

Integration of Green Chemistry and Digital Technology for Sustainable Development and Smart Cities

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ABSTRACT

Sustainable urban development is becoming a global issue due to the rising strain on natural resources, environmental quality, and public health caused by the rapid speed of urbanization and industrialization. An inventive strategy to create resilient, resource-efficient, and ecologically sustainable smart cities is through the integration of digital technology and green chemistry. While digital technologies like artificial intelligence (AI), the Internet of Things (IoT), big data analytics, blockchain, digital twins, geographic information systems (GIS), cloud computing, robotics, and smart sensors enable intelligent monitoring, optimization, and management of urban systems, green chemistry encourages the design of safer chemicals, cleaner production methods, waste minimization, renewable feedstocks, and energy-efficient processes. When combined, these technologies help with pollution control, smart waste management, green transportation, circular economy principles, sustainable water management, and the integration of renewable energy. The Sustainable Development Goals (SDGs) of the United Nations, especially SDGs 3, 6, 7, 9, 11, 12, 13, and 17, are greatly aided by their convergence. This multidisciplinary approach is a key component of future smart and sustainable cities since it not only improves environmental sustainability but also urban governance, industrial competitiveness, and people's quality of life.

Keywords : Artificial Intelligence, Internet of Things, Circular Economy, Industry 4.0, Digital Twins, Sustainable Urban Development, Green Chemistry, Smart Cities, and SDGs

1. Introduction

By 2050, around 70% of the world's population is predicted to live in urban areas, which will raise demand for energy, water, transportation, housing, and industrial production. Innovative solutions that strike a balance between environmental preservation and economic growth are needed to address these issues.

Green chemistry offers environmentally friendly chemical processes that lessen dangerous compounds, preserve resources, and encourage the use of renewable materials. Data-driven urban planning, real-time environmental monitoring, predictive maintenance, and intelligent infrastructure management are all made possible concurrently by digital technologies.

Smart Sustainable Cities, where technology and eco-friendly chemistry collaborate to maximize resource usage, lower pollution, and enhance public health, are built on the integration of various disciplines.

In many different industries, the search for ecologically conscious and sustainable methods has grown in importance. By providing the instruments and information required to comprehend, prevent, and lessen environmental damage, chemistry is one of the important fields in promoting sustainable and ecologically responsible behaviors.

Green chemistry, a field that focuses on creating chemical products and processes that minimize or completely do away with the usage and production of hazardous compounds, is the main example of this link. A key component of creating a more sustainable future is green chemistry (GC), which employs techniques and procedures to minimize or completely eradicate the usage of hazardous materials and the production of hazardous waste. GC strives for economic efficiency, conserving natural resources, and safeguarding human health by giving priority to the creation of chemical products and processes that have less of an impact on the environment.

For example, the following are some significant connections between chemistry and sustainability:

(a) Pollution Prevention: By developing procedures that reduce waste and hazardous byproducts, green chemistry seeks to stop pollution at its source. This reduces the need for costly and energy-intensive waste management and cleanup operations, resulting in cleaner air, water, and soil.

(a) Renewable Resources: Chemistry makes it easier to switch from fossil fuels to renewable resources, such as biomass, for the production of materials, fuels, and chemicals. By decreasing dependency on non-renewable resources and carbon footprints, this shift promotes the growth of a bioeconomy.

(c) Degradable Materials: Scientists employ chemistry to create materials that decompose more readily in the environment or can be recycled effectively, lessening the impact of persistent pollutants like plastics and supporting the circular economy by encouraging material reuse.

(d) Biofuels and Bioenergy: Chemistry propels bioenergy innovation by creating cutting-edge biofuels (such as cellulosic ethanol and biodiesel) and other types of bioenergy, which are crucial for cutting greenhouse gas emissions and moving toward a low-carbon economy.

(e) Energy Solutions: Chemistry plays a significant role in the development of sustainable energy technologies that help lower greenhouse gas emissions and offer cleaner energy options than fossil fuels, such as solar cells, batteries, and fuel cells.

(f) Health applications: Green chemistry principles direct the development of safer goods for both the environment and human health. Chemistry helps create safer consumer goods and a better ecosystem by getting rid of dangerous compounds and lowering hazardous emissions.

It is evident that chemistry makes a wide range of contributions. With an emphasis on efficiency, safety, and reducing environmental effect, the concepts of green chemistry have become a key framework for reinventing the traditional approach to the chemical industry in this context.

