Resources, Conservation & Recycling 232 (2026) 108944

Contents lists available at ScienceDirect

Resources, Conservation & Recycling

journal homepage: www.sciencedirect.com/journal/resources-conservation-and-recycling

Full length article

The computational microscope: 28,000 pathway tests reveal how urban expansion triggers the hidden carbon-heat-haze cascade

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ARTICLE INFO

Keywords:
Urban expansion
Carbon-heat-haze nexus
Ecological efficiency
Nature-based solutions
Data-driven hypothesis testing
Precision urban governance

ABSTRACT

This study conducts the first comprehensive data-driven theoretical hypothesis testing in urban environmental science, systematically evaluating existing theories through 28,848 pathway combinations across a global sample of 6488 cities, encompassing 4 urban expansion drivers, 9 environmental variables, 10 temporal configurations, 7 geographic regions, and 3 socioeconomic strata. The empirical validation reveals that current theories show expected probability distributions, but data-driven refinement identifies robust patterns: vegetation dynamics, not economic activity, dominates urban environmental outcomes, establishing an ecological efficiency paradigm. Temperature emerges as the critical mediating hub, connecting 80% of environmental transmission pathways in the carbon-heat-haze nexus. Environmental impacts exhibit pronounced 10-year lag effects, with medium-term policies achieving 87.5% effectiveness. Geographic disparities reveal theory boundaries: Asian cities follow predictable patterns (70% conformity) while European cities have fundamentally restructured cause-effect relationships. Middle-income countries experience peak environmental stress while high-income nations successfully interrupt cascading processes. This study provides an empirical roadmap for precision urban governance aligned with sustainable development goals.

1. Introduction

Global urbanization represents one of this century's most transformative anthropogenic processes, fundamentally reshaping human-environment relationships at unprecedented speed and scale (Angel et al., 2011; United Nations, 2019). With urban populations projected to reach 68% globally by 2050 and cities generating over 70% of global carbon emissions, urban sustainability has emerged as pivotal to achieving the United Nations Sustainable Development Goals (SDGs), particularly SDG 11 (Sustainable Cities and Communities) and SDG 13 (Climate Action) (UN-Habitat, 2022). Yet current urban environmental theories face a predictive crisis—they fail to provide consistent explanations across diverse global contexts, thereby undermining evidence-based, climate-responsive urban governance (Bai et al., 2018).

Cities drive economic growth while simultaneously becoming epicenters of global environmental pressure. Among their multifaceted environmental impacts, three challenges directly threaten urban sustainability and resident health: increased carbon emissions, intensified Urban Heat Islands (UHIL), and deteriorating air pollution. These correspond respectively to global climate change, local climate degradation, and public health crises (Tuholske et al., 2021; Luo et al., 2024), constituting essential dimensions for assessing urban environmental performance.

Understanding how cities generate these environmental consequences requires precise definition of the core driver: "urban expansion." Rather than treating this as a monolithic concept, we recognize it as a dynamic, multidimensional process (Seto et al., 2012). This study systematically deconstructs urban expansion into independently measurable aspects: spatial extent growth (Annual Expansion Area, AEA), built-up area intensification (Built-up Density Rate, BUDR), economic activity intensity (Nighttime Light Intensity Rate, NLIR), land use efficiency (New Land-Use Efficiency, NLE), and ecological pattern evolution (NDVI Dynamic Rate, NDR) (Li et al., 2020). Different expansion modes—compact versus sprawling development—produce markedly different or even contradictory environmental outcomes (Ewing and Cervero, 2010; Güneralp et al., 2020).

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https://doi.org/10.1016/j.resconrec.2026.108944
Received 16 December 2025; Received in revised form 10 March 2026; Accepted 3 April 2026
Available online 21 April 2026

Urban expansion dimensions generate not isolated environmental problems but an interconnected "carbon-heat-haze" nexus through altered surface energy balance and material cycling (Seto et al., 2014; Creutzig et al., 2022). These three elements couple through complex physical and chemical processes, creating cascading effects that demand systematic thinking beyond sectoral approaches (Geels, 2019). Land use changes directly alter surface albedo and evapotranspiration with confirmed climate consequences (Pielke et al., 2011). This intensifies UHI effects, elevating temperatures that increase cooling-related energy consumption and drive up Total Carbon Emissions (TCAL) (Zhang et al., 2024). Simultaneously, high temperatures and precursor concentrations accelerate secondary pollutant formation through photochemical reactions, deteriorating Air Quality Index (AQI) (Zhang et al., 2025). Within this cascade, Temperature Average Level (TAL) functions as a crucial "mediating hub."

These relationships exhibit strong contextual dependence rather than universal applicability. Evidence demonstrates significant variation in urbanization-environmental quality relationships across geographical regions (Chen et al., 2020). Between cities, different socioeconomic development levels result in vastly different environmental outcomes and policy capacities (Zhong et al., 2021). This heterogeneity suggests that seeking singular "universal" theories proves futile. Research must pivot toward understanding theoretical applicability contexts and failure modes.

This compound problem poses escalating threats to human well-being (Tuholske et al., 2021), with confirmed causal links between urbanization and PM2.5 pollution creating serious public health risks (Lu et al., 2019). However, accurate impact measurement confronts profound methodological challenges. Traditional urban environmental studies rely on static stock variables, yet environmental systems respond to urban expansion through inherently dynamic processes. Consequences arise primarily from incremental expansion effects rather than stock states. Moreover, environmental responses exhibit Time-lagged Effects. Infrastructure construction creates "lock-in effects" (Seto et al., 2016), ecosystem responses to disturbances show delays (Seto et al., 2016), and urbanization's air pollution impacts demonstrate confirmed lag effects (Yang et al., 2022).

Existing theories and empirical research face systematic challenges when explaining complex real-world phenomena. This study addresses this gap through large-scale, data-driven empirical analysis targeting three cognitive deficits: From Conceptual Ambiguity to Dimensional Clarity (most studies employ singular, generalized urbanization variables, failing to address urban expansion's multifaceted nature); From Macroscopic Correlation to Mechanism Transmission (systematic, data-based testing of complex multi-step mediation pathways among "carbon-heat-haze" components remains virtually absent at global scales); and From Static Stocks to Dynamic Change Rates (research overwhelmingly employs static stock variables, ignoring temporal lag effects and dynamic change rate effects).

