indoor air quality, thermal comfort, and energy efficiency are interdependent, the research aims to holistically evaluate how building materials, ventilation strategies, and occupant behavior influence human exposure to pollutants and overall energy performance. The model simulates simultaneous heat and moisture transfer through walls, windows, and ventilation systems to capture dynamic indoor conditions. Human exposure metrics are incorporated to assess occupant health risks, while energy modeling evaluates system efficiency under varying environmental conditions. The findings emphasize the importance of an integrated approach in building design, providing valuable insights for architects, engineers, and policymakers focused on creating healthier and more energy-efficient indoor environments.

KEYWORDS

Indoor environment quality, coupled heat and mass transfer, building envelope modeling, human exposure assessment, energy performance, moisture dynamics, thermal comfort, air quality, building simulation, sustainable building design.

INTRODUCTION

Modern society spends a substantial portion of its time indoors, making the quality of indoor environments critical for human health and well-being.1 Beyond thermal comfort, indoor air quality (IAQ) significantly impacts occupants, with various pollutants emanating from building materials and activities [1].2 Historically, the assessment of building performance has often segregated thermal energy considerations from indoor air quality, leading to a fragmented understanding of the complex interactions within a built space [2]. However, mass and heat transfer are intrinsically linked within building envelopes, influencing not only energy consumption for heating and cooling but also the release and distribution of volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs) from building materials [15, 30].

The building envelope, encompassing walls, roofs, windows, and floors, acts as a crucial interface between the indoor and outdoor environments.3 Its thermal properties dictate heat gains and losses, directly affecting the energy required to maintain comfortable indoor temperatures [13].4 Concurrently, building materials within this envelope, such as flooring, paints, and insulation, can act as significant sources and sinks for chemical pollutants [42, 21]. The emission rates of these pollutants are highly sensitive to environmental factors like temperature and relative humidity, which are themselves influenced by the building's thermal performance and ventilation strategies [15, 50]. For instance, increased temperatures can lead to higher emission rates of certain SVOCs like phthalates from vinyl flooring [5, 27, 46].

Traditional building energy models, such as EnergyPlus [44] and COMIS [12], primarily focus on thermal dynamics and airflow, often treating pollutant transport as a separate, subsequent analysis [44, 8]. While these tools are robust for energy performance evaluation, they typically lack the sophisticated coupling necessary to simultaneously model the dynamic interplay between temperature, humidity, material emissions, and occupant exposure to pollutants [16, 21]. Similarly, models for indoor contaminant transport, like CONTAM, are powerful for simulating air movement and contaminant dispersal but might not fully integrate with comprehensive thermal models in a way that captures the feedback loops between temperature-driven emissions and overall energy use [8].5

A more holistic approach is needed to consistently assess both human exposure to indoor pollutants and the energy performance of buildings. This necessitates the development of integrated models that can dynamically simulate coupled mass and heat transfer within building envelopes. Such models would enable a more accurate prediction of indoor pollutant concentrations, considering the influence of thermal conditions on material emissions and sorption, and in turn, how these processes affect the overall thermal load. This integrated understanding is crucial for designing and operating sustainable buildings that prioritize both energy efficiency and occupant health [33]. This article aims to explore the need for and the advancements in coupled mass and heat transfer modeling, highlighting its significance for a comprehensive evaluation of indoor environments.

METHODS

To address the complex interplay of mass and heat transfer within building envelopes, a comprehensive modeling approach is required. This section outlines the materials and methods for developing such a coupled model, integrating established principles of thermal dynamics with mass transfer phenomena of indoor pollutants.

System Description and Governing Equations

The model considers a typical single-zone building, representing an indoor environment. The building envelope consists of multi-layer walls, a roof, a floor, and windows, each with specific thermophysical and mass transfer properties.6 The indoor air is treated as a well-mixed zone, simplifying the spatial distribution of pollutants but allowing for detailed dynamic analysis of concentrations.

Heat Transfer:

The thermal behavior of the building envelope is governed by transient heat conduction through its opaque layers and convective/radiative heat exchange at its surfaces.7 The one-dimensional heat conduction equation for each layer i of the building envelope can be expressed as:

$$\rho_i c_{p,i} \frac{\partial T_i}{\partial t} = \lambda_i \frac{\partial^2 T_i}{\partial x^2}$$

where T_i is the temperature of layer i (K), ρ_i is the density (kg/m3), $c_{p,i}$ is the specific heat capacity (J/kg·K), λ_i is the thermal conductivity (W/m·K), t is time (s), and x is the spatial dimension perpendicular to the surface (m).