In line with the goals of sustainable development, it is crucial to take into account sustainable practices both separately and as part of a larger development landscape.

It is crucial to take into account how smart cities (SC) might act as catalysts for constructive change within the framework of sustainable development. Smart cities are urban places that use data, technology, and creative design to increase sustainability, efficiency, and quality of life. As a practical application of sustainable development principles at the urban level, this category of urban agglomerations focuses on resource optimization, minimizing environmental consequences, and enhancing infrastructure and services. By implementing sustainable practices in energy, transportation, water management, waste management, and other areas, they want to create resilient, habitable, and ecologically friendly urban environments.

Consequently, the degree to which smart cities are in line with the Sustainable Development Goals (SDGs) can be used to gauge their success. Therefore, SC can become true "urban laboratories" by implementing cutting-edge technologies and effective procedures, turning them into areas where social well-being and environmental sustainability coexist.

The Sustainable Development Goals arose in a 21st-century setting that already prioritizes sustainability and the reinforcement of its three pillars (economic, social, and environmental). In this case, PGCs can be viewed as the foundation for more ethical and sustainable uses in addition to being seen from a restorative perspective.

Smart city evaluation indicators are standardized by the ISO 37122 standard. The integration of PGCs with the SDGs and the ISO 37122 indicators is the topic of this work. Therefore, integrating the Sustainable Development Goals with the principles of green chemistry (PGCs) becomes a crucial tactic to encourage important sustainable advancements. In this regard, it's critical to find indicators that can track cities' advancement through PGC-based actions. These metrics can help evaluate how adopted behaviors affect society and the environment.

Therefore, the goal of this research is to investigate how green chemistry can be used strategically to help achieve the Sustainable Development Goals. Our goal is to examine how applying its ideas can support particular SDG goals. Furthermore, we aim to identify and debate smart city indicators that could be impacted by implementing PGC-based sustainable practices. Our objective is to investigate the potential benefits of this integration for urban environmental behavior. However, as an additional goal, this study will assess Curitiba City's (PR) performance, which was named the world's smartest city in 2023. We will evaluate its standing and ratings in the Ranking Connected Smart Cities report, paying special attention to initiatives that have received recognition on a global scale for sustainability in line with PGCs.

Components of Integration

Green Chemistry Approach	Enabling Technology	Digital Contribution to Smart and Sustainable Cities
Renewable raw materials	Artificial Intelligence (AI)	Promotes environmentally responsible manufacturing systems
Low-energy chemical processes	Internet of Things (IoT)	Facilitates intelligent energy monitoring and management
Environmentally benign solvents	Digital Twin technology	Enhances process simulation, monitoring, and optimization
Waste minimization strategies	Big Data Analytics	Improves resource efficiency and operational performance
Catalytic and sustainable reactions	Robotics and Automation	Supports precise, safe, and eco-efficient production
Development of safer chemical products	Smart Sensors	Enables continuous environmental and pollution monitoring
Biodegradable and eco-friendly materials	Blockchain	Strengthens transparent and sustainable supply chain management
Circular chemical systems	Geographic Information Systems (GIS) and Remote Sensing	Assists in sustainable environmental assessment and urban planning

2. Methodology

We suggest a responsible roadmapping approach and examine its application in three distinct scenarios within the field of green chemistry in order to investigate whether and how it can aid in the development of broad research and innovation agendas that address technical, environmental, as well as social, ethical, economic, aspects in the complex transformations of industrial sectors.

Table for Data for roadmapping approach

System Component	Functional Objective	IoT / AI Methodology	Operational Benefit
Smart Bins / Cyber-Physical Assets	Real-time telemetry and fill monitoring	Sensor-mesh networks (ultrasonic sensors, GPS, NB-IoT/LoRaWAN)	Elimination of manual monitoring and increased transparency
Route Optimization Engine	Dynamic logistics scheduling and network efficiency	Graph-theoretic optimization (weighted bin networks and centrality measures)	Reduced fuel usage and decreased carbon emissions
Geospatial Risk Mapping	Geographic prioritization and hotspot detection	Spatial interpolation and risk scoring (heatmaps)	Targeted interventions in high-density zones
Waste Management Sensors	Methane monitoring and overflow prediction	Methane monitoring sensors and XBee wireless mesh	Reduction in fuel usage by eliminating unnecessary truck rolls
IoT / AI Methodology	Predictive Maintenance	Sensors for mass data collection, customized algorithms, and automated ticket systems	Increase plant availability and reduce total maintenance costs
Green Materials Discovery	Biodegradable plastic decomposition	AI-driven analysis of 100,000 polymers	Faster decomposition compared to conventional polymers
Supply Chain / Warehousing	Advanced Inventory Management	Real-time optimization via sensors and robotics	Reduction in storage costs
Manufacturing / Research	Digital Twin / Smart Plant	3D virtualization, simulation algorithms, and mass data aggregation	Risk-free simulation of plant conditions and reduced product introduction costs
Solvent Selection	Prediction of eco-friendly solvents	ML models	Decreased hazardous waste and reduced hazardous solvent use
Sales and Marketing	Demand-driven production / Advanced Forecasting	Mass data-based forecasting (historical, social media, and external economic data)	Reduced forecasting errors and optimized safety stock
Process Optimization	Pharmaceutical synthesis and biofuel production optimization	AI-driven optimization and implementation	Reduced energy consumption and increased biofuel yield
Logistics	Connected Logistics	Industrial Internet of Things (IIOT) platform, track-and-trace, and autonomous driving	Reduced waiting times and optimized material flow

