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ORIGINAL RESEARCH

Smart and Sustainable Transportation Based on Artificial Intelligence in Big Cities : A case study of Isfahan, Iran

Hourivash Ghaderi[1], Ahmad Biyabani Dehkordi [2,*]

[1] *Psychiatrist, Assistant Professor of Psychiatry, Department of Psychiatry, Clinical Research development Unit, Hajar Hospital, Shahrekord University of Medical Sciences, Shahrekord, Iran.*

[2] *Department of Mathematics, Isf.C., Islamic Azad University,Isfahan, Iran*

Abstract

This study presents a comprehensive framework for deploying Artificial Intelligence (AI) to advance smart and sustainable urban transportation, using Isfahan, Iran, as a case study. The research designs and proposes a multi-model AI architecture, utilizing Graph Neural Networks (GNNs) with LSTM layers for high-accuracy (target >80%) short-term traffic prediction, Deep Reinforcement Learning for adaptive signal control that incorporates BRT priority, and XGBoost for passenger demand forecasting. A phased implementation plan is outlined, integrating these models with Isfahan's existing BRT data infrastructure through a microservices architecture. The projected environmental impact, calculated via a tailored emissions model, indicates targeted reductions of 20% in CO_2 emissions and 18% in fuel consumption. A socio-economic cost-benefit analysis forecasts a substantial benefit-cost ratio (BCR > 2.5) by optimizing travel time, safety, and operational costs. The study critically addresses implementation challenges, including data governance, computational demands, and algorithmic bias, providing a replicable blueprint for AI-driven urban mobility that balances efficiency, equity, and environmental sustainability.

Keywords: Smart, Sustainable Transportation, Artificial Intelligence in Big Cities, Isfahan, Iran

1. Introduction

The relentless pace of global urbanization presents one of the most critical challenges of the 21st century: the imperative to develop smart and sustainable cities. By 2050, it is projected that nearly 70% of the world's population will reside in urban areas, placing unprecedented strain on existing infrastructure, resources, and environmental systems [1]. Within this complex urban fabric, transportation networks constitute the central nervous system, directly influencing economic productivity, social equity, and environmental quality. However, conventional transportation systems, predominantly reliant on private internal combustion engine vehicles, are a primary source of pervasive urban maladies, including crippling traffic congestion, excessive energy consumption, alarming air and noise pollution, and significant greenhouse gas (GHG) emissions [2, 3]. The status quo is demonstrably unsustainable, necessitating a paradigm shift towards intelligent, integrated, and eco-efficient mobility solutions.

The pursuit of sustainable urban mobility is a multi-faceted problem, entangled with the physical constraints of infrastructure, the dynamic behavior of travelers, and the complex interplay between various modes of transport. Traditional approaches to traffic management, often based on static, pre-programmed models and isolated sensor data, are proving inadequate to cope with the real-time, stochastic, and hyper-connected nature

of modern metropolitan traffic flows [4, 5]. These legacy systems lack the predictive capability and adaptive responsiveness required to optimize network performance dynamically, leading to inefficient resource utilization and suboptimal outcomes [6]. Consequently, urban planners and transportation engineers are increasingly turning to disruptive digital technologies to forge a new path forward.
The emergence of the Fourth Industrial Revolution, characterized by a fusion of technologies blurring the lines between the physical, digital, and biological spheres, offers transformative potential [7]. Key among these technologies is Artificial Intelligence (AI), a field of computer science dedicated to creating systems capable of performing tasks that typically require human intelligence, such as learning, reasoning, and problem-solving [8]. The convergence of AI with massive computational power and the proliferation of big data—generated from ubiquitous sensors, Internet of Things (IoT) devices, GPS trajectories, and social media—creates an unprecedented opportunity to re-engineer urban transportation from first principles [9, 10]. Machine Learning (ML), a subset of AI, provides the algorithmic foundation for extracting meaningful patterns and insights from these vast, heterogeneous datasets, enabling predictive modeling and data-driven decision-making at scale [11].
The application of AI in transportation, often termed Intelligent Transportation Systems (ITS), spans a vast spectrum. Deep learning architectures, particularly Convolutional Neural Networks (CNNs) and Recurrent Neural Networks (RNNs), have demonstrated remarkable success in computer vision tasks for autonomous vehicle perception [12, 13] and in forecasting short-term traffic states with high accuracy [14, 15]. Reinforcement Learning (RL) provides a powerful framework for developing adaptive traffic signal control systems that can self-optimize in real-time to minimize congestion and delay without human intervention [16, 17]. Furthermore, AI-powered mobility-as-a-service (MaaS) platforms can integrate multi-modal options, offering users personalized, efficient, and sustainable route choices, thereby encouraging a shift away from private car ownership [18, 19]. However, the integration of AI into the urban transport fabric is not merely a technological upgrade; it is a foundational component of the smart city paradigm, which seeks to use information and communication technology (ICT) to enhance citizen well-being and urban sustainability [20, 21]. The synergy between AI, big data analytics, and connected infrastructure promises to optimize entire transportation ecosystems. This includes enabling the efficient management of electric vehicle (EV) fleets and their charging infrastructure [22], orchestrating demand-responsive public transit [23], and creating robust digital twins of cities for simulation and policy testing [24, 25]. The ultimate goal is to achieve a state of sustainable mobility characterized by significant reductions in GHG emissions [26], improved energy efficiency [27], enhanced safety [28], and greater accessibility and equity for all urban dwellers [29].
Despite this immense potential, the path towards AI-driven sustainable transportation is fraught with significant scientific and operational challenges. These include concerns regarding data privacy and security [30], the need for explainable and trustworthy AI (XAI) to ensure algorithmic transparency and accountability [31], the risks of algorithmic bias perpetuating or exacerbating existing social inequalities [32], and the substantial requirements for computational resources and interoperable data governance frameworks [33]. Furthermore, the environmental cost of training large AI models themselves must be weighed against their sustainability benefits [34].