To address these cognitive gaps, this study implements a systematic "data-driven theoretical hypothesis testing" framework using a global database of 6488 cities encompassing multiple urbanization dimensions. Rather than developing new theories, we systematically test existing theoretical predictions against empirical reality through unprecedented computational scale. Our analytical scope encompasses 28,848 individual pathway tests across 4 core urban expansion drivers (after multicollinearity control), 9 environmental response variables, 10 temporal configurations (including concurrent and various lag structures), 7 geographic regions, and 3 socioeconomic strata, employing both Simple and Sequential Mediation approaches. This massive computational investigation represents the most comprehensive theoretical testing in urban environmental science conducted to date. Through this systematic investigation, we provide scientific pathways for unlocking global cities' unexploited potential in climate change mitigation, offering empirically-validated theoretical foundations and targeted policy guidance for global urban sustainable development. Specifically, this study addresses three testable research questions:

RQ1: Among the multiple dimensions of urban expansion—ecological dynamics, economic metabolism, and spatial morphology—which dimensions and variable combinations constitute the most robust analytical framework for explaining the carbon-heat-haze environmental cascade across global cities? Competing theoretical perspectives suggest that economic activity intensity may dominate (the traditional economic metabolism view) or that ecological process variables may prove more predictive (the emerging ecological efficiency view); we empirically adjudicate between these alternatives through systematic combinatorial framework selection and validation (Sections 2.2–2.3).

RQ2: Does temperature function as a systemic mediating hub connecting urban expansion drivers to multiple downstream environmental outcomes (carbon emissions, air quality), or do parallel, independent transmission pathways better characterize the urban environmental system? We evaluate the relative frequency and strength of temperature-mediated versus non-temperature pathways across all conforming transmission chains (Section 2.3.2).

RQ3: To what extent does the theoretical consistency of urban environmental transmission pathways vary across temporal lags, geographic regions, and socioeconomic strata? We examine whether pathway conformity rates exhibit systematic contextual dependencies, thereby delineating the applicability boundaries of the identified framework (Section 2.4).

2. Results

2.1. Analytical framework and theoretical foundation

This study employs a dynamic change rate-oriented design that successfully eliminated urban scale differences, achieving true cross-city comparability. The dynamic design converted traditional stock variables into standardized annual change rates, capturing actual process effects of urban expansion rather than cumulative state effects while providing reliable foundations for lag effect analysis.

Our theoretical framework tests established urban environmental theory predictions: environmental degradation variables should exhibit positive relationships with each other, while ecological improvement variables should show negative relationships with environmental degradation. The unprecedented scope encompasses systematic testing of 4 core urban expansion drivers across 9 environmental response variables under 10 distinct temporal configurations, stratified across 7 geographic regions and 3 socioeconomic strata—generating over 8000 pathway combinations for comprehensive theoretical validation (Fig. 1).

We established strict criteria for pathway "theoretical conformity": all links must be statistically significant ($p < 0.05$) with impact directions completely consistent with existing scientific theory. For Sequential Mediation models ($X \rightarrow M1 \rightarrow M2 \rightarrow Y$), all three links must meet theoretical expectations.

2.2. Initial comprehensive analysis and framework refinement

The results in this section are reported using the theoretical conformity rate, defined as the proportion of statistically significant pathways ($p < 0.05$) whose coefficient directions are fully consistent with a priori theoretical predictions, as the primary evaluation metric. Our initial analysis tested over 8000 pathway combinations across 4 core urban expansion drivers and 9 environmental variables. In initial Simple Mediation analysis, only 34 out of 132 significant pathways (37.1%) conformed to theoretical expectations. Sequential Mediation analysis showed theoretical conformity rates of 19.4% (21 conforming pathways out of 108 significant). While these rates are consistent with expected probability distributions for complex multi-pathway systems, they indicated substantial room for optimization.

Based on theoretical conformity, pathway stability, and explanatory

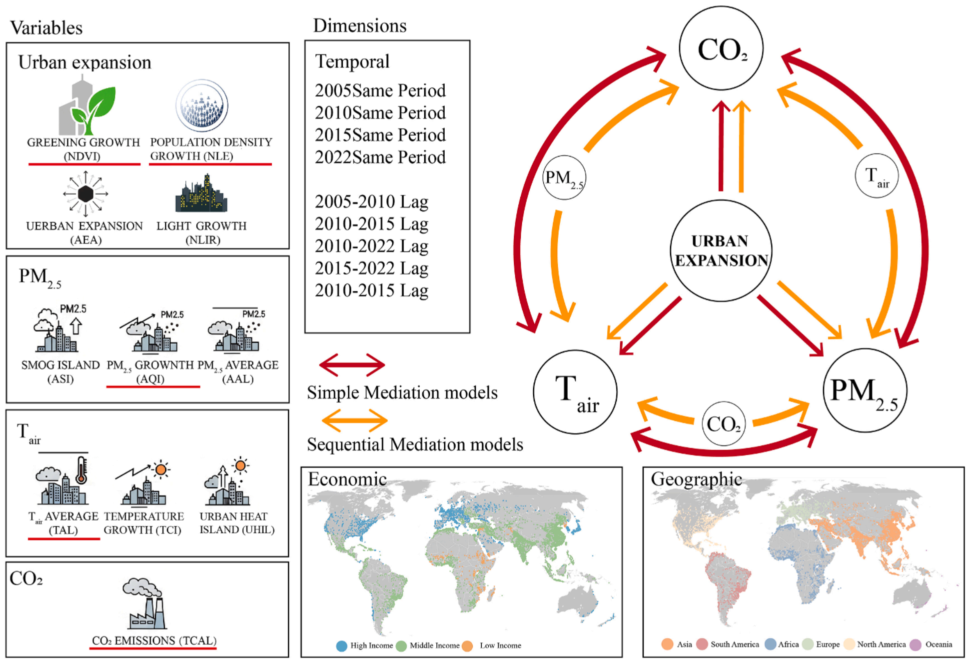

Fig. 1. Theoretical Framework and Analytical Design.

power analysis, we identified a streamlined framework consisting of 2 core driving forces (NDR, NLE) and 3 core environmental state variables (TCAL, TAL, AQI). This framework achieved a fundamental transformation: Simple Mediation pathway conformity reached 63.6% (71% improvement), while Sequential Mediation conformity reached 77.8% (300% improvement) (Fig. 2).

