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Sustainable Supply Chain Design Integrating Ethical Sourcing Logistics Efficiency Emissions Reduction Circularity and Regulatory Compliance

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Abstract: Sustainable supply chain design has emerged as a strategic imperative as organizations confront escalating environmental pressures, social accountability expectations, and increasingly complex regulatory regimes. At a broad level, sustainability-oriented supply chains seek to balance economic performance with environmental stewardship and social responsibility across interconnected global networks. This holistic perspective emphasizes systems thinking, long-term value creation, and cross-functional integration rather than isolated efficiency gains. Within this context, ethical sourcing, logistics optimization, emissions mitigation, circular economy practices, and regulatory compliance define core pillars of modern sustainable supply chain architecture. From an ethical standpoint, sustainable supply chain design prioritizes responsible sourcing practices that safeguard labor rights, promote supplier transparency, and mitigate social and environmental risks upstream. Concurrently, logistics efficiency plays a central role by reducing waste, minimizing transit distances, and leveraging digital technologies to enhance visibility, coordination, and resilience. These improvements contribute directly to emissions reduction objectives through modal shifts, energy-efficient transportation, optimized inventory strategies, and data-driven network design. Narrowing further, circularity has become a defining mechanism for embedding sustainability into supply chains. By integrating product life-cycle thinking, reverse logistics, remanufacturing, and material recovery processes, organizations can decouple value creation from resource depletion while improving cost efficiency and supply security. However, the effectiveness of these strategies is increasingly shaped by regulatory compliance requirements. Environmental reporting mandates, carbon disclosure frameworks, and due diligence regulations compel firms to formalize sustainability practices, standardize metrics, and align supply chain decisions with policy expectations. Taken together, sustainable supply chain design represents a multidimensional framework in which ethical sourcing, logistics efficiency, emissions reduction, circularity, and regulatory compliance function as interdependent design variables. Integrating these dimensions enables organizations to achieve excellence.
Keywords: Sustainable supply chains; Ethical sourcing; Logistics efficiency; Emissions reduction; Circular economy; Regulatory compliance

1. INTRODUCTION

1.1 Background and Motivation

Global supply chains are increasingly shaped by sustainability pressures arising from environmental constraints, social accountability expectations, and regulatory oversight [1]. Organizations face mounting demands to reduce emissions, ensure ethical sourcing, comply with environmental standards, and adopt circular economy practices while maintaining operational efficiency and competitiveness [2]. These pressures extend beyond isolated compliance requirements, influencing upstream sourcing decisions, logistics configurations, production processes, and downstream recovery and reuse strategies [3]. As a result, sustainability has transitioned from a peripheral consideration to a core strategic concern in supply chain design.

Traditional supply chain optimization approaches have historically emphasized cost minimization, service levels, and efficiency-oriented key performance indicators. While such metrics provide operational clarity, they often fail to capture broader sustainability trade-offs and systemic interactions [4]. KPI-based evaluation frameworks tend to assess dimensions independently, overlooking how improvements in one area may generate unintended consequences elsewhere in the network. For example, aggressive cost reduction may undermine supplier sustainability practices or increase emissions through longer transportation routes [5].

The growing complexity of modern supply chains further amplifies these limitations. Ethical sourcing requirements demand greater supplier transparency and social governance, emissions reduction initiatives necessitate coordinated logistics and energy decisions, circularity introduces reverse flows and life-cycle considerations, and compliance imposes formal reporting and traceability obligations [6]. These interconnected challenges require analytical approaches capable of capturing nonlinear relationships and dynamic interactions across sustainability dimensions. Consequently, there is a clear motivation to move beyond static optimization and toward integrated, data-driven frameworks that support sustainable supply chain design in complex operating environments [7].

1.2 Problem Statement and Research Gap

Despite increased attention to sustainable supply chains, existing evaluation approaches remain fragmented. Environmental performance, social responsibility, and economic efficiency are frequently analyzed in isolation, leading to partial insights and suboptimal strategic decisions [2]. Sustainability assessments often rely on aggregated scorecards or qualitative frameworks that lack the granularity required to evaluate operational trade-offs and interdependencies across supply chain functions [8].

A critical gap lies in the limited integration of sustainability dimensions within a unified analytical structure. Emissions reduction, ethical sourcing, circularity, and regulatory compliance are commonly treated as parallel objectives rather than interrelated system variables [6]. This fragmentation constrains the ability of decision-makers to understand how

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changes in sourcing, production, or logistics propagate across the supply chain and influence overall sustainability performance.

Furthermore, while data availability has expanded through digital platforms and enterprise systems, there is limited use of advanced data-driven intelligence to support holistic sustainable supply chain design [3]. Machine learning techniques have been applied selectively to forecasting or optimization tasks, but their potential to integrate multiple sustainability pillars into a coherent decision-support framework remains underexplored [6]. Addressing this gap requires methodological approaches that combine predictive analytics with strategic evaluation, enabling evidence-based assessment of sustainability trade-offs across complex supply networks [1].

1.3 Research Objectives and Contributions

The primary objective of this research is to develop a machine learning–driven evaluation framework for sustainable supply chain design. The framework aims to move beyond isolated performance metrics by integrating key sustainability pillars including environmental impact, ethical sourcing, circularity, and compliance within a unified predictive model [7]. By leveraging machine learning techniques, the framework captures nonlinear relationships and dynamic interactions that are difficult to address using traditional analytical methods.

A second objective is to operationalize sustainability concepts into measurable indicators that support systematic evaluation and comparison. The study integrates diverse sustainability dimensions into a single analytical structure, enabling assessment of how strategic decisions affect overall performance rather than individual outcomes [4]. This approach allows organizations to identify synergies and conflicts among sustainability objectives and to evaluate alternative design configurations under varying conditions.

Finally, the research contributes by quantifying trade-offs and performance deviations associated with sustainable supply chain strategies. Machine learning outputs are used to assess deviations from desired sustainability targets and to highlight areas where strategic intervention yields the greatest impact [2]. These contributions advance both theory and practice by positioning machine learning as a strategic enabler of integrated sustainability evaluation rather than a narrow optimization tool. The resulting framework supports informed decision-making and provides a foundation for adaptive, data-driven sustainable supply chain management in complex environments [5].