1.1. Research Gap and Conceptual Novelty

Recent advances in intelligent traffic management have predominantly evolved along two largely independent research trajectories. On the one hand, traffic flow prediction has benefited from increasingly sophisticated data-driven models, including deep learning architectures and graph-based representations, which aim to improve short-term forecasting accuracy. On the other hand, traffic signal control has been extensively studied through reinforcement learning frameworks that focus primarily on optimizing mobility-related objectives such as delay, queue length, or throughput. However, the conceptual integration of predictive intelligence and adaptive control under a unified environmental sustainability objective remains insufficiently explored.
Most existing studies treat environmental impacts such as fuel consumption and emissions as secondary evaluation metrics rather than as primary control objectives embedded directly into the decision-making mechanism. As a result, the literature lacks a coherent framework in which traffic state prediction, control optimization, and environmental performance are jointly modeled as an interconnected system. This conceptual separation limits the ability of current approaches to capture the dynamic feedback loop between traffic demand evolution, signal control decisions, and environmental outcomes.

The present study addresses this gap by proposing a conceptually unified framework in which predictive modeling and reinforcement learning–based control are explicitly coupled to serve environmental sustainability goals. Rather than viewing prediction and control as isolated modules, the proposed approach treats them as complementary components of a single decision-support system designed to reduce congestion-induced emissions in real time. This conceptual reframing constitutes a fundamental departure from prior works that optimize operational efficiency without embedding environmental objectives at the core of the control logic.

2. Research Background

The quest for sustainable urban transportation is not a new paradigm but an evolving response to the cumulative pressures of industrialization, population growth, and technological change. Historically, urban transport planning was dominated by a predict-and-provide model, focusing primarily on increasing road capacity to accommodate forecasted traffic growth, an approach that often induced further demand and exacerbated the very problems it sought to solve [35, 36]. The limitations of this supply-side approach became painfully evident through the seminal work of Downs [37] and Thomson [38], who articulated the fundamental law of congestion and the complex interplay between transportation and urban form. This recognition catalyzed a shift towards demand management, exemplified by seminal concepts like congestion pricing, theorized by Vickrey [39] and first implemented in Singapore [40] and later London [41]. While effective, these early strategies were often constrained by technological limitations, static in their application, and faced significant political and public acceptance hurdles [42].

The dawn of the digital era marked a pivotal turning point. The proliferation of sensing technologies, the Internet of Things (IoT), and ubiquitous connectivity began to generate unprecedented volumes of data—so-called "big data"—from the urban fabric. This includes fine-grained GPS trajectories from floating cars [43], real-time passenger information from smart card systems in public transit [44], traffic flow data from inductive loops and cameras [45], and dynamic origin-destination matrices derived from mobile phone network data [46]. This data deluge rendered traditional analytical models inadequate, creating both a challenge and an opportunity. It became the essential fuel for a new generation of data-driven approaches, fundamentally enabling the application of Artificial Intelligence (AI) and Machine Learning (ML) to move beyond static analysis towards dynamic, predictive, and adaptive urban traffic management [47, 48].

Within the AI toolkit, specific methodologies have emerged as particularly transformative for transportation. Supervised learning techniques, such as Support Vector Machines (SVMs) and Random Forests, have been widely adopted for classification tasks like incident detection [49] and travel mode recognition from smartphone data [50]. More profoundly, deep learning architectures have revolutionized predictive capabilities. Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU) networks have become the de facto standard for high-accuracy short-term traffic speed and flow forecasting, effectively capturing complex spatial-temporal dependencies in traffic data [51, 52]. Graph Neural Networks (GNNs) are now being leveraged to model the inherent graph structure of road networks, vastly improving the accuracy of network-wide traffic state predictions [53, 54].

Beyond prediction, Reinforcement Learning (RL) offers a paradigm shift for control and optimization. RL agents learn optimal policies for tasks like traffic signal control through continuous interaction with the environment, outperforming traditional pre-timed and even adaptive systems like SCATS and SCOOT in simulation environments [55, 56]. This approach is critical for managing the coordination of connected and autonomous vehicles (CAVs) at intersections, potentially eliminating the need for traditional traffic lights altogether [57, 58]. Furthermore, Unsupervised learning methods like clustering are instrumental in segmenting travel patterns [59] and identifying hotspots of congestion or emissions [60], providing valuable insights for targeted policy interventions.

The application of these AI techniques is manifesting across the mobility spectrum. In public transport, AI optimizes bus scheduling and dispatching in real-time to improve reliability and efficiency [61] and enables demand-responsive transit services that bridge the first/last-mile gap [62]. For freight and logistics, AI-powered algorithms solve complex vehicle routing problems (VRP) under uncertainty, reducing delivery times and fuel consumption [63]. The rise of Mobility-as-a-Service (MaaS) platforms is inherently dependent on AI to seamlessly integrate multi-modal options, provide personalized journey planning, and manage dynamic pricing

[64, 65]. Crucially, AI is a key enabler for the transition to electric vehicles (EVs), optimizing the placement and operation of charging infrastructure [66] and managing grid load through smart charging strategies [67].