2.3. *Core pathway validation and variable functions*

2.3.1. *Systematic validation of transmission pathways*

The results in this section report the number and proportion of theoretically conforming pathways attributed to each driver and mediator variable. A driver is considered dominant when it accounts for the majority (≥50%, as defined in this study) of all conforming pathways across both Simple and Sequential Mediation analyses. Our refined framework demonstrated robust performance across both analytical approaches. Simple Mediation analysis identified 7 stable and

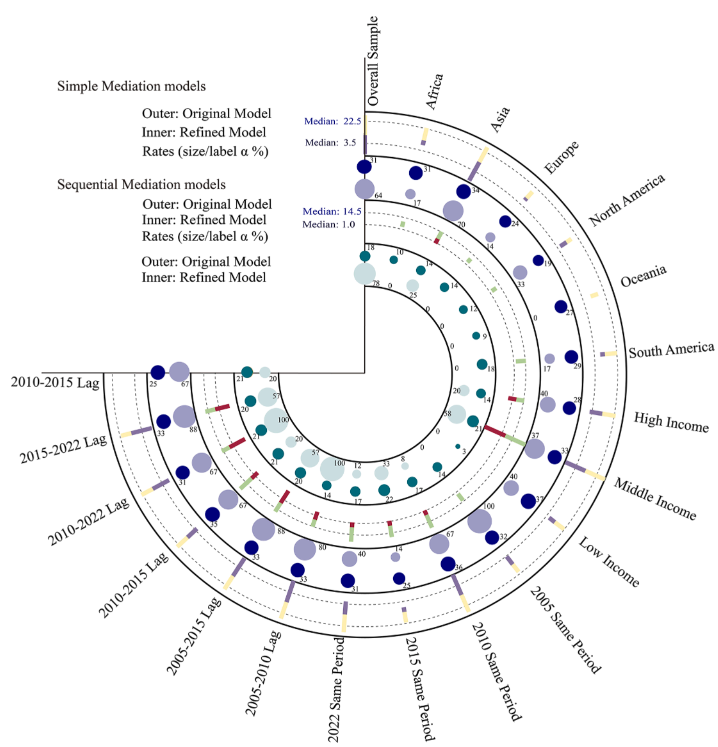

Fig. 2. Comparative analysis of theoretical conformity between the initial and refined models.

theoretically conforming pathways, while Sequential Mediation analysis revealed 7 complex transmission pathways.

NDR accounted for 71.4% (5 out of 7) of conforming pathways in both Simple and Sequential Mediation analyses, exceeding the dominance threshold (≥50%) defined above, driving 5 out of 7 conforming pathways in both analyses. NDR pathways demonstrated diverse regulatory functions: thermal regulation (NDR→TAL→TCAL, NDR→TAL→AQI), carbon sink effects (NDR→AQI→TCAL, NDR→TCAL→TAL), and air purification (NDR→TCAL→AQI). The strongest pathway was NDR→TAL→AQI→TCAL, representing comprehensive ecological regulation cascade.

NLE emerged as consistent secondary driving force, contributing 2 pathways in both approaches. All NLE pathways consistently followed efficiency-to-thermal-to-downstream transmission patterns, confirming land use efficiency's direct and predictable environmental impacts.

2.3.2. Environmental variable functional roles

The results in this section report the frequency with which each environmental variable functions as a mediator versus a terminal outcome across all conforming pathways, expressed as a percentage of total conforming pathways in each mediation approach. TAL assumed the role of core mediating hub in urban environmental systems. TAL appeared as mediating variable in 80% of Simple Mediation pathways and served as either first or second mediator in 85.7% of Sequential Mediation pathways, confirming the critical position of urban thermal environment (Fig. 3).

TCAL showed balanced but outcome-oriented characteristics. In Simple Mediation, TCAL served as mediating variable in 40% of pathways and final outcome in 60%. Sequential Mediation revealed TCAL's dual nature: 42.9% intermediate function, 57.1% terminal function.

AQI clearly exhibited terminal outcome variable characteristics. AQI served as final outcome in 75% of Simple Mediation pathways and 71.4% of Sequential Mediation chains, aligning with theoretical expectations of air quality as a final state variable.

2.3.3. Quantitative transmission characteristics

The results in this section report standardized path coefficients (β) from the mediation models, which allow direct comparison of effect magnitudes across different pathways and variables. Standardized coefficient analysis revealed quantitative patterns across transmission mechanisms (Fig. 4). NDR demonstrated significantly stronger influence with direct impact coefficient on AQI (−1.304) far exceeding NLE's impact on TAL (0.070). TAL showed strong downstream transmission capacity with impact coefficients on AQI (0.127) and TCAL (0.025). Sequential Mediation revealed stronger thermal-to-air quality transmission (0.093) compared to thermal-to-carbon pathways (0.019).

2.4. Contextual boundaries: deviations from overall patterns

The results in this section use the theoretical conformity rate as the primary metric, comparing subgroup-specific rates against the overall baseline rates (63.6% for Simple Mediation, 77.8% for Sequential Mediation) to identify systematic contextual deviations.

2.4.1. Temporal dimension variations

Temporal analysis revealed critical deviations from overall patterns. Medium-term lag models dramatically outperformed overall conformity rates, achieving 87.5% conformity in Sequential Mediation versus the overall 77.8%. Lag conditions enhanced standardized path coefficients (average 0.156) compared to concurrent models (average 0.089), indicating temporal accumulation effects.

Concurrent analysis showed dramatic temporal variations that diverged from stable overall patterns. Sequential Mediation conformity fluctuated from 100% (2005) to 8.3% (2010) to 33.3% (2015) to 12.5%

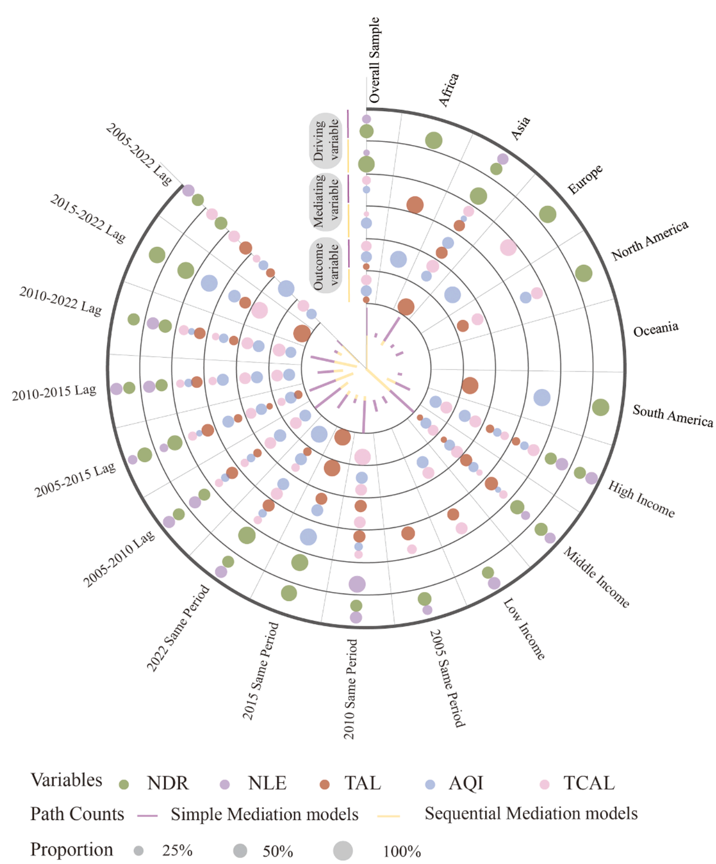

Fig. 3. Frequency and contextual heterogeneity of core variables in causal pathways.

