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Development of an Optimization Model for the Identification of Sources of Organic Atmospheric Pollutants

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Dedication

in the name of ALLAH, the Most Gracious, the Most Merciful.

To my beloved mother, for her endless love and prayers.

To my father, for his strength, sacrifices, and support.

To my brothers and sisters, for their encouragement and kindness.

To my nephews and nieces, my family, and my dear friends, for their love, support, and beautiful memories.

To my teachers, for the knowledge they shared.

And to every silent soul who supported me along the way.

I dedicate this humble achievement to you all.

Aridj

Dedication

in the name of ALLAH, the Most Gracious, the Most Merciful.

To my beloved mother, whose sincere prayers, endless sacrifices, boundless patience, and unwavering support have been the source of my strength and perseverance. May God protect her and reward her abundantly for all her efforts.

To my dear father, who worked tirelessly and made countless sacrifices to provide me with the best conditions for success. May God bless him with health, happiness, and a long life.

To my sister, my support and companion, who always believed in me and stood by my side during the most difficult moments.

To my brothers, for their love, encouragement, and constant support throughout my journey.

To a precious person whose support, encouragement, and presence have been a source of motivation and strength.

To everyone who contributed, directly or indirectly, to the completion of this dissertation.

With all my gratitude, love, and appreciation.

DEHBIA

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Abstract

This study addresses the development of a mathematical and optimization model for identifying the sources of organic atmospheric pollutants in the city of Ouargla, based on environmental modeling and simulation techniques. The study focuses on volatile organic compounds (VOCs), polycyclic aromatic hydrocarbons (PAHs), and wax compounds (WAX), which are used as indicators for distinguishing biogenic and natural pollution sources. In addition, mass conservation equations, Monte Carlo simulation techniques, and the Particle Swarm Optimization (PSO) algorithm were employed to analyze pollutant transport and estimate the contribution of different pollution sources. The results revealed that traffic emissions and indoor pollution sources represent the major factors influencing health risks associated with air pollution. The study also demonstrated the effectiveness of CPI and WAX indicators in differentiating between natural and petroleum-related pollution sources. Furthermore, improving ventilation and reducing traffic-related emissions were shown to significantly enhance air quality and mitigate the environmental and health impacts associated with atmospheric pollution.

Keyword: Air Pollution, Organic Atmospheric Pollutants, Volatile Organic Compounds Polycyclic Aromatic Hydrocarbons, Modeling and Simulation, Monte Carlo Method, Particle Swarm Optimization , Source Apportionment, Air Quality, Ouargla.

Résumé

Cette étude porte sur le développement d’un modèle mathématique et d’optimisation visant à identifier les sources des polluants organiques dans l’atmosphère de la ville de Ouargla, en s’appuyant sur des techniques de modélisation et de simulation environnementale. Elle se concentre sur l’étude des composés organiques volatils (COV), des hydrocarbures aromatiques polycycliques (HAP), ainsi que des composés cireux (WAX) utilisés comme indicateurs pour déterminer les sources biogéniques et naturelles des polluants. L’étude repose également sur les équations de conservation de la masse, les techniques de simulation de Monte Carlo et l’algorithme d’optimisation PSO afin d’analyser le transport des polluants et d’estimer la contribution des différentes sources de pollution. Les résultats ont montré que les émissions liées au trafic routier et les sources intérieures constituent parmi les principaux facteurs influençant les risques sanitaires associés à la pollution atmosphérique. L’étude a également démontré l’efficacité des indices CPI et WAX dans la distinction entre les sources naturelles et pétrolières des polluants. De plus, l’amélioration de la ventilation et la réduction des émissions du trafic contribuent de manière significative à l’amélioration de la qualité de l’air ainsi qu’à la diminution des impacts sanitaires et environnementaux liés à la pollution atmosphérique.