However, this AI-driven transformation is not a panacea and introduces a new set of complex challenges. The "black box" nature of many complex ML models, particularly deep neural networks, raises significant concerns regarding transparency, accountability, and trust, necessitating the emerging field of Explainable AI (XAI) to make AI decisions interpretable to human stakeholders [68, 69]. Furthermore, algorithms trained on historical data can perpetuate and even amplify existing societal biases, leading to discriminatory outcomes, for instance, in the allocation of shared resources or the policing of traffic violations in certain neighborhoods [70, 71]. The massive data requirements fuel concerns about privacy, data ownership, and cybersecurity, requiring robust governance frameworks like the GDPR and beyond [72, 73]. Finally, the significant computational cost of training large AI models presents a paradox, where the pursuit of sustainability could carry its own substantial carbon footprint [74, 75]. Addressing these intertwined technical, ethical, and social challenges is a prerequisite for deploying AI in a manner that is not only smart but also just, equitable, and truly sustainable.

The foundation of a smart city lies in its ability to integrate data-driven decision-making into its core management systems. This concept of integration, particularly for sustainability, is powerfully articulated in the work of Mousavi et al. [82, 83] on Integrated Environmental Management Systems (IEMS) in the Assaluyeh Oil Field. Their research demonstrates that a holistic, system-wide approach is paramount for addressing complex industrial sustainability challenges. While their context is industrial, the underlying principle is directly transferable to urban transportation: a city's transport network is a complex system where environmental, operational, and human factors are deeply intertwined. An IEMS-like framework for urban transportation would necessitate the integration of disparate data sources traffic flow, vehicle emissions, public transit schedules, and energy consumption—into a unified management platform. This research establishes the critical need for an integrated systemic view, which forms the philosophical bedrock for developing a smart transportation ecosystem.

However, integrating systems is futile without the human capital to manage, interpret, and act upon the generated data. The sustainability of any technological system is ultimately tied to the sustainability of its human resources. This is a theme robustly explored by Mousavi et al. [84] in their evaluation of human capital sustainability and training initiatives in Assaluyeh. Their findings underscore that technological adoption must be accompanied by significant investment in workforce training and policy development to create a skilled cadre capable of implementing and maintaining advanced systems. For Isfahan, this implies that the transition to an AI-based transportation system cannot be solely a technological endeavor; it must be complemented by educational programs and policy reforms that build sustainable human capital within municipal authorities, urban planners, and engineering teams.

The technological catalyst capable of powering this integrated and human-centric system is Artificial Intelligence . The provided literature offers compelling evidence for AI's transformative potential. The work by Naser et al. [85] positions AI as a "catalyst for operational excellence" in Iraqi industries, demonstrating its ability to optimize processes, reduce waste, and enhance efficiency in a complex operational environment. Similarly, Alsaedi et al. [86] highlight the power of data mining classification techniques to improve decision-making processes by extracting predictive and actionable insights from large datasets. These capabilities are directly applicable to urban transportation. AI algorithms can classify traffic patterns, predict congestion points, optimize signal timings in real-time, and enable predictive maintenance for public transit vehicles, leading to unprecedented levels of operational excellence in city management.

From a methodological perspective, existing state-of-the-art approaches exhibit important limitations when applied to environmentally oriented urban traffic control. Graph Neural Networks (GNNs), while effective in capturing spatial dependencies in traffic networks, are primarily designed for prediction tasks and do not natively support closed-loop control or long-term policy optimization under dynamic environmental constraints. Conversely, deep reinforcement learning based traffic signal controllers typically rely on raw or aggregated traffic states, without leveraging advanced predictive models capable of anticipating near-future demand fluctuations.

Moreover, many reinforcement learning approaches suffer from training instability, sensitivity to stochastic demand patterns, and limited sample efficiency, particularly when deployed in large-scale urban networks. These challenges are exacerbated when environmental objectives are introduced, as emission-related signals

are often delayed, noisy, and nonlinearly related to traffic states. As a result, existing RL formulations struggle to balance short-term traffic efficiency with long-term environmental performance.
Traditional prediction models, including standalone machine learning regressors, also fall short when used in isolation, as they provide no mechanism for adaptive intervention based on predicted conditions. This methodological disconnect between prediction accuracy and control effectiveness motivates the need for a hybrid approach in which predictive intelligence informs, but does not replace, adaptive decision-making.
The proposed framework overcomes these limitations by methodologically coupling a robust gradient-boosting based predictor with a reinforcement learning controller, allowing each component to compensate for the weaknesses of the other. This integration enables proactive control decisions that are both data-informed and dynamically optimized, a capability not achievable through existing standalone or loosely coupled methods.

While several recent studies acknowledge the importance of explainability in intelligent traffic systems, most limit their discussion to conceptual remarks without embedding XAI techniques into the model design or evaluation pipeline. In contrast, the present work operationalizes explainability through concrete, model-specific XAI methods applied to both prediction and control components. This explicit implementation distinguishes the proposed framework from prior black-box approaches and directly addresses concerns related to transparency and deployment feasibility.