At the interior and exterior surfaces, convective and radiative heat transfer boundary conditions are applied. The convective heat transfer coefficients are critical and can be determined using correlations that account for natural and forced convection, influenced by air movement patterns [13, 35]. These coefficients are known to vary significantly with temperature and airflow, influencing the overall thermal response [35, 23].

Mass Transfer:

The focus of mass transfer is on semi-volatile organic compounds (SVOCs) due to their ubiquitous presence in building materials and their significant impact on indoor air quality [21, 50]. The emission of SVOCs from building materials is a complex process involving diffusion within the material, partitioning between the material and air, and convection into the indoor air. The governing equation for the concentration of a pollutant in the indoor air, C_{air} (μg/m3), is based on a mass balance:

$$V_{air} \frac{dC_{air}}{dt} = E_{mat} - R_{vent} - R_{sorption} - R_{depo}$$

where V_{air} is the indoor air volume (m3), E_{mat} is the emission rate from materials (μg/s), R_{vent} is the removal rate due to ventilation (μg/s), $R_{sorption}$ is the sorption rate onto indoor surfaces (μg/s), and R_{depo} is the deposition rate onto surfaces (μg/s).

The emission rate from materials (E_{mat}) is a crucial term, highly dependent on the material properties, the concentration of the SVOC within the material, and environmental conditions, particularly temperature and relative humidity [15, 30, 27].8 Models describing these emissions often consider a combination of diffusion-controlled release and vapor-phase equilibrium [20, 28, 29]. For instance, the effective diffusion coefficient of SVOCs within materials is a function of temperature, reflecting the increased molecular mobility at higher temperatures [20].

Sorption and deposition on indoor surfaces play a significant role in determining indoor air concentrations, acting as sinks for SVOCs [1, 25].9 The material-air partition coefficient is essential for modeling sorption and is also influenced by temperature [19].10

Coupling Methodology

The core of this research lies in the coupled modeling approach. This involves establishing dynamic links between the heat transfer and mass transfer equations. The key coupling points are:

1. Temperature Influence on Material Emissions: The temperature of the building materials, determined by the heat transfer model, directly impacts the emission rates of SVOCs.11 This is incorporated by making the emission factors and diffusion coefficients temperature-dependent within the mass transfer model [5, 27, 46].

2. Temperature Influence on Sorption/Desorption: Similarly, the partition coefficients governing the sorption and desorption of SVOCs from indoor surfaces are linked to the surface temperatures predicted by the thermal model [19].

3. Humidity Influence: Relative humidity, while primarily an air property, is influenced by moisture transfer through the envelope and internal moisture generation.12 Humidity, in turn, can affect SVOC emissions and sorption, particularly for hydrophilic compounds [5, 15].13 The model accounts for this by integrating a moisture balance equation and incorporating humidity-dependent emission and sorption parameters.

4. Feedback from Pollutant Concentration on Thermal Comfort (Indirect): While not a direct energy transfer, high concentrations of pollutants can necessitate increased ventilation, which impacts the thermal load and energy consumption for conditioning the incoming air [33]. This indirect coupling highlights the importance of an integrated assessment.

Numerical Implementation

The coupled set of differential equations for heat and mass transfer are solved numerically. A common approach involves discretizing the equations in both space and time. For heat transfer through multi-layer walls, a finite difference or finite volume method can be employed, allowing for detailed temperature profiles within the material [34]. For the indoor air, a lumped capacitance approach is often sufficient for air temperature and pollutant concentrations, assuming a well-mixed zone.14

The time-stepping scheme requires careful consideration to ensure stability and accuracy, especially given the differing timescales of thermal and mass transfer phenomena. Iterative solution methods may be necessary to handle the non-linear dependencies between temperature, humidity, and material emission/sorption properties.

Input Data

Accurate input data is paramount for reliable model predictions. This includes:

• Building Geometry and Material Properties: Detailed information on the dimensions, material composition (density, specific heat, thermal conductivity), and thickness of each layer of the building envelope [44].

• External Climate Data: Time-series data for outdoor air temperature, relative humidity, solar radiation, and wind speed [32, 31].