Mots-clés : Pollution de l’air, polluants organiques atmosphériques, composés organiques volatils, hydrocarbures aromatiques polycycliques , modélisation et simulation, méthode de Monte Carlo, optimisation par essaim particulaire , identification des sources de pollution, qualité de l’air, Ouargla.

ملخص

تتناول هذه الدراسة تطوير نموذج رياضي وتحسيني لتحديد مصادر الملوثات العضوية في الغلاف الجوي بمدينة ورقلة، بالاعتماد على تقنيات النمذجة والمحاكاة البيئية. وتركّز على دراسة المركبات العضوية المتطايرة (VOCs)، والهيدروكربونات العطرية متعددة الحلقات(PAHs) ، إضافة إلى مركبات الشمع (WAX) المستخدمة كمؤشر لتحديد المصادر البيوجينية والطبيعية للملوثات. كما تعتمد الدراسة على معادلات حفظ الكتلة، وتقنيات محاكاة مونتي كارلو، وخوارزمية التحسين. PSO لتحليل انتقال الملوثات وتقدير مساهمة مصادر التلوث المختلفة .وقد أظهرت النتائج أن الانبعاثات المرورية والمصادر الداخلية تُعد من أبرز العوامل المؤثرة في المخاطر الصحية المرتبطة بتلوث الهواء. كما بيّنت الدراسة فعالية مؤشري CPI و WAXفي التمييز بين المصادر الطبيعية والبترولية للملوثات، إضافة إلى أن تحسين التهوية وتقليل الانبعاثات المرورية يساهمان بشكل ملحوظ في تحسين جودة الهواء والحد من التأثيرات الصحية والبيئية المرتبطة بتلوث الغلاف الجوي.

الكلمات المفتاحية: تلوث الهواء، الملوثات العضوية الجوية، المركبات العضوية المتطايرة ، الهيدروكربونات العطرية متعددة الحلقات، النمذجة والمحاكاة، مونت كارلو، خوارزمية سرب الجسيمات تحديد مصادر التلوث، جودة الهواء، ورقلة.

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Abbreviations

CDF: Cumulative Distribution Function

COPD: Chronic Obstructive Pulmonary Disease

CPI: Carbon Preference Index

DOE: Design of Experiments

ECDF: Empirical Cumulative Distribution Function

EPA: Environmental Protection Agency

F(r): Cumulative Distribution Function

f(x): Probability Density Function

I/O: Indoor/Outdoor Ratio

MAE: Mean Absolute Error

M&S: Modeling and Simulation

μ: Mean (average) of a distribution

n: Number of samples

PAHs: Polycyclic Aromatic Hydrocarbons

PDF: Probability Density Function

$PM_{2.5}$: Particulate Matter with diameter ≤ 2.5 μm

PM_{10}: Particulate Matter with diameter ≤ 10 μm

PSO: Particle Swarm Optimization

r(XY): Pearson Correlation Coefficient between variables X and Y

RMSE: Root Mean Square Error

SPM: Suspended Particulate Matter

σ: Standard Deviation

V&V: Verification and Validation

VOCs: Volatile Organic Compounds

WAX: High Molecular Weight Wax Compounds

WHO: World Health Organization

$\bar{x}$ / $\bar{y}$: Sample Means

General Introduction:

Air pollution is considered one of the most prominent contemporary environmental challenges, as it is classified among the greatest environmental threats to human health worldwide. According to the World Health Organization, ambient and household air pollution together cause seven million premature deaths annually, making it more deadly than a combination of diseases including malaria, tuberculosis, and AIDS. In this context, the need has emerged to develop methodological and scientific tools capable of understanding this complex phenomenon, predicting its evolution, assessing its impacts, and proposing effective measures to reduce its harmful effects.