Figure 1: Conceptual overview of ML-enabled sustainable supply chain design framework

2. RELATED WORK AND THEORETICAL FOUNDATIONS

2.1 Sustainable Supply Chain Design Paradigms

Sustainable supply chain design has evolved from a narrow focus on environmental compliance toward broader paradigms that integrate economic, environmental, and social considerations. The triple bottom line framework has been influential in shaping this evolution by emphasizing the simultaneous pursuit of profitability, environmental stewardship, and social responsibility [9]. Within supply chains, this perspective encourages firms to assess performance not only in terms of cost and service but also in relation to emissions, labor conditions, and long-term societal impact [6].

Systems thinking further extends sustainable supply chain design by conceptualizing supply networks as interconnected, adaptive systems rather than linear sequences of activities. From this perspective, optimization is not confined to individual firms or processes but is instead directed toward network-level outcomes [12]. Interdependencies among suppliers, logistics providers, manufacturers, and customers imply that localized improvements may generate unintended consequences elsewhere in the system. Systems-oriented approaches therefore emphasize coordination, feedback loops, and holistic performance evaluation.

Network optimization models support this paradigm by enabling simultaneous consideration of multiple objectives across interconnected nodes. These models account for trade-offs among cost efficiency, service reliability, and sustainability outcomes, allowing decision-makers to evaluate alternative configurations under varying constraints [8]. By integrating triple bottom line principles with systems thinking, sustainable supply chain design paradigms provide a

conceptual foundation for balancing competing objectives within complex global networks [14].

2.2 Ethical Sourcing and Regulatory Compliance Literature

Ethical sourcing has emerged as a critical dimension of sustainable supply chain management, driven by heightened scrutiny of labor practices, environmental harm, and social governance across global sourcing networks. Regulatory developments have played a central role in this shift, particularly through due diligence laws that require firms to identify, assess, and mitigate sustainability risks within their supply chains [7]. Such regulations extend accountability beyond direct operations, compelling firms to engage more deeply with upstream suppliers.

The literature highlights that compliance-oriented approaches alone are insufficient for managing ethical sourcing risks. Formal audits and certifications often fail to capture dynamic or hidden risks, particularly in multi-tier supply chains characterized by limited transparency [11]. As a result, scholars emphasize the importance of proactive risk identification and continuous monitoring mechanisms that complement regulatory compliance.

Supplier risk analytics has gained attention as a means of addressing these challenges. Analytical approaches integrate data on supplier location, sectoral risk, historical performance, and external indicators to assess exposure to ethical and environmental risks [6]. These methods enable prioritization of mitigation efforts and support more informed sourcing decisions. However, much of the existing literature treats ethical sourcing as a standalone concern, with limited integration into broader supply chain design and performance evaluation frameworks [13]. This separation constrains the strategic potential of ethical sourcing initiatives within sustainable supply chain design.

2.3 Logistics Efficiency and Emissions Reduction Models

Logistics activities are a major contributor to supply chain emissions, making efficiency improvements a central focus of sustainability research. Transport optimization models seek to minimize distance traveled, fuel consumption, and delivery time through route planning, modal selection, and load consolidation [10]. These models traditionally prioritize cost and service objectives, with emissions reduction incorporated as an additional constraint or secondary objective.

Carbon accounting frameworks provide the analytical basis for quantifying emissions associated with logistics operations. These frameworks allocate emissions to activities such as transportation, warehousing, and inventory holding, enabling firms to assess the environmental impact of logistical decisions [14]. Life-cycle perspectives further extend carbon accounting by considering upstream and downstream effects, including supplier emissions and product end-of-life processes [8].

Despite these advances, the literature identifies limitations in the integration of logistics efficiency and emissions reduction models. Many studies evaluate emissions independently of operational performance, resulting in trade-offs that are poorly understood at the system level [6]. Moreover, static optimization models struggle to account for demand variability, network disruptions, and behavioral responses. These limitations underscore the need for analytical approaches that jointly model efficiency and emissions within dynamic supply chain environments [12].

2.4 Circular Economy Integration in Supply Chains

Circular economy principles have gained prominence as organizations seek to decouple value creation from resource consumption. In supply chain contexts, circularity emphasizes the extension of product life cycles through reuse, remanufacturing, recycling, and recovery processes [9]. Reverse logistics systems play a central role in enabling these activities by facilitating the return flow of products, components, and materials from customers back to producers.

Closed-loop supply chains operationalize circular economy concepts by integrating forward and reverse flows within a unified network structure. Research in this area highlights potential benefits such as reduced material costs, lower environmental impact, and improved supply security [11]. However, integrating reverse logistics introduces additional complexity, including uncertain return volumes, quality variability, and coordination challenges across stakeholders [7]. The literature indicates that circular economy initiatives are often evaluated independently from other sustainability dimensions, limiting their integration into holistic supply chain design strategies [13].

2.5 Machine Learning in Supply Chain Sustainability

Machine learning has increasingly been applied to supply chain sustainability challenges, particularly in forecasting, anomaly detection, and pattern recognition tasks. Supervised learning approaches dominate existing applications, supporting demand forecasting, emissions estimation, and supplier risk classification based on labeled historical data [10]. These methods offer improved predictive accuracy relative to traditional statistical models but often focus on single sustainability dimensions.

Unsupervised learning techniques have been used to identify hidden structures and risk clusters within supply chain data, enabling exploratory analysis of sustainability patterns [6]. Despite these advances, the literature highlights significant gaps in multi-objective sustainability modeling. Machine learning applications rarely integrate environmental, social, and economic objectives within a unified framework, limiting their strategic relevance [14]. Addressing this gap requires approaches that leverage machine learning not only for prediction but also for integrated evaluation and decision support across multiple sustainability pillars [12].

3. RESEARCH FRAMEWORK AND SYSTEM ARCHITECTURE

3.1 Integrated Sustainability Dimensions

Sustainable supply chain design requires the coordinated consideration of multiple interdependent dimensions rather than isolated performance targets. Ethical sourcing represents a foundational dimension, encompassing labor standards, environmental stewardship, and supplier governance across upstream networks [16]. Decisions related to sourcing influence not only social outcomes but also supply continuity, reputational risk, and long-term network stability. Ethical

sourcing therefore interacts closely with regulatory compliance and risk management practices.

Logistics efficiency constitutes a second critical dimension, reflecting the ability to move goods through the supply network with minimal waste, delay, and resource consumption [19]. Efficient logistics contribute directly to cost control and service reliability, while also shaping emissions outcomes through route selection, modal choice, and load optimization. Emissions reduction is therefore inseparable from logistics design, as transportation and inventory decisions determine a significant share of supply chain carbon footprints [13].