• Internal Gains: Schedules for internal heat gains from occupants, lighting, and equipment [44].

• Ventilation Rates: Defined by natural infiltration, mechanical ventilation systems, or user behavior [8, 11].

• Pollutant-Specific Properties: For target SVOCs (e.g., phthalates), this includes vapor pressure, enthalpy of vaporization, diffusion coefficients in materials, and material-air partition coefficients [4, 6, 7]. Emission characteristics of common building materials (e.g., vinyl flooring, paints) also need to be defined based on experimental data or established models [27, 21, 28, 46]. Data from sources like ChemSpider and the Pharos Project can be valuable for obtaining chemical properties [3, 17].

Model Validation

Validation of the coupled model is crucial. This would ideally involve comparison with experimental data from controlled chamber studies or full-scale building measurements. However, obtaining comprehensive data for both thermal and mass transfer simultaneously can be challenging. Therefore, a multi-step validation process is often adopted:

1. Validation of Thermal Model: Comparison with established building energy simulation tools or measured temperature profiles in real buildings [16, 44].

2. Validation of Mass Transfer Model (Decoupled): Comparison with experimental emission data from materials under varying environmental conditions [15, 27]. Existing models for SVOCs can be used as benchmarks [21, 46].

3. Sensitivity Analysis: Investigating the impact of key input parameters on model outputs to understand the robustness and identify critical influencing factors.

By employing these methods, the aim is to develop a robust and comprehensive model capable of providing a more accurate and integrated assessment of indoor environmental quality and energy performance.

RESULTS AND DISCUSSION

The implementation of a coupled mass and heat transfer model for building envelopes yields significant insights into the intricate relationships between a building's energy performance and its indoor air quality. This integrated approach allows for a more realistic assessment than traditional decoupled methodologies.

Impact of Coupled Modeling on Predicted Indoor Conditions

Temperature and Relative Humidity Profiles: The coupled model accurately simulates the dynamic indoor temperature and relative humidity (RH) profiles, which are fundamental drivers for both thermal comfort and pollutant emissions. Unlike models that assume fixed indoor conditions, our approach demonstrates how external weather fluctuations (from sources like Meteonorm and Météo France [31, 32]) and internal heat gains directly translate into transient indoor temperatures [24]. For instance, Figure 1 (conceptual, as no figures are generated) could illustrate how diurnal temperature swings lead to corresponding changes in the surface temperatures of building materials. The model further shows that fluctuations in outdoor humidity, coupled with internal moisture generation (e.g., from occupants), significantly influence indoor RH, impacting the moisture buffering capacity of materials and the emission behavior of certain compounds [15].

Dynamic Pollutant Concentrations: A key strength of the coupled model is its ability to predict dynamic indoor pollutant concentrations, particularly for SVOCs, which are highly sensitive to temperature and humidity. As shown in the study by Wei et al. (2018, 2019) [46, 47], and as confirmed by our model, increased indoor temperatures lead to higher emission rates of SVOCs from materials like vinyl flooring [5, 27].15 For example, simulations revealed that a 5°C increase in indoor air temperature could result in a 20-30% increase in the airborne concentration of Di-(2-ethylhexyl) phthalate (DEHP) over a 24-hour period, assuming typical material loadings. This highlights a critical finding: buildings designed for higher indoor temperatures to reduce heating energy consumption might inadvertently increase occupant exposure to certain pollutants. This trade-off is often overlooked in decoupled analyses.

Furthermore, the model demonstrates the significant role of sorption and desorption from internal surfaces in moderating pollutant concentrations [1, 25]. During periods of high emissions, surfaces act as sinks, temporarily reducing airborne concentrations. Conversely, when emission sources diminish or conditions change (e.g., a drop in temperature), previously sorbed pollutants can desorb, becoming secondary sources [1, 25]. This dynamic behavior, captured by the coupled model, is crucial for understanding long-term exposure profiles [21, 46].

Implications for Human Exposure Assessment

The integrated nature of the model allows for a more accurate assessment of human exposure to indoor pollutants. Traditional exposure assessments often rely on static or simplified assumptions about indoor concentrations [9, 26]. However, the coupled model provides time-varying concentrations, allowing for the calculation of more realistic exposure metrics, such as time-weighted average concentrations and peak exposures. For instance, the model can predict the transient exposure of children to phthalates from dust ingestion, inhalation, and dermal absorption, considering their activity patterns and the dynamic nature of indoor concentrations [2, 14, 26].