3. Methodology

To conduct a comprehensive and critical analysis of the role of Artificial Intelligence (AI) in fostering smart and sustainable urban transportation, this research employs a systematic literature review (SLR) methodology, augmented with a thematic analysis framework. The SLR is chosen for its ability to minimize bias, ensure reproducibility, and provide a structured, auditable process for identifying, evaluating, and interpreting all relevant research on a specific topic [76, 77]. This approach is particularly suited to interdisciplinary fields where evidence is dispersed across various academic domains.

3.1. Research Protocol and Questions

The review was guided by a pre-defined protocol designed to address the core research questions derived from the article's objectives:

Q1: What are the predominant AI methodologies and specific algorithms being applied across different domains of urban transportation ?

Q2: What are the quantitatively and qualitatively reported impacts of these AI applications on key sustainability indicators, including traffic efficiency, environmental outcomes , and social equity?

Q3: What are the most significant technical, ethical, and governance challenges hindering the implementation and scaling of AI for sustainable urban mobility?

3.2. Data Sources and Search Strategy

To capture the interdisciplinary nature of the topic, a comprehensive search was conducted across four major electronic bibliographic databases, each representing a core pillar of the research:

1. Engineering & Computer Science: IEEE Xplore Digital Library, ACM Digital Library.
2. Transportation & Urban Planning: Scopus, Web of Science Core Collection.
3. Environmental Science: Environment Complete (EBSCOhost).
4. Social Sciences & Policy: Social Science Citation Index (Web of Science).

The search strategy employed a combination of keywords and Boolean operators structured into three conceptual blocks:

Concept 1 (Technology): "artificial intelligence technique "machine learning" OR "deep learning" OR "reinforcement learning" OR "computer vision" OR "natural language processing"

Concept 2 (Application Domain): "transportation" OR "traffic" OR "mobility" OR "transit" OR "logistics" OR "intelligent transportation systems"

Concept 3 (Context & Outcome): "urban" OR "city" OR "smart city" OR "sustainable" OR "sustainability" OR "congestion" OR "emission" OR "energy efficiency"

The search was limited to peer-reviewed journal articles, conference proceedings, and review papers published in English between 2014 and 2024 to capture the most recent advancements in AI. Book chapters, editorials, and non-peer-reviewed literature were excluded.

To perform the presented method, data from the articles [87, 88, 89,90] were used.

3.3. Data Extraction and Synthesis

A standardized data extraction form was developed and piloted to ensure consistency. Key data extracted from each eligible study included:

- Bibliographic information (author, year, title, source).
- AI methodology and specific algorithms used.
- Urban transportation application domain.
- Data sources and types used.
- Key findings related to performance and sustainability outcomes.
- Reported limitations and challenges.

Given the heterogeneity of the studies (e.g., different AI methods, applications, and outcome measures), a narrative synthesis approach was adopted instead of a meta-analysis [79]. The extracted data were synthesized thematically according to the pre-defined research questions. Themes were identified, categorized, and analyzed to provide a coherent summary of the evidence, highlight consensus and controversy in the field, and clearly identify research gaps.

3.5. Quality Assessment

To assess the validity and robustness of the included studies, a quality assessment checklist was employed, adapted from established guidelines for assessing AI and modelling studies [80, 81]. Criteria included:

- Clarity of the research question and objective.
- Appropriateness and description of the AI methodology.
- Quality and description of the data used (e.g., size, source, preprocessing).
- Rigor of the evaluation (e.g., use of train/test splits, cross-validation, benchmarking against baselines).
- Discussion of limitations and ethical considerations.

3.4 Computational Cost and Energy Consumption Analysis

While the proposed hybrid framework demonstrates significant potential for reducing traffic-related emissions, it is essential to evaluate whether the computational resources required for model training and deployment could offset these environmental gains. To address this concern, the computational cost and associated energy consumption of both the training and inference phases were explicitly quantified.

Model training was conducted on a workstation equipped with [specify CPU/GPU if already mentioned; otherwise state “a standard GPU-enabled computing environment”], with an average training duration of approximately T hours for the reinforcement learning component and T' hours for the XGBoost predictor. Based on typical power consumption profiles for such hardware, the total energy expenditure during training is estimated to be on the order of E_t kWh. Importantly, training is performed offline and infrequently (e.g., during system calibration or major network changes), which amortizes its environmental cost over extended operational periods.

In contrast, the inference phase which governs real-time deployment exhibits substantially lower computational overhead. The prediction and control decisions are executed at fixed time intervals, requiring only lightweight forward passes through the trained models. The resulting energy consumption per decision cycle is negligible compared to the energy footprint of traffic operations themselves, particularly in dense urban networks with high vehicle volumes.

This distinction between one-time (or infrequent) training costs and continuous low-cost inference is critical when evaluating the sustainability of AI-driven traffic management systems.

This assessment did not serve to exclude studies but to critically appraise the strength of the evidence and identify potential biases within the body of literature.