Catalyst Design	Hydrogen production efficiency	AI-designed catalysts	Improved reaction efficiency and reduced energy consumption
Water Distribution Grid	Leak detection and proactive maintenance	Internet of Things (IoT), AI, and predictive analytics	Early detection of leaks and improved system efficiency
Urban Infrastructure Management	Dynamic allocation and real-time monitoring	IoT sensors and data analytics for demand forecasting	Optimized water distribution and reduced waste
Traffic Flow Management Systems	Urban emission reduction	IoT mesh connectivity for traffic management	Massive reduction in vehicle emissions and cleaner air
Municipal Water Treatment	Contamination control and overflow prevention	Digi Connect Sensor + and Remote Manager	Prevention of overflows and environmental compliance
Toxic Gas Detection Systems	Predictive detection of contaminants	IoT-enabled gas concentration sensors	Automated shut-off of valves and chemical mitigation



Mind map for Different stages

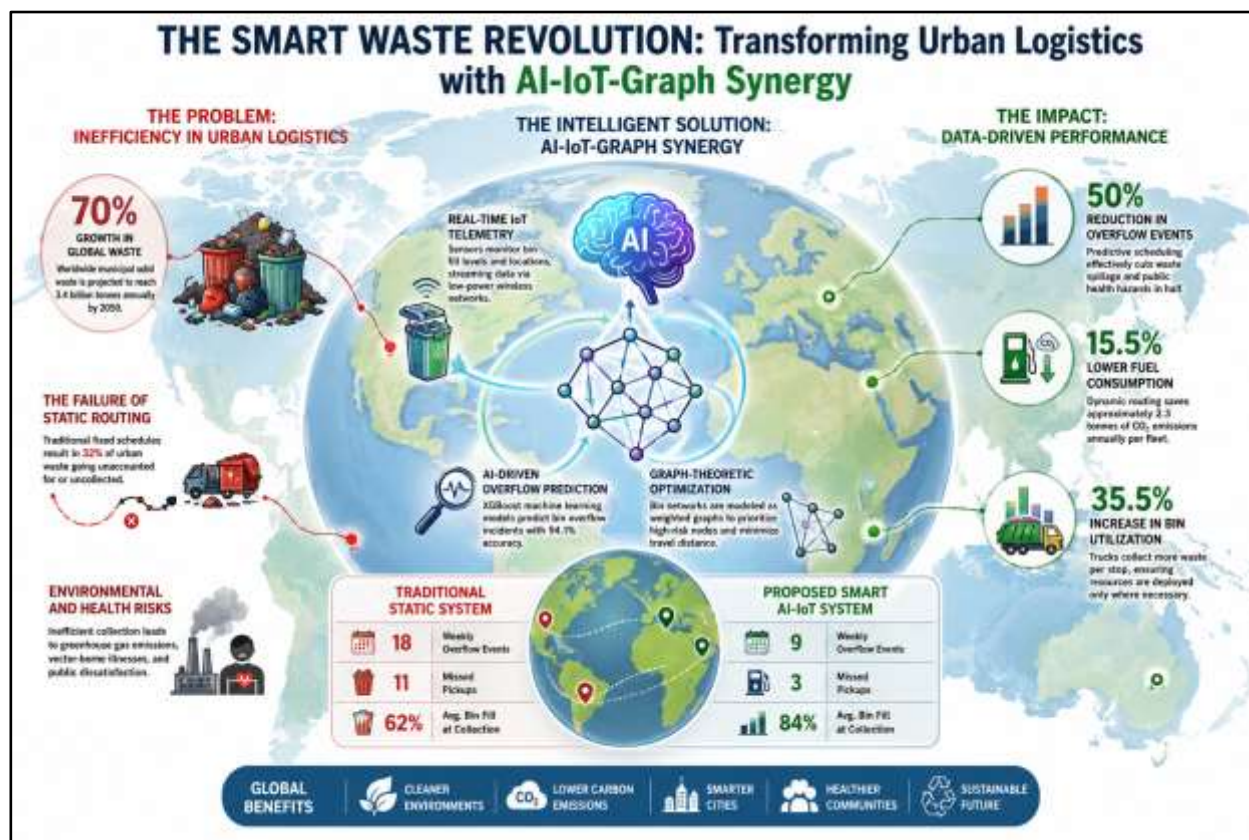


Diagram for Digital-Green Transformation and AI-IoT-Graph Synergy in Urban Systems

3. Data Analysis and Results

By taking socio-ethical, policy, and economic factors into account, the researchers also discovered factors that go beyond the 12 principles of green chemistry. In light of socio-ethical considerations, industry, wastewater treatment plant operators, and cities will be consulted in order to address the issue of future users' approval of the novel materials. An innovation system analysis and the identification and cooperation of regulatory specialists will be used to address policy issues such as the legislation of innovative materials. By evaluating the costs already in the early phases of their R&D process, economic considerations, that is, financial viability and competitiveness in comparison to alternative water treatment materials and processes—will be examined.

The "digital-green dual transformation" is being used in sustainable chemistry, energy conservation, and air and water quality monitoring in addition to waste logistics. The Sustainable Development Goals (SDGs) of the United Nations are in line with these developments, especially SDGs 11 (Sustainable Cities) and 12 (Responsible Consumption). A multi-layered strategy is necessary for success in various domains:

1. Technological Integration: Real-time sensing and decision-making using Cyber-Physical Systems (CPS) and machine learning (e.g., XGBoost).
2. Structural Optimization: Using graph theory to control intricate metropolitan networks.