Modeling and simulation constitute two fundamental methodologies in modern scientific and engineering research, as they enable the representation, analysis, and understanding of complex systems without direct intervention in them. A model is defined as an abstract representation of a real system that captures its essential characteristics while simplifying less important details, and it can be expressed through mathematical equations, logical rules, or computational structures. Simulation, on the other hand, is defined as the dynamic execution of the model over time in order to study the behavior of the system under different conditions, thereby allowing virtual experiments to be conducted at lower cost and without the risks associated with real-world experiments.

The importance of modeling and simulation in the field of air pollution is reflected in their ability to represent pollutant emissions from various sources, track their dispersion pathways in the atmosphere, estimate their concentrations across space and time, and evaluate their impacts on human health and the environment. These models take into account a range of influencing factors including wind speed and direction, temperature, humidity, altitude, topography, and the chemical reactions undergone by pollutants during their transport in the atmosphere.

The air pollutants studied in this context vary and include gases such as carbon monoxide, sulfur dioxide, and nitrogen oxides, as well as volatile organic compounds such as benzene and toluene, alkanes, and polycyclic aromatic hydrocarbons, which are characterized by their significant health hazards due to their toxicity and carcinogenic and mutagenic effects. Each of these pollutants possesses specific physical and chemical properties that influence its behavior in the atmosphere, thereby requiring the development of specialized models tailored to each type individually.

This thesis aims to provide a comprehensive theoretical framework integrating the concepts of modeling and simulation on one hand with air pollution sciences on the other. Different types and classifications of models, the life cycle of simulation model development, and the concepts of verification and validation as essential steps to ensure the credibility of results will be reviewed, along with the computational tools used in this field. This theoretical framework constitutes the basis for practical applications in subsequent chapters, particularly in modeling the evolution of atmospheric pollutant c7oncentrations while considering the specific desert climatic conditions of the study area.

Chapter I: General information of air pollution

I.1 Introduction:

Environmental pollution refers to the introduction of harmful substances or forms of energy into the environment at levels capable of causing adverse effects on human health, ecosystems, and natural resources. Pollution may affect air, water, and soil, leading to environmental degradation and disturbances in ecological balance. Rapid industrialization, urbanization, and technological development have significantly increased the emission of pollutants into the environment, making pollution one of the most serious global environmental challenges of the modern era. In particular, chemical pollution has become a major concern due to the widespread release of hazardous substances from industrial and anthropogenic activities, which negatively impact living organisms and environmental quality. Consequently, international organizations and governments have adopted various environmental regulations and sustainable development strategies to reduce pollution and protect environmental health. [1, 2]

I.2 Forms of pollution:

The major forms of pollution include soil pollution, water pollution, and air pollution.

I.2.1. Soil pollution:

Soil pollution refers to the degradation of soil quality caused by the accumulation of harmful chemicals, waste materials, and other contaminants. Healthy soil contains microorganisms such as bacteria and fungi that help decompose organic matter and maintain nutrient cycling necessary for plant growth. Excessive use of pesticides, fertilizers, and industrial chemicals may reduce soil fertility and negatively affect agricultural productivity and ecosystem stability. [3]

I.2.2. Water pollution:

Water pollution occurs when contaminants are introduced into water bodies such as rivers, lakes, seas, and groundwater, making the water unsuitable for human consumption and aquatic life. Pollutants may include chemicals, waste materials, heavy metals, microorganisms, and organic compounds. Water pollution can result in serious environmental and health problems due to the persistence and toxicity of many pollutants, particularly non-biodegradable substances. (5)

I.2.3. Air pollution:

Air pollution is considered one of the greatest environmental threats to human health worldwide. According to the World Health Organization, exposure to ambient and household air pollution is responsible for millions of premature deaths annually. Air pollution results from the presence of harmful gases, particulate matter, and biological contaminants in the atmosphere at concentrations that may adversely affect human health, ecosystems, and climate. Major pollutants include particulate matter ($PM_{2.5}$ and PM_{10}), nitrogen oxides (NOx), sulfur dioxide (SO_2), carbon monoxide (CO), ozone (O_3), and volatile organic compounds (VOCs). Long-term exposure to these pollutants has been associated with respiratory diseases, cardiovascular disorders, lung cancer, and environmental degradation .[1, 4]