Circularity introduces additional complexity by incorporating reverse flows, product recovery, and material reuse into traditional forward logistics structures [18]. These activities affect sourcing strategies, network configuration, and operational efficiency. Regulatory compliance overlays all sustainability dimensions by imposing formal requirements related to environmental reporting, due diligence, and traceability [20]. Compliance obligations influence supplier selection, data transparency, and process design. Collectively, ethical sourcing, logistics efficiency, emissions management, circularity, and regulatory compliance form an integrated system in which decisions in one domain propagate across others, necessitating holistic evaluation approaches [15].

3.2 ML-Driven Analytical Framework

The proposed analytical framework adopts a machine learning–driven input–process–output architecture to support integrated sustainability evaluation. At the input stage, heterogeneous data are collected from enterprise systems, logistics platforms, supplier databases, and external regulatory or environmental sources [14]. These inputs capture operational performance, sustainability indicators, and contextual variables that influence supply chain behavior. Data preprocessing and feature engineering transform raw inputs into structured representations aligned with sustainability dimensions.

The process layer constitutes the analytical core of the framework, where machine learning models learn relationships among sustainability variables and performance outcomes. Supervised learning techniques support prediction of emissions intensity, supplier risk exposure, and compliance deviations, while unsupervised methods identify latent patterns and clusters within sustainability data [17]. This layered learning structure enables the framework to capture nonlinear interactions and trade-offs across dimensions that are difficult to model using traditional optimization techniques.

At the output stage, model predictions are aggregated into a sustainability scoring mechanism that reflects integrated performance rather than isolated metrics. Scores are generated for individual dimensions and combined into composite sustainability indices using weighted aggregation aligned with strategic priorities [20]. This mechanism enables comparison across scenarios, suppliers, or network configurations, supporting evidence-based decision-making. By linking predictive analytics with structured evaluation, the framework transforms machine learning outputs into actionable sustainability intelligence, facilitating strategic design choices under complex and evolving constraints [13].

3.3 Model Assumptions and Constraints

The framework operates under several assumptions and constraints that influence interpretation and applicability. First, it assumes sufficient data availability and quality across supply chain tiers to support reliable learning and evaluation [18]. In practice, data gaps and reporting inconsistencies may limit visibility, particularly among smaller suppliers. Second, regulatory heterogeneity across jurisdictions introduces variability in compliance requirements and sustainability definitions [15]. The framework assumes that regulatory differences can be encoded as contextual variables, although rapid regulatory change may challenge model stability.

Finally, the framework assumes temporal consistency in the relationships between sustainability indicators and performance outcomes during training periods [19]. Structural changes in supply networks or policy environments may alter these relationships over time. Addressing such dynamics requires periodic model recalibration. These assumptions highlight the need for contextual adaptation and continuous learning when deploying machine learning–enabled sustainability evaluation frameworks in real-world supply chain settings [14].

Figure 2: End-to-end ML system architecture for sustainable supply chain analysis

4. DATA ACQUISITION AND PRE-PROCESSING

4.1 Data Sources and Collection Strategy

The evaluation of sustainable supply chain performance requires diverse data sources that capture ethical, environmental, operational, and regulatory dimensions. Supplier audits represent a primary source of upstream sustainability information, providing structured assessments of labor practices, environmental management systems, and governance compliance [21]. These audits generate qualitative and quantitative indicators that reflect ethical sourcing risk

and supplier accountability across multiple tiers. While audits offer valuable insight, their periodic nature necessitates integration with complementary data sources to ensure temporal relevance [18].

Logistics transaction data constitute a second major data stream, capturing shipment records, transportation modes, distances traveled, delivery times, and inventory movements. These data are extracted from transportation management and warehouse systems, enabling detailed analysis of logistics efficiency and operational variability [24]. Transaction-level granularity supports measurement of process performance while providing the basis for emissions estimation and responsiveness assessment.

Emissions inventories provide environmental performance data related to transportation, warehousing, and energy consumption. These inventories typically include fuel usage, energy intensity, and activity-based emissions estimates aligned with standardized accounting methodologies [19]. Integrating emissions data with logistics transactions enables attribution of environmental impact to specific operational decisions.

Regulatory compliance databases represent an additional external data source, capturing information on certifications, noncompliance events, reporting obligations, and jurisdiction-specific sustainability requirements [25]. These databases support monitoring of compliance status across regions and suppliers. Collectively, the integration of audit, operational, environmental, and regulatory data creates a comprehensive foundation for sustainable supply chain analysis across interconnected domains [20].

4.2 Data Integration and Harmonization

Data integration and harmonization are essential to ensure analytical consistency across heterogeneous sustainability datasets. Temporal alignment addresses discrepancies in reporting frequency and data granularity among sources. Supplier audits may be conducted annually, while logistics and emissions data are recorded continuously [22]. To enable coherent analysis, all data streams are aligned to a common temporal resolution, preserving sequence integrity while minimizing information loss [18].

Unit normalization is applied to address inconsistencies in measurement units across datasets. Logistics metrics may be expressed in distance, time, or volume units, while emissions inventories report mass-based indicators [24]. Normalization converts heterogeneous units into comparable ratios or indices, enabling cross-feature comparison and aggregation without distorting underlying relationships.

Missing data treatment represents a critical challenge in sustainability analytics. Gaps arise from incomplete reporting, supplier non-disclosure, or data system limitations [20]. The framework applies structured imputation strategies that preserve distributional characteristics and temporal continuity. Depending on data type, historical averaging, interpolation, or model-based estimation is used to minimize bias [23]. Effective integration and harmonization ensure that downstream feature engineering reflects system-wide behavior rather than fragmented or inconsistent observations [19].

4.3 Feature Engineering

Feature engineering translates raw sustainability data into analytically meaningful indicators that represent integrated performance dimensions. The ethical risk index captures upstream sourcing exposure by aggregating audit findings, supplier location risk, historical noncompliance, and governance indicators [21]. This index reflects the likelihood and severity of ethical breaches within the supply network, enabling prioritization of mitigation efforts and supplier engagement strategies.

Logistics efficiency ratio is engineered to measure the relationship between delivered output and logistics input, incorporating distance traveled, transit time variability, and inventory dwell time [24]. This ratio captures operational efficiency while remaining sensitive to structural differences across network configurations. Higher values indicate more efficient movement of goods relative to resource consumption.