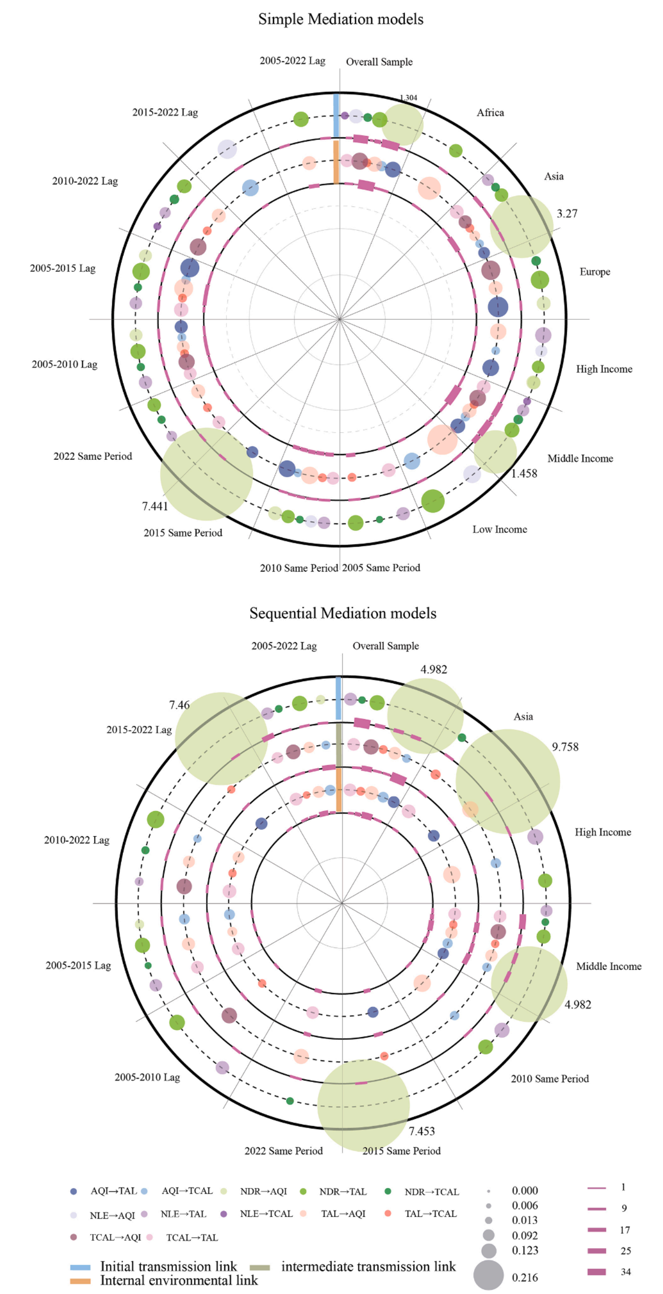

Fig. 4. Coefficient heterogeneity of simple mediation paths and sequential mediation paths.

(2022), revealing a critical "decoupling transition" period during 2010–2015 that systematically disrupted traditional environmental relationships.

2.4.2. Geographic dimension variations

Geographic analysis revealed substantial regional deviations from overall conformity patterns. Asia exceeded overall performance with 70.0% conformity in Simple Mediation compared to overall 63.6%, while maintaining moderate Sequential Mediation performance (25.0%). Asian contexts preserved traditional variable hierarchies with NDR dominating 80% of pathways and TAL serving as primary mediator in 75% of cases.

Europe showed complete divergence from overall patterns, achieving only 14.3% Simple Mediation conformity and 0.0% Sequential Mediation conformity versus overall rates of 63.6% and 77.8%. European variable patterns fundamentally differed from overall structures, with traditional driver-mediator-outcome hierarchies largely disrupted and inverted coefficient patterns indicating systematic environmental management interventions.

2.4.3. Socioeconomic dimension variations

Socioeconomic analysis revealed inverted-U patterns that deviated significantly from overall averages. Middle-income groups exceeded overall conformity with 66.7% Simple Mediation and 58.3% Sequential Mediation rates. Middle-income contexts displayed classic theoretical structures with NDR serving as primary driver in 71.4% of pathways and strongest average pathway coefficients (0.167).

High-income groups showed contrasting deviations with reduced Simple Mediation conformity (40.0%) and substantially lower Sequential Mediation conformity (20.0%) compared to overall patterns. Variable role analysis revealed systematic disruptions: NDR coefficients were substantially reduced (0.078 vs overall average), TAL's mediating function decreased to 40%, while TCAL emerged as alternative mediator, indicating advanced environmental management systems that fundamentally alter traditional transmission pathways.

Low-income groups demonstrated complete sequential pathway failure (0.0% conformity) despite moderate simple pathway performance (40.0%), suggesting fundamentally different environmental dynamics driven by infrastructure deficits rather than urban expansion processes.

3. Discussion

Through systematic "explore-refine-validate" data-driven processes involving 28,848 pathway tests across 4 core urban expansion drivers, 9 environmental response variables, 10 temporal configurations, 7 geographic regions, and 3 socioeconomic strata, this study refined a robust theoretical framework for global urban environmental impacts while profoundly revealing the contextual dependency boundaries of this theory's applicability. Our findings provide new scientific evidence for reconstructing urban sustainable development theory and guiding precise governance practices.

3.1. Theoretical paradigm shift: from economic metabolism to ecological efficiency

This study's most significant contribution lies in provides preliminary evidence suggesting in urban environmental science. The systematic refinement from initial probability-consistent conformity (19.4–37.1%) to robust frameworks (63.6–77.8%) through massive computational analysis confirms that current urban environmental theories require fundamental reconceptualization rather than incremental modification. The data-driven approach demonstrated that while initial theory performance follows expected statistical distributions, substantial improvements are achievable through systematic variable refinement and contextual understanding.

The emergence of vegetation dynamics (NDR) as the dominant driving force across both analytical approaches challenges the traditional "economic metabolism paradigm" that emphasizes economic activity intensity and expansion scale. This finding aligns with mounting evidence for urban ecosystem services (Li et al., 2024; Wang et al., 2024; Wu et al., 2023) and the demonstrated co-mitigation effects of greenspace on both PM2.5 and surface temperature (Li et al., 2023). The thermal regulation pathway (NDR→TAL→AQI) achieving consistent effects across development contexts suggests that NDR pathways exhibited relatively consistent performance across the contexts examined in this study, though the generalizability of this pattern to contexts beyond our sample requires further investigation.