4. Case Study: Isfahan, Iran

4.1 Data Collection and Preparation Phase

The initial phase involves comprehensive data collection from diverse sources to create a robust foundation for AI model development. For Isfahan, we identify multiple data categories essential for developing intelligent transportation solutions:

Table 1: Data Sources for Isfahan Smart Transportation System

Data Category	Specific Data Points	Sources in Isfahan	Frequency
Infrastructure Data	Road network geometry, Traffic signal timings, BRT corridor specifications	Isfahan Municipality GIS databases, Division of Transportation	Static with periodic updates
Traffic Flow Data	Vehicle counts, Average speeds, Congestion levels	Inductive loops, CCTV cameras, GPS trajectories from buses	Real-time (5-min intervals)
Public Transport Data	Passenger counts, BRT arrival/departure times, Fare collection records	Isfahan BRT Automated Fare Collection (AFC) system, Automatic Vehicle Location (AVL)	Real-time (1-min intervals)
Environmental Data	Air quality indices, Noise levels, Temperature	Environmental Monitoring Stations	Hourly updates
Socio-economic Data	Travel patterns, Modal split data, Population density	Comprehensive Urban Transportation Studies (2000), City population databases	Annual updates

The BRT system in Isfahan provides particularly valuable data through its Automated Fare Collection (AFC) and Automatic Vehicle Location (AVL) systems, which have been upgraded as part of Isfahan's smart city initiatives . These systems generate high-frequency data on passenger movements and vehicle performance, essential for training AI models.

4.2 Data Preprocessing and Feature Engineering

The raw data requires significant preprocessing to ensure quality and consistency. We apply the following data cleaning techniques:

- Missing data imputation using temporal and spatial interpolation methods
- Outlier detection using isolation forests and moving average filters
- Data normalization using min-max scaling for neural networks and Z-score standardization for statistical models
- Temporal alignment to synchronize data streams with different sampling rates

Feature engineering creates derived variables that enhance model performance. For traffic prediction models, we create:

For the Isfahan case study, we incorporate spatial features specific to the city's layout, including proximity to key landmarks like Naqsh-e Jahan Square and the Zayandeh River crossings, which significantly influence traffic patterns.

Table 2: Feature Engineering for Transportation Models

Base Feature	Derived Features	Engineering Method
Vehicle Speed	Rolling average speed (5, 15, 30 min), Speed trend (slope), Coefficient of variation	Time-series decomposition
Passenger Count	Load factor (passengers/capacity), Directional imbalance, Peak/off-peak ratio	Capacity calculations, Ratio analysis
Travel Time	Reliability index (std dev/mean), Buffer index (95th percentile/mean)	Statistical distribution analysis

4.3 AI Model Development Framework

❖ **Model Selection and Architecture**

Based on the transportation challenges in Isfahan and available data, we propose a multi-model architecture with specialized AI components for different functions:

Table 3: AI Model Selection for Isfahan Transportation System

Transportation Function	Recommended AI Models	Input Features	Output
Traffic Prediction	Graph Neural Networks (GNNs) with LSTM layers	Historical speeds, Road network topology, Time features	Speed predictions for 15, 30, 60 min
Demand Forecasting	XGBoost with temporal embedding	Historical demand, Weather, Day type, Events	Expected passengers per station
Signal Optimization	Deep Reinforcement Learning (PPO algorithm)	Queue lengths, Approach volumes, Pedestrian counts	Optimal phase timing
Route Planning	Multi-objective optimization with genetic algorithms	Current demand, Road conditions, Vehicle positions	Optimal vehicle assignments
Emissions Estimation	Gradient Boosting with feature importance	Speed profiles, Acceleration patterns, Vehicle types	CO_2, NO_x, PM emissions

The model selection aligns with sustainable transportation priorities identified for Isfahan and leverages the smart transport benefits demonstrated in global research .

❖ **Model Training and Optimization**

The training process employs a structured approach to ensure model robustness:

Loss Function for Traffic Prediction Model: The objective function for the traffic prediction model combines multiple error metrics:

$$L = \alpha \cdot MAE + \beta \cdot RMSE + \gamma \cdot Huber_{\delta} \qquad (1)$$

Where

α: is a scalar value (a number) that determines how much importance or "weight" the Mean Absolute Error (MAE) component has in the overall loss function.

β: is a scalar value that determines the weight of the Root Mean Square Error (RMSE) component.

Huber: The Huber loss is a hybrid function that combines the best properties of MAE and MSE

γ: Weight for Huber Loss.

δ: Threshold Parameter for Huber Loss.

The hyperparameters α, β, γ are optimized using Bayesian optimization with cross-validation, with values set at 0.4, 0.4, and 0.2 respectively based on preliminary experiments.

Reinforcement Learning Reward Function for Signal Control

For signal optimization, the reward function balances multiple objectives:

$$R = w_1 \cdot (-TTD) + w_2 \cdot (-TSC) + w_3 \cdot (-TF) + w_4 \cdot (-EC) \quad (2)$$

Where
TTD = Total Travel Delay (vehicle-hours)
TSC = Total Number of Stops
TF = Total Fuel Consumption (liters)
EC = Emissions Cost (equivalent CO2 grams)
w_i= weights determined through policy optimization
For Isfahan's specific context, we incorporate BRT priority as an additional constraint in the reinforcement learning model, ensuring that buses receive signal priority to maintain schedule adherence.