I.3 Pollutants:

Air pollution is generally caused by gaseous pollutants such as ozone (O_3), nitrogen dioxide (NO_2), sulfur dioxide (SO_2), and carbon monoxide (CO), in addition to particulate matter, especially particles smaller than 2.5 μm in diameter ($PM_{2.5}$). In recent decades, reductions in indoor air pollution have contributed to a decline in global mortality associated with air pollution. However, outdoor particulate matter and ozone pollution continue to pose serious environmental and public health concerns. [2, 5]

I.3.1. Primary Pollutants:

Primary air pollutants are substances directly emitted into the atmosphere from natural or anthropogenic sources without undergoing chemical transformation. Examples include carbon monoxide (CO), carbon dioxide (CO_2), methane (CH_4), volatile organic compounds (VOCs), ammonia (NH_3), sulfur dioxide (SO_2), and nitric oxide (NO). [5]

I.3.2. Secondary Pollutants:

Secondary air pollutants are not emitted directly into the atmosphere but are formed through chemical reactions between primary pollutants, often in the presence of sunlight. Examples include ozone (O_3), nitric acid (HNO_3), sulfuric acid (H_2SO_4), sulfates (SO_4^{2-}), and secondary particulate matter (PM) . [5, 6]

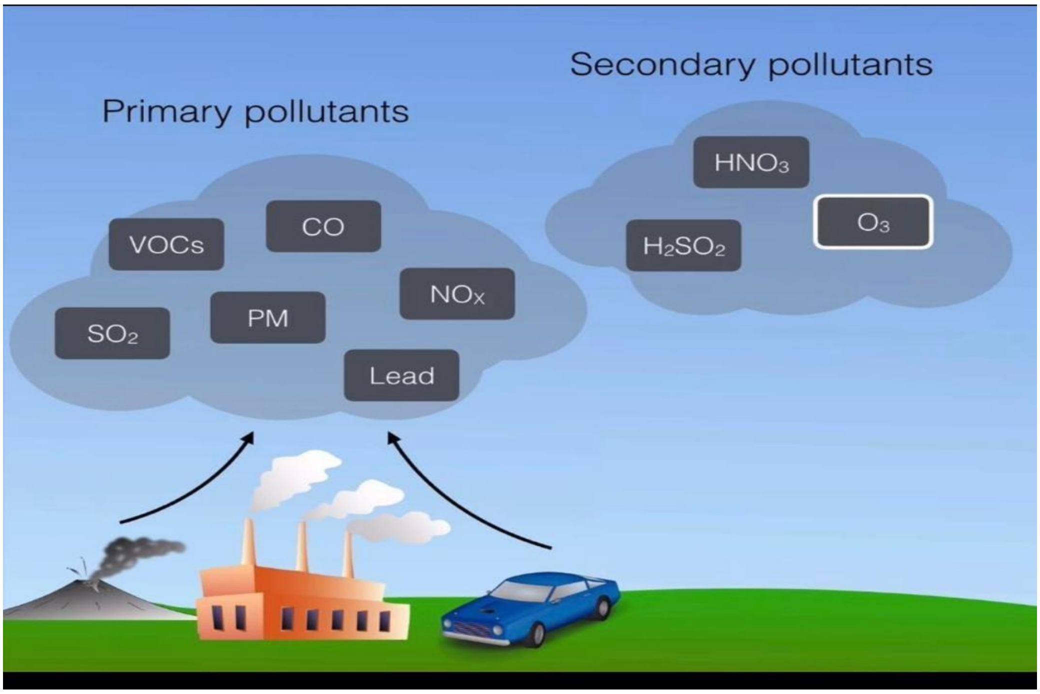

Figure (I. 1): Two Types of pollution.