These findings are consistent with an 'ecological efficiency' perspective in which vegetation dynamics play a more prominent role than conventionally assumed, though we note that this interpretation is based on the specific variable set and analytical framework employed here. Traditional approaches focused on technological interventions and end-of-pipe solutions, but our empirical evidence demonstrates that ecological processes provide more robust and predictable environmental regulation. This paradigm shift has profound implications for urban planning practices, suggesting that nature-based solutions should receive priority in resource allocation rather than being treated as supplementary measures (Gómez-Baggethun and Barton, 2013).

New Land-Use Efficiency's (NLE) secondary but stable role validates compact city theories (Ewing and Cervero, 2010) while revealing the "compact city paradox" (Sarkar and Webster, 2017). Our pathway analysis demonstrates that efficiency improvements simultaneously reduce carbon emissions and increase local heat exposure, requiring coordinated ecological infrastructure development. This finding provides empirical evidence for the need to move beyond single-objective optimization toward integrated sustainability strategies that address multiple environmental dimensions simultaneously (IPCC, 2022).

Notably, traditional drivers like economic activity (NLIR) and spatial scale (AEA) did not enter our final refined framework. This does not negate their importance but rather reveals their indirectness. In a multidimensional model, their effects are largely mediated by "eco-efficiency" variables that are closer to the underlying surface physical processes. Therefore, focusing on these direct ecological and efficiency levers offers a more precise and actionable entry point for sustainable urban governance than intervening on macro-level economic and scale indicators.

3.2. Mechanistic discovery: temperature as environmental system hub

The identification of temperature as the critical mediating hub (80% mediator function in Simple Mediation, 85.7% in Sequential Mediation) reveals a notable empirical pattern with far-reaching implications for urban environmental management. This finding validates emerging theories about thermal environments' central role in urban systems (Santamouris, 2014; Haddad et al., 2024) while providing unprecedented quantitative evidence for policy prioritization.

The stronger thermal-to-air quality transmission compared to thermal-to-carbon pathways suggests that UHIL mitigation strategies offer more immediate air quality benefits than carbon reduction alone, which may inform the relative prioritization of thermal management strategies, pending confirmation from intervention studies. This thermal-to-carbon link is further supported by evidence that summer heat is a strong predictor of residential electricity consumption (Zhang et al., 2024). The observed mediating pattern is consistent with thermal management functioning as a leverage point for multiple environmental outcomes, extending beyond environmental quality to urban mobility and climate resilience (Zhang et al., 2026), though causal confirmation would require experimental or quasi-experimental designs. The finding challenges sectoral approaches to environmental management and supports integrated strategies that leverage thermal dynamics as central organizing principles (Rosenzweig et al., 2018).

The hub function of temperature also reveals why previous studies showed inconsistent results—by focusing on direct driver-outcome relationships, they missed the critical mediating role of thermal processes (e.g., Zhao et al., 2019). Our systematic analysis demonstrates that understanding environmental transmission mechanisms requires explicit modeling of thermal dynamics, providing methodological guidance for future urban environmental research.

3.3. Temporal dynamics: the 10-Year lag pattern and decoupling transitions

The pronounced 10-year lag effects (87.5% conformity in medium-term scenarios) provide large-scale empirical evidence consistent with the "urban environmental policy lag hypothesis" (e.g., Yang et al., 2022). The higher conformity rates observed under lagged configurations compared to concurrent analyses (87.5% vs. 77.8% for Sequential Mediation) suggest that concurrent analyses may systematically underestimate intervention impacts, though we note that this comparison is based on conformity rates rather than direct causal estimation of policy effects. The temporal pattern is also consistent with infrastructure "lock-in" effects theory (Seto et al., 2016) suggesting that longer evaluation horizons may be warranted when assessing urban environmental interventions.

The observation of non-linear temporal evolution patterns, particularly the 2010–2015 "decoupling transition" period, provides new insights into global sustainability transformations. The dramatic decline in theoretical conformity during this period, followed by partial recovery, suggests that global policy interventions and technological transitions may have created systematic disruptions in traditional environmental relationships. This pattern is consistent with successful policy intervention but also highlights the complexity of managing transitions toward sustainability (Turnheim et al., 2015). However, alternative explanations—such as data quality shifts between satellite sensor generations or global economic shocks (e.g., the 2008 financial crisis aftermath)—cannot be excluded without further analysis.

The temporal findings suggest that longer-term evaluation frameworks may better capture the delayed effects of urban environmental interventions, though the specific policy implications require confirmation through longitudinal or quasi-experimental studies.

3.4. Geographic and socioeconomic context dependencies: beyond universal theories

The stark geographic disparities—Asian predictability (70% conformity) versus European theory breakdown (0–14% conformity)—are consistent with "development model bifurcation" theories while revealing their mechanistic basis. Europe's low conformity rates are compatible with the notion of successful "environmental decoupling" (European Environment Agency, 2020; Nagorny-Koring and Nochta, 2018) potentially achieved through policy innovation rather than technological advancement alone. However, we acknowledge that our cross-sectional mediation design cannot identify the specific mechanisms behind Europe's divergence; alternative explanations, such as differences in urban form, energy mix, or data measurement characteristics across regions, may also contribute to this pattern.

The geographic analysis suggests that universal theories may be insufficient for global application. Instead, our findings support development of region-specific theoretical frameworks that account for different development trajectories, institutional contexts, and environmental management capabilities, echoing the principle that institutional context shapes long-run outcomes (Acemoglu et al., 2005). This challenges the dominant approach in urban environmental science of seeking universal laws and supports more contextualized theoretical development (Bai et al., 2018).

The socioeconomic inverted-U pattern provides correlational evidence consistent with Environmental Kuznets Curve theory (Grossman and Krueger, 1995) while revealing the underlying causal processes. The observation that high-income countries show reduced pathway conformity alongside shifted variable roles (e.g., TCAL emerging as alternative mediator, TAL's mediating function decreasing to 40%) suggests that different environmental management mechanisms may operate across income strata—potentially involving "cascading process interruption" rather than "source control modification". However, our cross-sectional design cannot establish these mechanisms causally, and this interpretation requires confirmation through longitudinal or quasi-experimental studies (e.g., Le Quéré et al., 2019; Liu et al., 2023).

Middle-income countries exhibited peak conformity rates (66.7% Simple Mediation, 58.3% Sequential Mediation) alongside the strongest average pathway coefficients (0.167), suggesting that traditional urban environmental transmission mechanisms operate most predictably in these contexts. This finding warrants further investigation into whether targeted interventions at this development stage could yield the greatest environmental returns.