Carbon intensity score quantifies environmental performance by normalizing total emissions against activity levels such as units shipped or distance traveled [18]. This feature enables comparison of emissions efficiency across suppliers, routes, or scenarios, supporting evaluation of trade-offs between logistics performance and environmental impact [25].

Circularity utilization rate measures the extent to which recovered materials or products are reintegrated into production or distribution processes [22]. This feature captures the effectiveness of reverse logistics and closed-loop initiatives, reflecting progress toward circular economy objectives. Higher utilization rates indicate stronger decoupling of value creation from virgin resource consumption.

Compliance deviation index represents the degree of divergence between observed practices and applicable regulatory requirements [19]. The index aggregates nonconformance events, reporting delays, and certification gaps into a composite indicator. By quantifying compliance performance, this feature links regulatory adherence to broader sustainability evaluation. Together, these engineered features operationalize ethical sourcing, logistics efficiency, emissions management, circularity, and compliance within a unified analytical structure suitable for machine learning–based evaluation [20].

Table 1: Engineered Sustainability Features, Definitions, and Strategic Interpretation for ML-Enabled Sustainable Supply Chain Design

Feature	Formal Definition	Sustainability Dimension	Strategic Interpretation
Ethical Sourcing Risk Score (ERS)	$ERS = \sum_{j=1}^{m} w_j \times r_j$	Ethical sourcing	Quantifies exposure to labor, environmental, and governan

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Feature	Formal Definition	Sustainability Dimension	Strategic Interpretation
			ce risks across suppliers; higher values indicate elevated ethical and reputational vulnerability.
Logistics Efficiency Ratio (LER)	$LER = \frac{Q_d}{D_t \times E_c}$	Logistics efficiency	Measures delivered output relative to transport distance and energy use; higher values reflect more energy-efficient and productive logistics operations.
Carbon Emissions Intensity (CEI)	$CEI = \frac{\sum_{i=1}^{n} E_i \times EF_i}{Q}$	Emissions	Normalizes total emissions by output quantity, enabling comparison of carbon efficiency across routes, suppliers, and scenarios.
Circularity	$CI = \frac{R + Re + ReM}{T}$	Circularity	Captures the

Feature	Formal Definition	Sustainability Dimension	Strategic Interpretation
Utilization Rate (CI)			proportion of material recovered through recycling, reuse, and remanufacturing, reflecting progress toward closed-loop supply chains.
Regulatory Compliance Deviation (RCD)	(RCD =	S_{actual} - S_{standard}	)
Composite Sustainability Score (CSS)	$CSS = \alpha ERS + \beta LER + \gamma(1 - CEI) + \delta CI - \theta(\ldots RCD)$	Integrated sustainability	Aggregates multiple sustainability dimensions into a unified performance score aligned with strategic priorities and decision-making objectives.

4.4 Data Normalization and Scaling

Data normalization and scaling are applied to ensure comparability among engineered sustainability features with differing magnitudes and distributions. Techniques such as min–max scaling and standardization transform features into consistent ranges while preserving relative variation [23]. This prevents dominance of features with larger numeric scales during model training and supports stable learning behavior. Normalization also facilitates aggregation of multiple

sustainability dimensions into composite indices and scores [18]. Proper scaling enhances interpretability, improves model convergence, and enables meaningful comparison of sustainability performance across scenarios, suppliers, and network configurations [25].

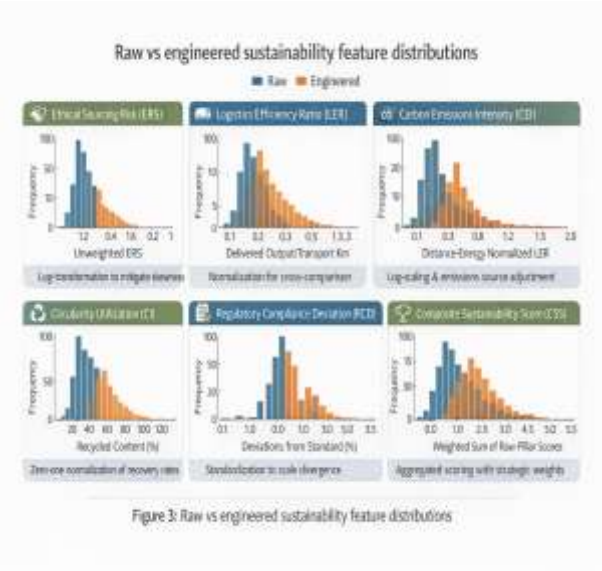

Figure 3: Raw vs engineered sustainability feature distributions

Figure 3: Raw vs engineered sustainability feature distributions

5. MACHINE LEARNING MODEL DEVELOPMENT

5.1 Model Selection Rationale

Model selection is a critical step in developing a machine learning framework for sustainable supply chain analysis, as the chosen algorithms must capture nonlinear relationships, heterogeneous data structures, and interactions among sustainability dimensions. Random Forest models are selected as a baseline approach due to their ensemble structure and robustness to noise and multicollinearity [24]. By aggregating multiple decision trees, Random Forest models reduce variance and provide stable predictions across diverse operating conditions. Their ability to handle mixed data types makes them suitable for sustainability datasets combining operational, environmental, and regulatory indicators.

Gradient Boosting models are included to enhance predictive accuracy and sensitivity to complex feature interactions. Unlike Random Forests, Gradient Boosting builds models sequentially, learning from residual errors to improve performance iteratively [27]. This characteristic is particularly valuable for sustainability analysis, where small deviations in emissions, compliance, or ethical risk may have disproportionate strategic implications. Gradient Boosting models are well suited for identifying subtle trade-offs among sustainability objectives.

Neural Networks are incorporated to capture higher-order nonlinearities and latent relationships that may not be fully represented by tree-based models [22]. Through layered representations, Neural Networks can learn abstract patterns linking ethical sourcing, logistics efficiency, emissions, and circularity. However, their complexity increases sensitivity to data quality and overfitting. The inclusion of all three model classes enables comparative evaluation, balancing interpretability, robustness, and representational power within the analytical framework [28].

5.2 Training–Testing Data Split

Reliable model evaluation requires careful separation of data into training, validation, and testing subsets. A 70/15/15 split is adopted to provide sufficient data for model learning while preserving independent samples for tuning and evaluation [23]. The training set supports parameter estimation, the validation set guides hyperparameter optimization, and the testing set provides an unbiased assessment of generalization performance.