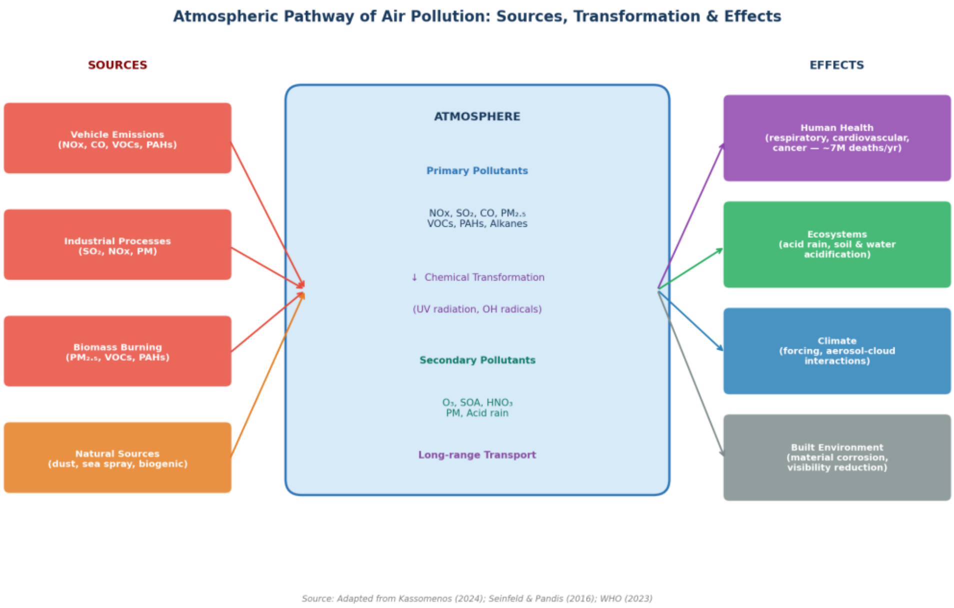

Figure (I. 2): Atmospheric pathway of air pollution.

I.3.3. Sources:

Air pollution originates from both natural and anthropogenic sources. In some cases, pollutants emitted from one region may be transported by atmospheric currents to distant locations, making it difficult to identify the original source. [5]

I.3.3.1 Natural Sources:

Natural sources of air pollution originate from environmental processes that occur without human intervention. These sources include volcanic eruptions, forest fires, dust storms, sea spray, biological decomposition, and emissions from vegetation. Although natural emissions can significantly affect air quality under certain conditions, their impacts are generally temporary and regulated by natural environmental cycles. [5, 6]

I.3.3.2 Anthropogenic Sources:

Anthropogenic sources are human-generated activities that release pollutants into the atmosphere. These sources are considered the primary contributors to modern air pollution due to rapid industrialization, urban growth, transportation, and energy consumption. Major anthropogenic sources include industrial emissions, fossil fuel combustion, vehicle exhaust, agricultural practices, waste incineration, and the use of chemical products such as solvents, paints, and aerosols. These activities contribute significantly to atmospheric contamination and environmental imbalance. [2, 5]

A. Stationary Sources :

These include emissions from power plants, factories, industrial facilities, waste incinerators, and domestic heating systems that burn fossil fuels.

B. Mobile Sources :

Mobile sources include cars, trucks, buses, motorcycles, ships, boats, and aircraft that release pollutants through fuel combustion.

C. Agricultural and Forestry Practices:

Agricultural activities contribute to air pollution through the use of pesticides, fertilizers, biomass burning, and livestock emissions. Forestry practices such as controlled burning may also release pollutants into the atmosphere.

D. Household and Consumer Products :

Household products such as paints, varnishes, cleaning agents, aerosol sprays, cosmetics, adhesives, and solvents release volatile organic compounds (VOCs) into indoor and outdoor environments.