3.5. Methodological contributions and policy directions

This study's core methodological contribution lies in establishing a systematic 'data-driven theoretical hypothesis testing' framework for urban environmental research. By testing 28,848 pathway combinations across multiple urban expansion drivers, environmental variables, temporal configurations, geographic regions, and socioeconomic strata, the process-oriented variable design responds to recent calls for strengthening causal inference and process understanding in urban science (Pacheco-Romero et al., 2022), paralleling emerging data-driven approaches in other urban domains such as sustainable mobility (Li et al., 2026). The integration of Simple and Sequential Mediation approaches provides complementary insights into direct and cascading environmental effects, offering a template that can be adapted for systematic theory testing in other complex urban systems.

Our empirical findings point to several policy-relevant directions that warrant further investigation. The consistent role of vegetation dynamics suggests that ecological infrastructure may deserve greater priority in urban environmental governance, particularly in middle-income contexts where pathway conformity is highest. The mediating role of temperature indicates that thermal management strategies could potentially yield co-benefits across multiple environmental dimensions. Geographic and socioeconomic heterogeneity in pathway conformity underscores the importance of context-adaptive policy design over universal prescriptions (Kitchin, 2014). Finally, the superior performance of medium-term lag configurations suggests that extended policy evaluation horizons may better capture the delayed effects of urban environmental interventions. These directions should be interpreted as empirically-grounded hypotheses for future policy research rather than definitive prescriptions.

3.6. Limitations

Several limitations should be noted when interpreting our findings. First, our mediation analysis employs a repeated cross-sectional design rather than a formal panel mediation framework. Although the temporal lag configurations provide partial support for the assumed causal ordering and the dynamic change rate design partially mitigates the influence of time-invariant city-level heterogeneity, we cannot fully rule out reverse causality or unmeasured confounding. Future studies using cross-lagged panel models or instrumental variable approaches would strengthen causal inference.

Second, the conversion of static stock variables into dynamic change rates, while enabling cross-city comparability and capturing process-level effects, may obscure information contained in absolute levels. Cities with similar rates of change but vastly different baseline conditions (e.g., megacities vs. small cities) are treated equivalently, which may mask important scale-dependent dynamics.

Third, the composite score weights used for framework selection (40% theoretical conformity, 30% stability, 20% significance, 10% parsimony) were assigned based on the research objectives of this study rather than derived from objective statistical methods. Although our sensitivity analysis (Supplementary Table S2) demonstrates that the top-ranking framework remains stable under alternative weighting schemes (±10% perturbation on each weight), future studies could employ methods such as entropy weighting or the Analytic Hierarchy Process for more objective weight determination.

Fourth, the spatiotemporal cross-validation yielded a geographic generalization accuracy of 36.6% and temporal extrapolation accuracy of 18.6%. These values, while reflecting the substantial global heterogeneity documented throughout our analysis (e.g., the 0–70% range in regional conformity rates), indicate that our framework performs best when applied to specific regional and temporal contexts rather than as a universal predictive model. This limited generalizability underscores the need for region-specific calibration before any practical application of the framework.

Fifth, data availability constrains our temporal resolution to approximately 5-year intervals, precluding analysis of shorter-term dynamics. The reliance on globally gridded datasets, while necessary for cross-country comparability, may introduce measurement uncertainties in regions with sparse ground-truth observations. Finally, the exclusion of cities with built-up areas <5 km^2 or populations $<50,000$ limits the generalizability of our findings to smaller urban settlements.

4. Methods

4.1. Study area and city sample selection

The analytical units for this study are global cities. We first extracted boundaries based on the Global Urban Boundary (GUB) product (Li et al., 2020). To ensure a continuous time series, we further utilized the Global Artificial Impervious Area (GAIA) data to dynamically update the urban boundaries after 2018. The final sample includes cities with a built-up area >5 km^2 and population $>50,000$, yielding a total of 6488 cities distributed across all inhabited continents.

4.2. Variable definition and data processing

This study employs a "process-oriented" variable design, systematically converting traditional static stock variables into dynamic rates of change. All geospatial data were co-registered and resampled to a uniform 1-km resolution.

The dynamic change rate for each variable was calculated using the following standardized formula:

$$\text{Rate}_i = (V_i, t2 - - V_i, t1) \ / \ (\Delta t)$$

where V_i,t1 and V_i,t2 represent the mean value of variable V for city i during the start-period and end-period time windows (e.g., 2000–2005 and 2005–2010 for a short-term lag configuration), respectively, and Δt is the number of years between the midpoints of the two time windows (e.g., $\Delta t = 5$ for consecutive 5-year periods). This annual rate of change formulation ensures comparability across cities of different sizes and baseline conditions by measuring the pace of change rather than absolute levels.

4.2.1. Urban expansion drivers

We quantified the multi-dimensional process of urban expansion. The Annual Expansion Area (AEA) and Built-up Density Rate (BUDR) were used to characterize changes in spatial morphology, with data (Urban Area A, Built-up Area BU) sourced from the GUB and GAIA datasets. The Expansion Intensity Index (EII) and New Land-Use Efficiency (NLE) measure the coupling of expansion with population, with population data (P) sourced from the high-resolution LandScan Global Population Database. The intensity of economic activity was represented by the Nighttime Light Intensity Rate (NLIR), with data from the dataset detailed in Li et al. (2020). Economic development was further characterized by GDP per capita, using the downscaled gridded global dataset for Gross Domestic Product (GDP) by Kummu et al. (2018). Finally, the ecological dimension of expansion was captured by the NDVI Dynamic Rate (NDR), with data from the MODIS Vegetation Indices product (MOD13A2). The NDVI calculation utilized growing season averages calculated separately for three latitudinal zones: Northern Hemisphere temperate and boreal zones (>23.5°N): March–October; Southern Hemisphere temperate zones (<23.5°S): September–April; and Equatorial/tropical zones (23.5°S–23.5°N): year-round (January–December), ensuring accurate vegetation dynamics capture across diverse climatic conditions.

4.2.2. Environmental response and control variables

The three core environmental responses were measured as follows: TCAL data were derived from the Open-source Data Inventory for

Anthropogenic CO2 (ODIAC) dataset. TAL data were sourced from the ERA5-Land monthly averaged reanalysis dataset from the Copernicus Climate Change Service. AQI, represented by PM2.5 concentration, was sourced from the Global Surface PM2.5 Grids from the Atmospheric Composition Analysis Group at Washington University (van Donkelaar et al., 2021). To account for the influence of natural background conditions, we included precipitation and wind speed from the ERA5-Land dataset, and elevation data from the ASTER Global Digital Elevation Model V003 (ASTGTM V003).