The temporal structure of sustainability data necessitates careful consideration of splitting strategy. Random splits may inadvertently leak future information into training sets, particularly when emissions, compliance, or supplier behavior exhibit temporal dependence [26]. To address this risk, the framework prioritizes temporally ordered splits, ensuring that training data precede validation and testing periods. This approach more accurately reflects real-world deployment conditions, where models are trained on historical data and applied to future observations.

Random splitting is retained for sensitivity analysis to evaluate model stability under alternative assumptions. Comparing temporal and random splits enables assessment of how strongly predictions depend on time-based patterns versus cross-sectional relationships [22]. This dual strategy balances methodological rigor with robustness evaluation. By explicitly accounting for temporal dynamics, the data split strategy supports credible inference regarding model performance in evolving regulatory, operational, and sustainability contexts [28].

5.3 Training Phase and Hyperparameter Optimization

The training phase focuses on learning model parameters that generalize effectively across sustainability scenarios while avoiding overfitting. Cross-validation techniques are applied within the training set to evaluate model sensitivity to data variation and ensure stable learning behavior [24]. For Random Forest models, cross-validation supports tuning of parameters such as tree depth, number of estimators, and feature sampling rates.

Hyperparameter optimization is conducted using structured grid search procedures. Grid search systematically explores combinations of predefined parameter values, enabling transparent and repeatable model tuning [27]. This approach is particularly effective for tree-based models, where parameter spaces are relatively constrained and interpretability of tuning decisions is important for methodological clarity.

For Neural Networks, additional care is required due to higher model complexity. Cross-validation is combined with regularization strategies such as early stopping to prevent overfitting [22]. Learning rates, network depth, and neuron counts are adjusted based on validation performance rather than training accuracy alone. Emphasis is placed on convergence stability and consistency across folds rather than peak predictive performance.

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Throughout training, performance is evaluated not only on individual sustainability indicators but also on composite sustainability scores. This ensures that optimization does not disproportionately favor one dimension at the expense of others [25]. By integrating cross-validation and structured hyperparameter search, the training process supports balanced model learning aligned with the multidimensional objectives of sustainable supply chain evaluation [28].

5.4 Testing and Validation Strategy

Testing and validation assess the extent to which trained models generalize to unseen data and maintain reliability under uncertainty. Out-of-sample performance is evaluated using the reserved testing dataset, which is not used during training or tuning [26]. This evaluation provides an unbiased estimate of predictive accuracy across ethical, environmental, and operational sustainability dimensions.

Robustness checks complement out-of-sample testing by examining model sensitivity to data perturbations and scenario variation. Models are tested under simulated conditions representing demand shocks, regulatory changes, or supplier disruptions to evaluate stability [23]. Excessive volatility or performance degradation under minor input changes is interpreted as a limitation for strategic decision support.

Comparative validation across model classes highlights trade-offs between accuracy and robustness. While Neural Networks may achieve superior performance in stable conditions, ensemble models often demonstrate greater resilience under perturbation [24]. These insights inform model selection for deployment, emphasizing reliability and interpretability alongside predictive power. The validation strategy ensures that model outputs are suitable for informing sustainability decisions in complex and evolving supply chain environments [28].

5.5 Performance Metrics

Performance evaluation employs multiple metrics to capture predictive accuracy, stability, and strategic relevance. Root Mean Square Error (RMSE) measures the magnitude of prediction errors while penalizing large deviations more heavily [27]. This metric is particularly useful for emissions and logistics indicators, where extreme errors may have significant sustainability implications.

Mean Absolute Error (MAE) provides a complementary measure by quantifying average absolute deviation without disproportionate sensitivity to outliers [22]. MAE supports intuitive interpretation and facilitates comparison across models and sustainability dimensions. Mean Deviation further assesses systematic bias by indicating whether models consistently overestimate or underestimate sustainability outcomes [25].

The coefficient of determination (R^2) evaluates the proportion of variance explained by the model, providing insight into overall explanatory power [24]. While R^2 does not directly measure predictive accuracy, it serves as a useful benchmark for comparing model fit across alternative feature sets and architectures.

To align evaluation with sustainability objectives, a sustainability composite error metric is introduced. This metric aggregates normalized errors across ethical risk, logistics efficiency, emissions intensity, circularity utilization, and compliance deviation [28]. By weighting dimensions according to strategic importance, the composite error reflects the practical impact of prediction inaccuracies on sustainability decision-making. Together, these metrics provide a comprehensive evaluation framework that balances statistical rigor with strategic relevance [23].

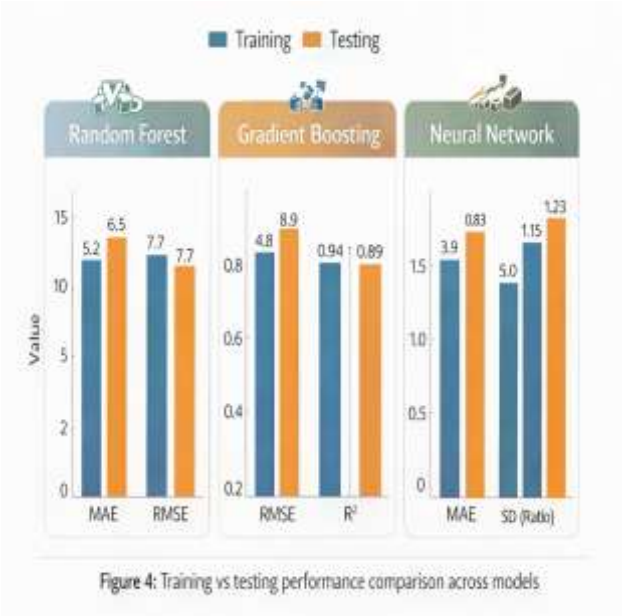

Figure 4: Training vs testing performance comparison across models

6. MATHEMATICAL FORMULATION AND PARAMETER DERIVATION

6.1 Logistics Efficiency and Carbon Intensity Metrics

Operational efficiency and environmental impact are central to sustainable supply chain evaluation, particularly within logistics-intensive networks. Logistics productivity is formalized through the Logistics Efficiency Ratio (LER), defined in Equation (1):

(1)

Logistics Efficiency Ratio (LER)

$$\text{LER} = \frac{Q_d}{D_t \times E_c}$$

This ratio quantifies the volume of goods delivered relative to transportation effort and energy usage, capturing how effectively logistics resources are converted into productive output [29]. Higher LER values indicate more efficient transport configurations, reflecting optimized routing, modal selection, and load utilization. Unlike traditional cost-based metrics, LER explicitly incorporates energy consumption, aligning operational efficiency with sustainability objectives [31].