3. Policy Alignment: Integrating digital-green planning to manage biodiversity preservation and low-carbon development.

AI-IoT-Graph Framework for Smart Waste Management - Static routing and human monitoring are features of traditional municipal solid waste (MSW) systems that result in inefficiencies and hazards to public health. These are replaced with an integrated, scalable design in the suggested smart waste management system (SWMS).

1.1 Predictive analytics and methodology - Predictive models are trained by the framework using simulated smart bin telemetry in five urban zones.

* Predictive Engine: To handle structured tabular data, the system uses the XGBoost classifier, which was selected for its efficiency, accuracy, and transparency (interpretability).

* Performance Metrics: High-risk (overflow-prone) bins are rarely overlooked thanks to the AI model's 91.7% precision and 95.8% recall.

* Spatial Intelligence: Municipal planners can identify high-density overflow zones and service shortfalls by using heatmaps for risk mapping.

1.2 Optimization via Graph Theory - The system models the urban bin network as a directed, weighted graph $G = (V, E)$ in order to go beyond simple prediction.

* Nodes (V): Show smart bins with risk ratings and centrality metrics.

* Edges (E): Show routes that are prioritized for overflow, congestion fines, and distance.

* Multi-Objective Function: Optimization tries to decrease total journey distance and missed pickups while maximizing the prioritizing of high-risk nodes.

1.3 Impact on Comparative Operations - Significant improvements were found in a benchmarking study that contrasted the smart system with conventional static scheduling:

Metric Improvement with Smart System Overflow Events -50.0%

Missed Pickups -72.7% Average Bin Fill at Collection +35.5% Fuel Consumption -15.5% Labor Man-hours -41.7%

2. IoT-Powered Clean Technology and Environmental Monitoring - By using edge computing, remote connectivity, and sensor deployment, the use of IoT for environmental stewardship expands to more extensive ecological protection.

2.1 Essential Components of Monitoring

Four pillars are necessary for IoT environmental systems to be successful:

1. Monitor: Sensors installed in water systems, industrial facilities, or fields.
2. Measure: Evaluating data points for leaks, failure, or impact.
3. Catalog: Utilizing cloud/data centers to store enormous datasets (e.g., Microsoft Planetary Computer).
4. Insight: Data delivery for actionable warnings into software platforms (like Azure and AWS).