4.3. Mediation effect model

We used path analysis, a subset of Structural Equation Modeling (SEM) (e.g., Rosseel, 2012), to test for mediation effects. The analytical approach follows the causal steps method outlined by Baron and Kenny (1986), but employs modern bootstrapping techniques for significance testing of indirect effects to overcome the limitations of the traditional Sobel test, a practice strongly advocated in modern mediation analysis (Efron and Tibshirani, 1993; Preacher and Hayes, 2008). This study employed both Simple Mediation models, which test a single intervening variable (X → M → Y), and more complex Sequential Mediation models, which test a hypothesized causal chain with two mediators (X → M1 → M2 → Y).

Control variables (precipitation rate, wind speed rate, and elevation) were incorporated as covariates in all regression equations of the mediation model. Precipitation and wind speed were converted to dynamic change rates consistent with the process-oriented design of all other variables; elevation was retained as a static level variable as it does not vary meaningfully over the study period. Specifically, in the Simple Mediation model (X → M → Y), the model comprises two regression equations:

$$M_i = a_0 + a_1X_i + a_2Precip_i + a_3Wind_i + a_4Elev_i + e_i$$

$$Y_i = b_0 + b_1X_i + b_2M_i + b_3Precip_i + b_4Wind_i + b_5Elev_i + \varepsilon_i$$

where Precip and Wind represent the dynamic change rates of precipitation and wind speed, respectively, and Elev represents mean elevation. The indirect effect is calculated as $a_1 \times b_2$, and its significance is assessed via 1000-iteration bootstrap confidence intervals (Preacher and Hayes, 2008).

The Sequential Mediation model (X → M1 → M2 → Y) extends this to three regression equations:

$$M1_i = c_0 + c_1X_i + c_2Precip_i + c_3Wind_i + c_4Elev_i + e_{1i}$$

$$M2_i = d_0 + d_1X_i + d_2M1_i + d_3Precip_i + d_4Wind_i + d_5Elev_i + e_{2i}$$

$$Y_i = f_0 + f_1X_i + f_2M1_i + f_3M2_i + f_4Precip_i + f_5Wind_i + f_6Elev_i + \varepsilon_i$$

The sequential indirect effect is calculated as $c_1 \times d_2 \times f_3$, with significance assessed via 1000-iteration bootstrap confidence intervals.

Our analytical design employs a repeated cross-sectional approach: for each of the 10 temporal configurations (Table 1), a separate cross-sectional mediation analysis is conducted across the global city sample ($N = 6488$). We do not employ formal panel mediation models (e.g., random-intercept cross-lagged panel models), as our primary objective is to test the empirical consistency of theoretical predictions across diverse temporal and spatial contexts, rather than to estimate within-city dynamic causal effects. In addition, the temporal dimension of our dataset (four 5-year periods) provides insufficient panel depth for such models, which require substantially longer time series for stable parameter estimation.

Regarding city-level heterogeneity: although explicit city fixed effects are not included, our process-oriented variable design—converting static stock variables into dynamic rates of change (e.g., $\Delta NDVI/\Delta t$, $\Delta CO_2/\Delta t$)—partially mitigates the influence of time-invariant city-level characteristics (baseline climate, geography, institutional context) by focusing on within-period changes rather than absolute levels. While conceptually related to first-differencing in panel econometrics, this approach does not formally eliminate all sources of unobserved heterogeneity (see Section 3.7). Time trends are addressed through our analytical design: each temporal configuration is analyzed as an independent cross-sectional sample, thereby avoiding confounding from secular trends within any single analysis. Cross-period comparisons of conformity rates (Section 2.4.1) separately characterize how pathway structures evolve over time. Precipitation, wind speed, and elevation are included as control variables in all regression equations to account for spatial heterogeneity in natural background conditions.

We acknowledge that the causal ordering of the mediation sequence (X → M → Y) is grounded in established theory (e.g., urban expansion alters surface energy balance, which modifies thermal environment, which subsequently affects air quality) but is not statistically identified in a strict sense. The temporal lag configurations provide partial exogeneity support by ensuring that driver variables temporally precede mediators and outcomes. However, we cannot fully rule out reverse causality or unmeasured confounding, and this is discussed as a key limitation (see Section 3.7).

Table 1
The 10 temporal configurations used in this study.

No.	Configuration Type	Driver (X)	Mediator (M)	Outcome (Y)	Lag Structure
1	Concurrent-1	2000–2005	2000–2005	2000–2005	0-year
2	Concurrent-2	2005–2010	2005–2010	2005–2010	0-year
3	Concurrent-3	2010–2015	2010–2015	2010–2015	0-year
4	Concurrent-4	2015–2022	2015–2022	2015–2022	0-year
5	Short-term lag-1	2000–2005	2005–2010	2005–2010	5-year
6	Short-term lag-2	2005–2010	2010–2015	2010–2015	5-year
7	Short-term lag-3	2010–2015	2015–2022	2015–2022	5-year
8	Medium-term lag-1	2000–2005	2005–2010	2010–2015	5 + 5yr
9	Medium-term lag-2	2005–2010	2010–2015	2015–2022	5 + 5yr
10	Long-term lag	2000–2005	2010–2015	2015–2022	10+5yr

Notes:.
(a) Short-term lag configurations (No. 5–7): the driver is offset by one period, but the mediator and outcome are measured concurrently. The M→Y causal direction in these configurations relies on theoretical assumptions rather than temporal precedence. Example (Configuration 5, Simple Mediation): NDR change rate over 2000–2005 (X), TAL change rate over 2005–2010 (M), TCAL change rate over 2005–2010 (Y).
(b) Medium-term lag configurations (No. 8–9) assign driver, mediator, and outcome to three successive periods, providing the strongest temporal precedence support. Example (Configuration 8, Sequential Mediation): NDR change rate over 2000–2005 (X), TAL change rate over 2005–2010 (M), AQI change rate over 2010–2015 (Y). Their superior empirical performance (87.5% conformity vs. 77.8% overall; Section 2.4.1) is consistent with this stronger temporal identification.
(c) The long-term lag (No. 10) introduces a 10-year driver–mediator offset, testing whether urban expansion effects persist over extended horizons consistent with infrastructure "lock-in" theory (Seto et al., 2016).

4.4. Statistical analysis workflow: the "Explore-Refine-Validate" paradigm

Our analytical workflow followed an "Explore-Refine-Validate" paradigm. The core of this paradigm was a data-driven process to move from a comprehensive but low-performing set of initial variables to a parsimonious yet robust final framework. This was achieved through an integrated framework selection strategy, detailed below, followed by a stringent validation of the selected model.

To ensure transparency, we provide the explicit derivation of the pathway combination counts reported in this study:

The initial comprehensive analysis ("8000+ pathway combinations"): This count refers to the total number of individual mediation pathways tested during the initial exploration phase with the full variable set, before framework refinement. Across the full variable pool, multiple temporal configurations, and geographic/SES subsamples, the total exceeded 8000 individual pathway tests.