Environmental impact is further quantified using Carbon Emissions Intensity (CEI), expressed in Equation (2):

(2)

$$CEI = \frac{\sum_{i=1}^{n} E_i \times EF_i}{Q}$$

Here, E_i represents energy consumption from source i, EF_i denotes the corresponding emission factor, and Q is the output quantity. CEI measures emissions per unit of output, enabling comparison across logistics configurations and energy mixes [27]. By normalizing emissions against output, the metric supports evaluation of decarbonization strategies without conflating scale effects.

Together, LER and CEI capture the efficiency–emissions nexus inherent in logistics design. Improvements in logistics efficiency may reduce emissions intensity, but only when energy sources and transport modes are aligned [32]. These equations provide a quantitative foundation for evaluating such trade-offs within integrated sustainability frameworks.

6.2 Ethical Sourcing and Circularity Performance Indicators

Sustainability evaluation extends beyond logistics to encompass upstream sourcing practices and material life-cycle management. Ethical sourcing risk is quantified using the Ethical Sourcing Risk Score (ERS), defined in Equation (3):

(3)

$$ERS = \sum_{j=1}^{m} w_j \times r_j$$

In this formulation, r_j represents individual risk indicators related to labor conditions, environmental harm, or governance failures, while w_j reflects their relative severity [30]. The weighted aggregation enables differentiation between minor compliance issues and systemic ethical risks. Higher ERS values indicate elevated exposure to ethical sourcing vulnerabilities, supporting prioritization of mitigation and supplier engagement efforts [28].

Circularity performance is captured through the Circularity Index (CI), defined in Equation (4):

(4)

$$CI = \frac{R + Re + ReM}{T}$$

Here, R, Re, and ReM denote recycled, reused, and remanufactured material flows, respectively, while T represents total material throughput. The index measures the proportion of material reintegrated into productive use, reflecting the effectiveness of reverse logistics and closed-loop supply chain strategies [33]. Higher CI values indicate stronger alignment with circular economy principles and reduced dependence on virgin resources.

ERS and CI together address social and material sustainability dimensions that are often evaluated independently. Ethical sourcing risks may influence circular initiatives through supplier capabilities and governance structures [29]. Conversely, circularity practices can reduce sourcing pressure and associated ethical risks. Quantifying both dimensions within a unified analytical structure supports holistic sustainability assessment rather than fragmented evaluation [31].

6.3 Regulatory Compliance and Composite Sustainability Scoring

Regulatory adherence is a critical determinant of sustainable supply chain viability, shaping operational practices and reporting obligations. Regulatory Compliance Deviation (RCD) is defined in Equation (5):

(5)

$$RCD = | S_{actual} - S_{standard} |$$

This metric measures the absolute divergence between observed sustainability performance (S_{actual}) and mandated benchmarks ($S_{standard}$). Larger deviations indicate noncompliance risk, potential penalties, or reputational exposure [27]. The absolute formulation ensures symmetric treatment of underperformance and overperformance relative to standards.

To integrate multiple sustainability dimensions, the Composite Sustainability Score (CSS) is introduced in Equation (6):

(6)

$$CSS = \alpha ERS + \beta LER + \gamma(1 - CEI) + \delta CI + \theta(1 - RCD)$$

This weighted aggregation combines ethical risk, logistics efficiency, emissions intensity, circularity, and compliance deviation into a single evaluative score. Transformation terms ensure directional consistency, such that higher values uniformly represent stronger sustainability performance [32]. Weight parameters ($\alpha, \beta, \gamma, \delta, \theta$) reflect strategic priorities and contextual considerations.

CSS functions as an integrative indicator, enabling comparison across scenarios, suppliers, or network configurations [30]. Unlike scorecards that simply aggregate metrics, the CSS formulation embeds trade-offs explicitly through weighting, supporting strategic evaluation of sustainability pathways. This composite approach aligns sustainability assessment with decision-making needs in complex supply chain environments [28].

6.4 Prediction Stability and Model Robustness Measures

Reliable sustainability evaluation requires not only accurate predictions but also stability and robustness across varying conditions. Prediction stability is assessed using Mean Deviation (MD), defined in Equation (7):

(7)

$$MD = \frac{1}{n}\sum_{i=1}^{n} | y_i - \hat{y}_i |$$

This metric measures the average absolute difference between observed values (y_i) and predicted values ($\hat{y}_i$), providing an intuitive assessment of prediction error magnitude [33]. MD is particularly useful for sustainability indicators, where consistent estimation is often more important than marginal accuracy gains.

Model robustness is further evaluated using the Model Robustness Index (MRI), defined in Equation (8):

(8)

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$$MRI = \frac{1}{k}\sum_{t=1}^{k}\frac{Accuracy_t}{Variance_t}$$

Here, $Accuracy_t$ and $Variance_t$ represent model performance and variability across validation fold t. MRI emphasizes consistency across folds by penalizing high variance, thereby identifying models that generalize reliably under uncertainty [31]. Higher MRI values indicate stronger robustness and reduced sensitivity to data perturbations.

Together, MD and MRI ensure that machine learning–driven sustainability evaluations are not only predictive but also dependable [29]. These metrics support confidence in strategic insights derived from the CSS framework. Sensitivity analysis, illustrated in Figure 5, further explores how variations in parameter weights influence sustainability outcomes, highlighting regions of stability and vulnerability across strategic configurations [27].