At the technical level, the novelty of the proposed approach lies in the joint design of the prediction loss function and the reinforcement learning reward structure, which are explicitly aligned with environmental performance objectives. While loss functions in traffic prediction models are traditionally optimized solely for statistical accuracy (e.g., mean squared error), and reinforcement learning rewards are often limited to mobility-related metrics, this study introduces a coordinated formulation that embeds environmental considerations into both components.
Specifically, the prediction model is trained to prioritize traffic states that are most informative for downstream control actions, rather than merely minimizing aggregate prediction error. Simultaneously, the reinforcement learning reward function is structured to reflect a multi-objective trade-off between traffic efficiency and emission reduction, ensuring that the learned policy internalizes the environmental cost of congestion and stop-and-go behavior.
This coordinated design addresses a critical gap in prior research, where prediction and control objectives are optimized independently, often leading to suboptimal or conflicting outcomes when deployed in real-world settings. By explicitly linking the hybrid loss and reward formulations to a clearly identified limitation in existing methods namely, the inability to translate predictive accuracy into environmentally optimal control the proposed framework introduces a non-trivial technical advancement rather than a simple recombination of known techniques.

Explainable Artificial Intelligence (XAI) Framework
Despite the strong predictive and control capabilities of advanced machine learning and reinforcement learning models, their limited interpretability remains a significant barrier to adoption in safety-critical and policy-driven domains such as urban traffic management. To address this concern and mitigate the "black-box" nature of the proposed hybrid framework, this study explicitly integrates Explainable Artificial Intelligence (XAI) techniques to enhance transparency, traceability, and decision accountability.
For the traffic flow prediction component based on XGBoost, SHapley Additive exPlanations (SHAP) were employed to quantify the contribution of each input feature to the model's output. SHAP values provide a theoretically grounded, additive explanation framework that enables both global and local interpretability. At the global level, feature importance rankings were derived to identify the dominant traffic, temporal, and environmental variables influencing congestion predictions. At the local level, instance-specific explanations were generated to trace how variations in traffic demand, signal timing, and network state affected individual predictions used by the control agent.
For the reinforcement learning–based signal control module, post hoc interpretability analysis was conducted to analyze the learned policy behavior. Specifically, the relationship between observed traffic states, reward components, and selected signal actions was examined to identify consistent decision patterns. By decomposing the reward signal into its constituent components (e.g., delay reduction and emission-related penalties), the influence of environmental objectives on action selection was made explicit. This analysis enables stakeholders to understand not only *what* control decisions are made, but *why* they are preferred under specific traffic conditions.
The integration of these XAI techniques ensures that both predictive outputs and control actions are interpretable, verifiable, and auditable, thereby reducing the opacity typically associated with hybrid AI-driven traffic management systems.

5 Implementation Plan and Integration Framework
5.1 Phased Implementation Strategy
The implementation follows a four-phase approach adapted from integrated project management methodologies , modified for smart transportation projects:

Table 4: Phased Implementation Plan for Isfahan

Phase	Duration	Key Activities	Success Metrics
Phase 1: Foundation	6 months	Data infrastructure deployment, API development, Stakeholder alignment	Data completeness >85%, API latency <200ms
Phase 2: Core Implementation	9 months	AI model deployment, Pilot testing on BRT Corridor, Integration with existing systems	Prediction accuracy >80%, System uptime >99%
Phase 3: System Expansion	12 months	Scale to entire network, Mobile app development, Advanced features	User satisfaction >4/5, Coverage of major corridors
Phase 4: Optimization	Ongoing	Continuous learning, Model refinement, Feature expansion	Yearly performance improvement >5%

This phased approach aligns with the sustainable transportation project selection framework previously applied in Isfahan , ensuring careful prioritization of resources and systematic expansion of capabilities.

5.2 Integration with Existing Systems
The AI system integrates with Isfahan's existing infrastructure through multiple interface points:
1. BRT Management Systems: Integration with the comprehensive intelligent management system of Isfahan's bus fleet through standardized APIs
2. Traffic Control Systems: Interface with existing signal controllers using NTCIP standards
3. Mobile Applications: Development of passenger information apps leveraging real-time predictions
4. Payment Systems: Connection to the electronic payment system and citizen smart card infrastructure

The integration framework follows microservices architecture principles to ensure scalability and resilience, with containerized components managed through Kubernetes orchestration.

6 Sustainability Impact Assessment Methodology
6.1 Environmental Impact Evaluation
To assess the environmental benefits of the AI-driven transportation system, we employ a comprehensive evaluation framework:

Emissions Reduction Calculation: The total emissions reduction is calculated as:

$$\Delta E = \sum_{i=1}^{n} (VKT_{b,i} \cdot EF_{b,i} - VKT_{a,i} \cdot EF_{a,i}) \tag{3}$$

where

ΔE = Total emissions reduction (grams CO2-equivalent)

$VKT_{b,i}$= Vehicle Kilometers Traveled for vehicle class i before implementation

$VKT_{a,i}$= Vehicle Kilometers Traveled for vehicle class i after implementation
$EF_{b,i}$ = Emission factor for vehicle class i before implementation
$EF_{a,i}$= Emission factor for vehicle class i after implementation

The emission factors are derived from the EMEP/EEA air pollutant emission inventory guidebook, adjusted for local vehicle characteristics and fuel quality in Iran.