The total study-wide count ("28,848 pathway combinations"): After VIF-based multicollinearity diagnostics (threshold = 4.0), 4 treatment variables (drivers) survived. Simple Mediation: The code tests all cross-category mediator–outcome pairs from 3 environmental categories (carbon: 1 variable; heat: 3 variables; haze: 3 variables), yielding 30 pathway types per treatment. With 4 treatments × 30 pathways × 10 temporal configurations × 10 subsamples (1 global + 6 continents + 3 SES) = 12,000 tests. Sequential Mediation: 6 pathway orderings (all permutations of carbon→heat→haze categories) × 9 variable combinations per ordering = 54 pathways per treatment. Global sample: 4 × 54 × 14 temporal configurations = 3024; Continental subsamples (simplified 7 configs): 4 × 54 × 7 × 6 = 9072; SES subsamples: 4 × 54 × 7 × 3 = 4536. Sequential subtotal = 16,632. Validation tests (10-fold CV, temporal hold-out, bootstrap): ~216 tests. Grand total: 12,000 + 16,632 + 216 = 28,848.

To clarify: the 8000+ figure represents the breadth of the initial exploratory analysis with the full variable set, whereas 28,848 = 12,000 (Simple) + 16,632 (Sequential) + 216 (validation) represents the cumulative count of all completed individual mediation tests across the entire Explore–Refine–Validate paradigm.

4.4.1. Integrated framework selection via combinatorial optimization

To ensure a fully data-driven approach and account for potential interaction effects between drivers and environmental indicators, we developed and implemented an integrated framework selection strategy. This process moves beyond selecting variables sequentially and instead evaluates complete "pathway frameworks" to identify the optimal model in a single, unified process, drawing on principles from machine learning and predictive modeling (Guyon et al., 2002; Kuhn and Johnson, 2013). The workflow consists of four stages:

Pathway Framework Generation: We first defined the pools of candidate variables. The driver variable pool consisted of the four variables that passed multicollinearity diagnostics (NLIR, NLE, NDR, and AEA). The environmental indicator pool consisted of one carbon variable (TCAL), three heat variables (TAL, UHIL, TCI), and three haze variables (AAL, ASI, AQI). A full combinatorial product of these sets yielded 135 distinct pathway frameworks to be tested.

Standardized Framework Evaluation: Each of the 135 frameworks was subjected to a standardized simple mediation analysis using a mid-term lag configuration (2010–2015). This analysis was performed on the full global sample and on each of the six continental sub-samples to gather metrics for stability assessment.

Multi-Criteria Scoring: Each framework was scored based on a composite function S weighting four key metrics: (a) Theoretical Conformity (40% weight), assigned the highest weight because the primary objective of this study is to identify frameworks whose empirical behavior aligns with established theory; (b) Stability (30% weight), weighted second to prioritize frameworks that generalize across geographic contexts rather than fitting a single sample; (c) Significance (20% weight), the overall proportion of significant pathways; and (d) Parsimony (10% weight), calculated as the inverse of the number of driver variables. We acknowledge that these weights reflect the research priorities of this study rather than objective statistical derivation. To verify the robustness of this weight assignment, we conducted a systematic sensitivity analysis by perturbing each weight by ±10 percentage points (128 alternative weight combinations). The optimal framework {NDR, NLE} × {TCAL, TAL, AQI} ranked first in 93.8% of all scenarios, confirming that the framework selection is not sensitive to the specific weight values.

Optimal Framework Identification: All 135 pathway frameworks were ranked according to their composite score S. The screening process unequivocally identified the framework combining the {NDR, NLE} driver set with the {TCAL, TAL, AQI} environmental indicator set as the top-ranking model with the highest composite score (see Supplementary Table S1 for the full ranking results). This optimal framework was subsequently used for all in-depth analyses in this study.

4.4.2. Validation of the refined framework

The finalized framework, identified through the process above, underwent stringent validation. We define validation accuracy as the proportion of cross-validated subsamples in which the refined framework maintained its core theoretically conforming pathway structure—operationalized as ≥60% of pathways retaining both statistical significance ($p < 0.05$) and theoretical directional consistency. This threshold was chosen as a simple majority criterion, requiring that more than half of the framework's core pathways remain intact in each held-out subsample. Spatiotemporal cross-validation (leave-one-continent-out for geographic generalization; leave-one-period-out for temporal extrapolation) yielded a mean geographic generalization accuracy of 36.6% (95% CI: 27.3%–45.9%) and a temporal extrapolation accuracy of 18.6%. These values should be interpreted in the context of the substantial global heterogeneity documented in our results: regional conformity rates range from 0% (Europe) to 70% (Asia), and temporal conformity fluctuates from 8.3% to 100% across periods. The geographic accuracy of 36.6% indicates that the framework generalizes to approximately one-third of novel regional contexts, confirming that context-specific calibration (as discussed in Sections 2.4 and 3.4) is more appropriate than universal deployment. The temporal extrapolation accuracy of 18.6% is notably lower, attributable to two factors: (i) the leave-one-period-out design involves only four time periods, making the estimate highly sensitive to any single anomalous fold; and (ii) the 2010–2015 "decoupling transition" period, with Sequential Mediation conformity of only 8.3% (Section 2.4.1), substantially depresses the cross-validated average. This confirms that the framework captures stable cross-sectional patterns more reliably than it predicts temporal dynamics, and that temporal transferability remains an important direction for future research. Furthermore, a 1000-iteration bootstrap analysis confirmed the statistical robustness of the key indirect pathways in our model; for instance, the 95% confidence interval for the NDR→TAL→AQI pathway was found to be [−0.0245, −0.0031]. All analysis code (Python 3.9) is available from the corresponding author upon reasonable request.

CRediT authorship contribution statement

Yuyang Zhang: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. **Yazhou Hua:** Writing – review & editing, Writing – original draft, Visualization, Formal analysis. **Wenke Ma:** Writing – review & editing, Writing – original draft, Visualization, Methodology. **Zhenyu Luo:** Writing – review & editing, Writing – original draft, Methodology, Conceptualization. **Ying Long:** Conceptualization, Investigation, Resources, Validation, Writing – review & editing. **Yan Li:** Writing – review & editing, Writing – original draft, Resources, Methodology, Funding acquisition, Formal analysis, Data curation, Conceptualization.

Declaration of competing interest

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

Acknowledgments

We thank Tianqi Zang for improving the visualisation. This research was funded by the Fundamental Research Funds for the Central Universities (Grant No.: 2-9-2024-075) and the Youth Research Special Project of North China University of Technology (Grant No.: 2025NCUTYRSP027).

Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.resconrec.2026.108944.

Data availability

Data will be made available on request.

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