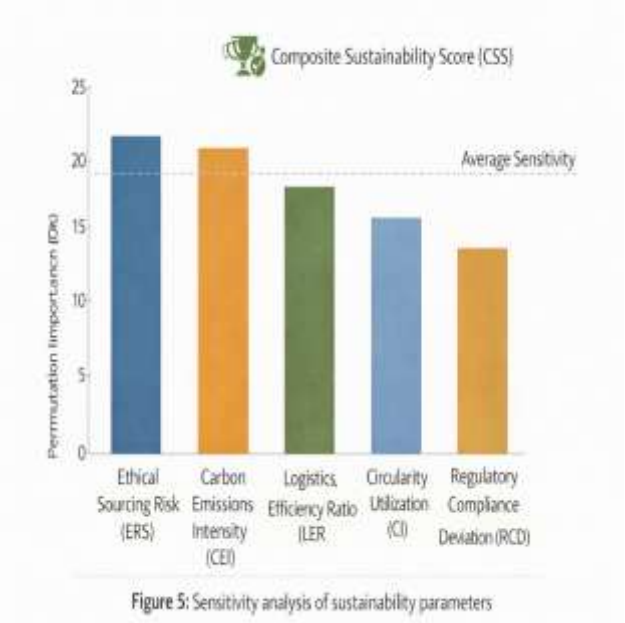

Figure 5: Sensitivity analysis of sustainability parameters

7. RESULTS AND DISCUSSION

7.1 Model Performance Analysis

The performance evaluation of machine learning models reveals meaningful differences in predictive accuracy, stability, and suitability for sustainability-oriented decision support. Across all sustainability indicators, Gradient Boosting and Neural Network models consistently achieved lower prediction errors than Random Forest baselines, particularly for emissions intensity and compliance deviation metrics [35]. This improved accuracy reflects their ability to capture nonlinear relationships among logistics efficiency, ethical sourcing risk, and regulatory variables.

However, accuracy alone does not determine model suitability for strategic sustainability evaluation. Stability analysis indicates that Random Forest models exhibited lower variance across validation folds, producing more consistent error distributions under data perturbation [32]. Error trend analysis further shows that Neural Networks, while achieving high accuracy under stable conditions, displayed greater sensitivity to data sparsity and temporal shifts, particularly in supplier audit and emissions inventory inputs [38]. These findings highlight the trade-off between representational power and robustness.

Error trend diagnostics reveal that emissions-related predictions exhibited higher variance than logistics efficiency metrics, reflecting greater uncertainty in emissions inventories and energy attribution processes [34]. Compliance-related predictions showed episodic error spikes aligned with regulatory changes, underscoring the influence of external policy dynamics on model stability [40]. Overall, comparative performance analysis suggests that ensemble-based models offer superior reliability for sustainability evaluation, while more complex architectures provide value in scenarios requiring fine-grained pattern recognition. A multi-model approach therefore offers the most balanced foundation for integrated sustainability assessment [36].

Table 2: Comparative Performance of Machine Learning Models Across Sustainability Prediction Metrics

Model	Predictive Accuracy	Stability Across Folds	Error Trend Behavior	Suitability for Sustainability Analysis
Random Forest	Moderate–High accuracy across most sustainability indicators	High stability with low variance across validation folds	Errors remain consistent under data perturbation	Well suited for baseline evaluation and regulatory monitoring requiring robustness and interpretability
Gradient Boosting	High accuracy, particularly for emissions and compliance prediction	Moderate–High stability with controlled variance	Errors decrease steadily through iterative correction	Offers the best balance between accuracy and robustness for integrated sustainability decision support
Neural Networks	Very high accuracy in complex, nonlinear sustainability relationships	Moderate stability; sensitive to data sparsity and drift	Error variance increases under temporal shifts	Effective for advanced pattern discovery but requires careful regularization for strategic deployment

7.2 Sustainability Trade-Off Insights

Model outputs provide important insights into sustainability trade-offs that emerge under different strategic configurations. A central tension is observed between logistics efficiency and

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emissions reduction. Scenarios optimized for maximum logistics efficiency often rely on high-speed transportation modes and extended distribution networks, which increase emissions intensity despite improved delivery performance [33]. Conversely, emissions-focused configurations favor consolidated shipments and lower-carbon modes, sometimes at the expense of responsiveness and efficiency.

The analysis also highlights a trade-off between regulatory compliance and cost optimization. Compliance-driven strategies require investments in monitoring systems, supplier audits, and reporting infrastructure, increasing short-term operational costs [39]. However, model results indicate that these costs are partially offset over time through reduced compliance deviation, lower disruption risk, and improved supplier reliability. In contrast, cost-minimization strategies that underinvest in compliance exhibit higher volatility and increased exposure to regulatory penalties [32].

Importantly, the results identify synergistic regimes in which trade-offs are mitigated. Enhanced visibility and data integration reduce emissions without substantial efficiency loss by enabling optimized routing and energy-aware planning [37]. Similarly, proactive compliance management improves cost stability by reducing corrective actions and supply interruptions. These findings demonstrate that sustainability trade-offs are context-dependent rather than absolute. Integrated strategies that align efficiency, emissions, and compliance objectives outperform fragmented optimization approaches across composite sustainability metrics [35].

7.3 Benchmarking Against Standards

Benchmarking analysis compares machine learning–predicted sustainability performance against established international standards. Alignment with ISO 14001 environmental management principles is evident in scenarios exhibiting systematic emissions monitoring, continuous improvement cycles, and corrective action responsiveness [34]. Models predicting lower carbon intensity and emissions volatility align closely with ISO 14001 expectations regarding environmental performance control.

Comparison with the Greenhouse Gas (GHG) Protocol highlights the framework's consistency in emissions attribution and normalization. Predicted emissions intensities fall within accepted reporting ranges for Scope 1 and Scope 2 activities, while deviations are primarily associated with upstream Scope 3 estimation uncertainty [38]. This alignment supports the credibility of ML-driven emissions evaluation.

OECD due diligence guidelines emphasize risk-based supplier engagement and continuous monitoring. Model predictions related to ethical sourcing risk and compliance deviation correspond closely with these principles, particularly in identifying high-risk supplier clusters requiring enhanced oversight [40]. Benchmark comparison indicates that ML-enabled sustainability evaluation not only meets baseline regulatory expectations but also approximates best-practice performance observed in mature sustainability programs [36].

7.4 Managerial and Policy Implications

The findings carry significant implications for managers and policymakers. For practitioners, the results underscore the importance of adopting integrated sustainability strategies rather than pursuing isolated efficiency or compliance targets. Investments in data integration and analytical capability enhance both environmental and economic performance by reducing uncertainty and enabling proactive decision-making [33]. Managers are encouraged to use ML outputs as decision-support tools to explore trade-offs and test sustainability scenarios before implementation.

From a policy perspective, the results suggest that regulatory frameworks benefit from encouraging data transparency and standardized reporting. Policies that support digital traceability and emissions disclosure reduce compliance costs while improving sustainability outcomes [39]. By aligning regulatory incentives with integrated performance metrics, policymakers can promote sustainable supply chain transformation without imposing disproportionate operational burdens [35].