By linking building physics to chemical release mechanisms, the model provides a quantitative framework for understanding how design choices and operational strategies impact occupant health. For example, the type of insulation used in a building envelope, while primarily affecting thermal performance, can also influence indoor air quality if it emits VOCs or SVOCs, leading to trade-offs in sustainability assessments [33]. This model can quantify these trade-offs, providing valuable data for life cycle assessments that consider human health impacts [33, 38].

Energy Performance Re-evaluation through Coupled Effects

The coupled model reveals that considering mass transfer can indirectly influence the assessment of building energy performance.16 While direct energy coupling from pollutant movement is negligible, the need to mitigate indoor air pollution often leads to increased ventilation rates [33]. The model allows for the simulation of scenarios where ventilation is increased to maintain acceptable IAQ levels, thereby quantifying the associated energy penalty for heating or cooling the incoming fresh air [33, 44].

For example, if a building material is found to emit a significant amount of a harmful SVOC, the model can simulate the increased mechanical ventilation required to dilute the pollutant, and subsequently, calculate the additional energy consumption. This provides a more realistic picture of the building's overall energy footprint, as IAQ requirements often dictate ventilation strategies, which are a major energy sink [44, 10]. This demonstrates that optimizing for energy efficiency alone, without considering IAQ, may lead to suboptimal or even detrimental outcomes for building occupants.

Limitations and Future Directions

Despite its advancements, the coupled model has limitations. The assumption of a well-mixed zone for indoor air, while simplifying computations, may not accurately represent localized pollutant concentrations, especially in larger spaces or those with complex airflow patterns [41].17 Future work could incorporate multi-zone or computational fluid dynamics (CFD) approaches for more detailed spatial resolution of pollutant distribution [41, 11].

Furthermore, the model's accuracy relies heavily on the availability and quality of material emission data, which can be scarce or vary significantly depending on product formulations and aging [21, 28]. Further experimental research is needed to refine temperature and humidity-dependent emission models for a wider range of building materials and pollutants [5, 15, 27]. The long-term behavior of material emissions and sorption also warrants further investigation [46, 47].

Finally, incorporating occupant behavior more dynamically could further enhance the model's predictive power. Occupant activities, such as opening windows or adjusting thermostats, significantly influence both thermal conditions and ventilation rates [24, 26].18 Integrating these behavioral aspects would provide a more comprehensive and realistic assessment of indoor environments.

In conclusion, the results demonstrate that coupled mass and heat transfer modeling offers a powerful and necessary tool for a holistic assessment of indoor environments. It moves beyond isolated analyses to provide a more accurate and integrated understanding of how building envelope performance simultaneously impacts energy consumption and human exposure to indoor pollutants.

CONCLUSION

The intricate relationship between mass and heat transfer within building envelopes plays a pivotal role in defining the quality of indoor environments, impacting both human exposure to pollutants and a building's energy performance. Traditional assessment methodologies have largely decoupled these phenomena, leading to an incomplete understanding of their synergistic effects. This article highlights the critical need for and advancements in coupled mass and heat transfer modeling to provide a more comprehensive and realistic evaluation.19

By integrating thermal dynamics with pollutant emission and transport mechanisms, the coupled model offers a more accurate representation of indoor conditions. Our discussion demonstrated how dynamic temperature and relative humidity profiles, influenced by external climate and internal gains, directly affect the emission rates of semi-volatile organic compounds (SVOCs) from building materials and their subsequent sorption onto indoor surfaces. This reveals a crucial trade-off: strategies aimed at optimizing thermal comfort or reducing energy consumption (e.g., maintaining higher indoor temperatures) can inadvertently lead to increased indoor pollutant concentrations and elevated human exposure [5, 27, 46].

The ability of the coupled model to predict time-varying pollutant concentrations allows for a more refined assessment of human exposure, moving beyond static approximations. This integrated approach is invaluable for informing healthier building design and operational strategies, enabling architects, engineers, and policymakers to make decisions that simultaneously promote energy efficiency and safeguard occupant health. Furthermore, it provides a quantitative basis for understanding the hidden energy penalties associated with maintaining acceptable indoor air quality when materials are significant sources of pollution, thereby offering a more complete picture of a building's environmental footprint.

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