2.2 Important Use Cases

* Water Quality: Contamination and pH levels in stormwater, municipal treatment, and agricultural irrigation are analyzed in real time.

* Air Quality: Monitoring toxic particulates, carbon monoxide, and methane to help with urban planning and lessen the effects of industry.

* Energy Conservation: Using renewable energy integration to stabilize the power system and avoid energy usage spikes.

* Toxic Gas Detection: Recognizing flammable or corrosive gases (such CO or H₂S) in petrochemical and refinery settings to initiate automated system shutdowns.

3. The Digital-Green Transition and Sustainable Chemistry - The development of "Sustainable Chemistry," a more comprehensive idea than conventional "Green Chemistry," reflects the move toward sustainable urban systems.

3.1 The Holistic Framework - Green chemistry is usually guided by 12 principles (developed in 1998), while sustainable chemistry addresses broader scientific and social elements.

- * Objectives: The UN Environment Programme (UNEP) has created 10 objectives to steer innovation, ensuring chemistry is compatible with the 2030 Sustainable Development Agenda.

- * Dual Transformation: "Sustainable Smart City" planning is becoming more and more popular. This integrates eco-friendly construction and effective transportation with low-carbon economic development.

3.2 Suggestions for Scale-Up Policies - Stakeholders must do the following in order to accomplish a "people-centered" digital and green transformation:

- * Mandate Smart Infrastructure: In high-density locations, smart bins and sensors must be installed.

- * Encourage contractors to embrace AI-driven solutions by offering tax rebates or performance-based bonuses.

- * Enhance Data Governance: Create thorough digital privacy and transparency by using real-time dashboards that are visible to the public.

4. Integration and Synergies in Industry 4.0 - These technologies come together to form a Cyber-real System (CPS), which is a closed-loop feedback system in which digital infrastructure and the real world interact.

4.1 AI Modeling Technique Comparison

Although XGBoost is given priority in the framework under study, other deep learning models, such as LSTM (Long Short-Term Memory), have distinct benefits for overflow prediction:

4.2 Advantages for the Socio-Environment - There are measurable benefits to integrating these frameworks:

- * Health: Lower overflows lessen odors and vector-borne diseases.

- * Emissions: An estimated 2.3 tonnes of CO₂ emissions are reduced annually in the trash sector alone for every 15.5% reduction in fuel consumption.

- * Economic: The initial investment in smart technology is justified by the reduction of overflow penalties (estimated at 60%) and operational man-hours (41.7%).

5. Restrictions and Prospects - Current frameworks encounter a number of difficulties despite their great prediction success:

- * Simulated vs. Real-World Data: A lot of research is based on simulated settings, which could not accurately reflect the complexity of mixed land use or the diversity of human behavior.

- * Urban Barriers: One-way streets, real-time traffic congestion, and physical accessibility barriers are frequently left out of current graph-theoretic models in order to simplify routing.

- * Contextual Gaps: To improve model robustness, future iterations must take into account contextual factors including public events, seasonal variations, and demographic changes.

In the end, a circular economy is made possible by the shift from reactive to intelligent urban systems, which move away from linear disposal models and toward resource recovery and sustainable urban living.

4. Conclusion

To sum up, chemical products and processes may be crucial in facilitating the shift to more sustainable manufacturing methods, promoting the circular economy, and tackling the SDGs. Green chemistry seeks to minimize and eradicate dangerous compounds while advancing human and environmental health, resource conservation, and economic sustainability. By proposing how to apply the responsible roadmapping technique to include the ideas of responsible research and innovation into green chemistry practices, this work closes a significant gap. Different action plans for trans- and inter-disciplinary research and responsible innovation were produced by applying this strategy to three research projects that focused on safer and more sustainable production methods. By adding pertinent social, ethical, political, legal, and/or economic elements, the interdisciplinary roadmapping process broadened the plans' scope. The study shows that by employing responsible roadmaps, researchers can be empowered to plan how to maximize the positive effects of their research and innovation while minimizing risks and bad effects, and to accept responsibility for co-creating sustainable futures through their R&D efforts.

Urban infrastructure is changing from reactive, static models to predictive, robust, and sustainable systems through the integration of Industry 4.0 technologies, particularly Artificial Intelligence (AI), the Internet of Things (IoT), and graph-theoretic optimization. An AI-IoT-graph architecture may reach a 94.1% predictive accuracy for bin overflows, resulting in a 50% decrease in overflow events, a 72.7% decrease in missed pickups, and a 15.5% reduction in fuel usage, according to a key case study in smart waste management.

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