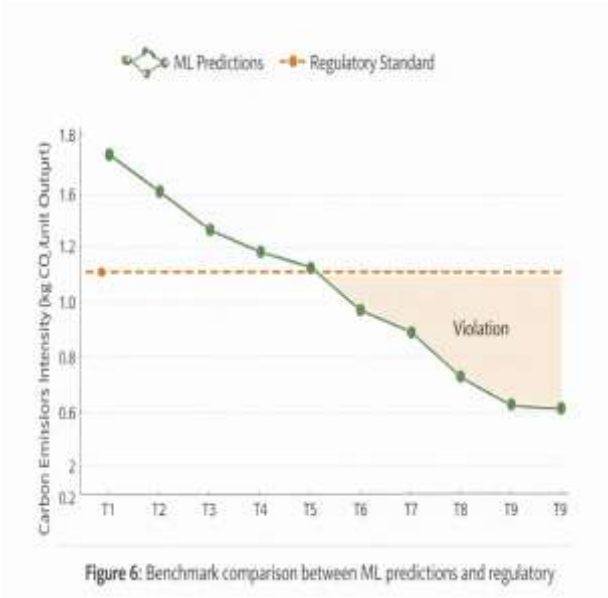

Figure 6: Benchmark comparison between ML predictions and regulatory standards

8. LIMITATIONS AND FUTURE RESEARCH DIRECTIONS

Despite its contributions, the study is subject to several limitations that warrant consideration. Data quality constraints represent a primary challenge. Sustainability data often suffer from reporting inconsistencies, estimation uncertainty, and incomplete coverage across supply chain tiers [37]. Emissions inventories and supplier audit data are particularly susceptible to gaps, which may affect model accuracy and bias sustainability assessments toward more digitally mature partners [32].

Cross-regional regulatory variability presents an additional limitation. Sustainability regulations differ significantly across jurisdictions, creating challenges in standardizing compliance indicators and interpreting deviation metrics [40]. While the framework encodes regulatory context as input variables, rapid policy changes and enforcement variability may reduce temporal stability of learned relationships. This limitation highlights the need for frequent model recalibration in dynamic regulatory environments [34].

Future research may extend the framework through reinforcement learning approaches. Reinforcement learning enables sequential decision-making under uncertainty, allowing sustainability policies to adapt based on observed outcomes rather than static optimization criteria [38]. Such approaches are well suited to supply chains characterized by delayed rewards, cumulative emissions impacts, and evolving compliance landscapes.

Another promising direction involves integration with digital supply chain twins. Digital twins provide virtual representations of physical supply networks, enabling simulation of sustainability interventions without operational risk [36]. Coupling machine learning models with digital twins would support scenario experimentation, stress testing, and real-time calibration, enhancing both predictive accuracy and strategic relevance. These extensions would strengthen the framework's role as a dynamic sustainability decision-support system and expand its applicability across industries and regulatory contexts [39].

Table 3: Summary of Key Findings, Contributions, and Strategic Value of ML-Enabled Sustainability Intelligence

Dimension	Summary Insight	Strategic Significance
Key Findings	Integrated evaluation of ethical sourcing, logistics efficiency, emissions, circularity, and compliance reveals system-level trade-offs and synergies not observable through isolated KPIs or compliance-only assessments.	Enables holistic sustainability diagnosis and avoids unintended consequences arising from fragmented optimization.
Theoretical and Practical Contributions	The study advances sustainability theory by operationalizing multiple sustainability pillars into a unified, data-driven evaluation framework supported by machine learning analytics.	Bridges the gap between conceptual sustainability models and actionable, measurable supply chain design decisions.
Strategic Value of ML-Enabled Intelligence	Machine learning captures nonlinear relationships, predicts performance deviations, and supports scenario-based sustainability decision-making under uncertainty.	Transforms sustainability from a reporting obligation into a source of strategic insight, resilience, and long-term competitive advantage.

9. CONCLUSION

This study has examined sustainable supply chain design through an integrated, data-driven lens, emphasizing the interdependence of ethical sourcing, logistics efficiency, emissions management, circularity, and regulatory compliance. The findings demonstrate that sustainability performance cannot be effectively assessed or improved through isolated metrics or compliance checklists alone. Instead, meaningful and resilient sustainability outcomes emerge when these dimensions are evaluated as a connected system, where decisions in one area propagate across the broader supply chain network. The results confirm that fragmented optimization approaches often generate hidden trade-offs, while integrated evaluation enables more balanced and robust sustainability performance.

From a theoretical standpoint, the study contributes to sustainable supply chain literature by advancing the conceptualization of sustainability as a multidimensional strategic capability rather than a collection of independent objectives. By operationalizing sustainability pillars into quantifiable indicators and combining them within a unified analytical framework, the research bridges the gap between abstract sustainability concepts and measurable operational behavior. The introduction of composite sustainability scoring and trade-off analysis provides a structured way to examine interactions among efficiency, emissions, compliance, and circularity, enriching systems-based perspectives on supply chain sustainability.

In terms of practical contribution, the framework offers managers a structured methodology for diagnosing sustainability strengths, weaknesses, and tensions across end-to-end supply chains. Rather than relying on static benchmarks or retrospective reporting, organizations can use the proposed approach to evaluate alternative design configurations, anticipate sustainability risks, and prioritize interventions with the greatest system-wide impact. The findings highlight that investments in data integration, visibility, and analytical capability often yield compounding benefits, improving environmental performance while stabilizing costs and reducing compliance volatility. This shifts sustainability management from reactive reporting toward proactive strategic planning.

A central contribution of this research lies in clarifying the strategic value of machine learning–enabled sustainability intelligence. Machine learning is shown not merely as a forecasting or automation tool, but as an enabler of integrated sustainability reasoning. By capturing nonlinear relationships, identifying hidden patterns, and quantifying trade-offs across sustainability dimensions, machine learning enhances managerial understanding of complex cause–effect dynamics that are difficult to address through traditional optimization or KPI-based approaches. When embedded within a structured evaluation framework, machine learning supports continuous learning, adaptive decision-making, and scenario exploration under uncertainty.

Overall, the study demonstrates that ML-enabled sustainability intelligence provides a powerful foundation for sustainable competitive advantage. Organizations that leverage integrated analytics to align ethical, environmental, and operational objectives are better positioned to navigate regulatory pressure, stakeholder expectations, and resource constraints. By transforming sustainability from a compliance obligation into a source of strategic insight, the framework

supports the development of supply chains that are not only more sustainable, but also more resilient, transparent, and strategically agile in complex operating environments.

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