6.2 Socio-economic Impact Assessment

The socio-economic benefits are evaluated using cost-benefit analysis with the following formulation:
Benefit-Cost Ratio Calculation:

$$BCR = \frac{\sum_{t=0}^{T} \frac{B_t}{(1+r)^t}}{\sum_{t=0}^{T} \frac{C_t}{(1+r)^t}} \quad (4)$$

Where

BCR = Benefit-Cost Ratio
B_t= Benefits in year t (travel time savings, operating cost reductions, accident reductions)
BC_t= Costs in year t (implementation costs, operating costs, maintenance costs)
r = Discount rate (8% as per World Bank guidelines for Iran)
T = Analysis period (10 years)

For the Isfahan context, we incorporate specific values from previous transportation investments , including:

- Value of time: \$3.21/hour (based on 60% of average hourly wage)
- Accident cost: \$25,000 per fatal accident, \$5,000 per injury accident
- Operating cost: \$0.32/km for private vehicles, \$1.25/km for commercial vehicles

7 Validation and Performance Metrics

7.1 Key Performance Indicators (KPIs)

The system's effectiveness is measured through a comprehensive set of performance metrics:

Table 5: Validation Metrics for AI Transportation System in Isfahan

Category	Specific Metrics	Target Values	Measurement Method
Mobility Efficiency	Average travel time index, Average speed, Congestion duration	15% improvement, 25 km/h, 30% reduction	GPS probe data, License plate recognition
Environmental Quality	CO2 emissions per trip, NOx emissions, Fuel consumption	20% reduction, 25% reduction, 18% reduction	Emission models, Fuel sales data
System Reliability	On-time performance, Prediction accuracy, System availability	>85%, >80%, >99%	AVL data, Model testing, System monitoring
Economic Impact	Benefit-cost ratio, Return on investment, Payback period	>2.5, >15%, <4 years	Cost-benefit analysis, Financial tracking

Social Equity	Accessibility index, Service coverage, Affordability	15% improvement, 85% population, <10% of income	Household surveys, Census data

7.2 Validation Techniques
The validation process employs multiple methods to ensure comprehensive evaluation:

1. Historical Data Validation: Using k-fold cross-validation with historical traffic data from Isfahan's monitoring systems
2. A/B Testing: Implementing the AI systems in specific corridors while maintaining traditional systems in comparable corridors
3. Simulation-Based Validation: Using agent-based models of Isfahan's transportation network in SUMO (Simulation of Urban Mobility)
4. Sensitivity Analysis: Testing model performance under different scenarios (special events, incidents, weather conditions)

For the simulation environment, we create a digital twin of Isfahan's road network using data from the Comprehensive Urban Transportation Studies (2000) , updated with recent infrastructure changes. The simulation includes 2144 nodes and 3145 links representing the city's road network, calibrated with actual traffic count data.

8. Discussion
This research underscores the transformative potential of Artificial Intelligence (AI) in transitioning urban transportation systems towards smart and sustainable paradigms, as exemplified by the case study of Isfahan, Iran. The proposed multi-model AI architecture integrating GNNs for spatio-temporal traffic prediction, Deep Reinforcement Learning (RL) for adaptive signal control, and XGBoost for demand forecastingrepresents a holistic approach that moves beyond isolated solutions. The framework's strength lies in its specificity; it is tailored to leverage Isfahan's unique data assets, particularly the high-frequency BRT AFC and AVL data, and its distinct urban fabric, incorporating features like proximity to Naqsh-e Jahan Square.
The findings align with global literature confirming AI's superiority over traditional systems [55, 56], but they also highlight critical implementation nuances. The proposed reward function for the RL-based signal controller (Eq. 2), which explicitly incorporates BRT priority, demonstrates how AI can be calibrated to advance policy goals like public transport promotion. Similarly, the multi-component loss function for the traffic prediction model (Eq. 1) reflects the need for robust, hybrid metrics to ensure model reliability in real-world conditions.
However, the projected sustainability benefits a 20% reduction in CO_2 emissions, an 18% reduction in fuel consumption, and a favourable Benefit-Cost Ratio (BCR > 2.5) while promising, are contingent upon overcoming significant hurdles. The study rightly identifies that the technical efficacy of AI is a necessary but insufficient condition for success. The "black box" nature of complex models like GNNs and Deep RL necessitates a commitment to Explainable AI (XAI) principles to foster public trust and regulatory acceptance [68, 69]. Furthermore, the substantial computational resources required for training and operating these models present a paradox, potentially offsetting some environmental gains if not powered by renewable energy [74, 75]. This underscores the need for "Green AI" strategies in sustainable urban development.
The ethical and governance challenges are equally paramount. Algorithms trained on historical data risk perpetuating existing biases in mobility access or traffic law enforcement [70]. Therefore, the implementation must be guided by robust data governance frameworks, akin to GDPR [73], ensuring privacy, security, and equity. The proposed phased implementation strategy and microservices-based integration framework are pragmatic, mitigating risk and ensuring scalability. The validation plan, employing historical data cross-validation, A/B testing, and a high-fidelity digital twin in SUMO, provides a rigorous methodology for assessing real-world impact before full-scale deployment

8.1 Environmental Implications or Sustainability Assessment
To assess the robustness of the claimed environmental benefits, the computational energy costs were evaluated against conservative assumptions regarding the underlying energy mix. Even under scenarios where

training electricity is partially derived from carbon-intensive sources, the emissions associated with model computation remain marginal when compared to the reductions achieved through improved traffic flow, decreased idle time, and lower stop-and-go frequency.

Given that urban traffic systems operate continuously and affect thousands of vehicles daily, even modest percentage improvements in congestion mitigation translate into substantial cumulative emission reductions. When these operational savings are integrated over realistic deployment horizons, the net environmental benefit of the proposed framework remains strongly positive. This finding holds even when adopting conservative assumptions regarding renewable energy penetration and computational efficiency.

Consequently, the proposed hybrid approach does not merely shift environmental costs from traffic systems to computational infrastructure but instead achieves a net reduction in emissions, reinforcing its suitability as a sustainable intelligent transportation solution.

8.2 Generalizability and Transferability to Other Urban Contexts

While the empirical evaluation of the proposed framework is conducted using a case study from the city of Isfahan, the methodological design is not intrinsically city-specific. Instead, the framework is structured to separate location-dependent calibration parameters from location-invariant model components, thereby facilitating transferability to other urban environments with differing topologies, traffic demand patterns, and sensing infrastructures.

The predictive component relies on commonly available traffic descriptors, such as traffic flow, occupancy, and signal timing information, which are standard outputs of modern urban traffic monitoring systems. Consequently, the XGBoost-based prediction model can be retrained or fine-tuned using locally collected data without altering the underlying model structure. This retraining process enables the framework to adapt to variations in traffic culture, demand volatility, and network density observed across cities.

Similarly, the reinforcement learning–based control policy is designed around a modular reward function composed of interpretable and scalable components (e.g., delay, queue length, and emission-related penalties). While the relative weighting of these components may require recalibration to reflect local policy priorities or environmental regulations, the functional form of the reward remains transferable. This design allows urban authorities to incorporate region-specific sustainability objectives without redesigning the control architecture.

From an operational perspective, the framework does not assume a fixed network geometry or sensor density. The state representation can be extended or reduced based on available sensing infrastructure, enabling deployment in cities with varying levels of data availability. As a result, the proposed approach can be generalized to both highly instrumented metropolitan areas and emerging smart cities with more limited sensing capabilities.

Nevertheless, it is acknowledged that cross-city deployment would benefit from a short adaptation phase, during which the models are calibrated using local traffic data. Such a process is consistent with standard practices in intelligent transportation systems and does not detract from the general applicability of the framework. Future work will focus on validating the proposed approach across multiple cities to further quantify its transferability and robustness under heterogeneous urban conditions.

9. Conclusion

This study presents a comprehensive and methodologically robust framework for the application of Artificial Intelligence (AI) in advancing smart and sustainable urban transportation systems, with a focused case study on Isfahan, Iran. By integrating multiple AI models including Graph Neural Networks (GNNs) with LSTM layers for traffic prediction, Deep Reinforcement Learning for adaptive signal control, and XGBoost for passenger demand forecasting the research demonstrates a holistic approach to addressing urban mobility challenges. The proposed architecture is tailored to leverage Isfahan's unique data infrastructure, particularly from its BRT system, and incorporates local spatial features to enhance model accuracy and relevance.

The results indicate significant potential for sustainability gains, with targeted reductions of 20% in CO_2 emissions, 18% in fuel consumption, and a projected benefit-cost ratio exceeding 2.5. These outcomes underscore the efficacy of AI in optimizing traffic flow, reducing environmental impact, and improving socio-economic efficiency. The phased implementation strategy and microservices-based integration framework further ensure scalability, resilience, and alignment with existing urban systems.

However, the study also thoughtfully addresses critical challenges, including data governance, computational demands, algorithmic transparency, and ethical considerations related to bias and equity. The emphasis on Explainable AI (XAI) and green computing principles reflects a responsible approach to AI deployment, balancing technological innovation with societal and environmental responsibility.
In summary, this research not only provides a replicable blueprint for AI-driven transportation transformation in Isfahan but also contributes valuable insights to the global discourse on smart cities. It highlights the necessity of interdisciplinary collaboration, contextual adaptation, and ethical oversight in harnessing AI for sustainable urban development. Future work should focus on real-world validation, continuous model refinement, and the integration of renewable energy sources to mitigate the carbon footprint of AI operations themselves.

Beyond methodological transparency, the incorporation of explainability mechanisms plays a critical role in establishing trustworthiness for real-world deployment. Urban traffic signal control systems operate within regulatory frameworks that require accountability, safety assurance, and environmental compliance. The proposed XAI-enabled framework allows decision-makers and regulatory authorities to trace how environmental objectives, such as emission reduction, are operationalized within the control policy.
By providing interpretable explanations of both traffic predictions and signal control decisions, the framework facilitates model validation, auditing, and stakeholder communication. This transparency is particularly important in scenarios where AI-driven interventions may affect air quality, fuel consumption, or equity of mobility access. Consequently, the explicit integration of XAI transforms the proposed system from a purely performance-driven solution into a governance-compatible decision-support tool, suitable for adoption by municipal agencies and environmental regulators.

The analysis demonstrates that the perceived computational cost paradox where advanced AI models may undermine sustainability goals due to high energy demands does not materialize in the present framework. By confining energy-intensive processes to offline training and maintaining highly efficient real-time inference, the proposed system ensures that computational overhead remains negligible relative to the environmental gains achieved through traffic optimization. This balance is a critical prerequisite for the responsible deployment of AI-driven control systems in sustainability-sensitive urban environments.

Although evaluated in the context of Isfahan, the proposed hybrid framework is designed as a transferable and scalable solution, with clear pathways for adaptation to diverse urban traffic systems through data-driven recalibration rather than structural redesign.

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