I.3.4. Volatile Organic Compounds (VOCs):

I.3.4.1 Definition:

Volatile Organic Compounds (VOCs) are a large group of carbon-containing organic chemicals characterized by high vapor pressure and low boiling points, allowing them to evaporate easily into the atmosphere at ambient temperature. VOCs originate from both natural and anthropogenic sources, including vegetation, industrial activities, fuel combustion, vehicle emissions, paints, solvents, and household products. These compounds play an important role in atmospheric photochemical reactions and contribute to the formation of ground-level ozone and photochemical smog. Some VOCs are also associated with toxic, carcinogenic, and mutagenic health effects. [7-10]

I.3.4.2 Indoor and Outdoor Sources:

Several studies have identified hazardous VOCs commonly present in indoor environments, including benzene, formaldehyde, acrolein, acetaldehyde, vinyl chloride, and 1,3-butadiene. Indoor VOC concentrations are strongly influenced by human activities such as cooking, smoking, cleaning, and the use of household chemicals. Additional sources include building materials, furniture, paints, adhesives, air fresheners, and poor ventilation.

Outdoor VOC pollution mainly originates from industrial emissions, fuel combustion, petroleum refining, and vehicle exhaust. Outdoor pollutants may infiltrate indoor environments and contribute significantly to indoor air contamination. [8, 10, 11]

I.3.5. Alkanes:

Alkanes are saturated hydrocarbons composed exclusively of carbon and hydrogen atoms linked by single covalent bonds. In the atmosphere, several alkanes are classified as volatile organic compounds (VOCs) and are emitted mainly from fossil fuel combustion, petroleum industries, natural gas leakage, and vehicle exhaust emissions. Although alkanes are generally less chemically reactive than unsaturated hydrocarbons, they contribute indirectly to air pollution through atmospheric oxidation reactions that promote the formation of ozone and photochemical smog. Continuous exposure to alkane-related emissions may negatively affect both environmental quality and human health. [8, 12, 13]

I.3.6. Polycyclic Aromatic Hydrocarbons (PAHs):

Polycyclic Aromatic Hydrocarbons (PAHs) are a group of organic pollutants composed of multiple fused aromatic rings. They are primarily generated during the incomplete combustion of organic materials such as coal, petroleum, gasoline, wood, tobacco, and waste. PAHs are commonly detected in vehicle exhaust emissions, industrial smoke, and urban atmospheric pollution. Many PAHs are toxic, persistent, mutagenic, and carcinogenic, posing serious risks to both human health and the environment. [14-16]

I.4 Health and Environmental Effects of Air Pollution:

Air pollution has significant impacts on both human health and the environment, affecting ecosystems, climate, biodiversity, and living organisms worldwide.

I.4.1. Health Effects:

Air pollution represents a major environmental and public health concern because airborne pollutants can adversely affect the human body following short-term or long-term exposure. Polluted air may irritate the respiratory tract, reduce lung function, and contribute to the development of chronic diseases. The severity of these effects depends on the type of pollutant, its concentration, and the duration of exposure.

Examples of diseases associated with air pollution include:

- Asthma
- Bronchitis
- Lung cancer
- Cardiovasculaire diseuses
- Chronic obstructive pulmonary disease (COPD). [1, 17, 18]

I.4.2. Environmental Effects:

Air pollution has significant environmental consequences that affect ecosystems, climate, water resources, and biodiversity. Emissions of sulfur dioxide (SO_2) and nitrogen oxides (NOx) contribute to the formation of acid rain, which damages forests, soil, freshwater ecosystems, and buildings. In addition, greenhouse gases and atmospheric pollutants intensify the greenhouse effect, leading to global warming and climate change. Air pollutants can also reduce visibility, contaminate water and soil, and disturb ecological balance by affecting plant growth and animal life. [19-21]

Table (I.1): Gaseous air pollutants: their sources and effects

Pollutant	Source	Harmful effects
Carbon compounds (CO, CO2)	Automobile exhaust, burning of wood and coal	Respiratory problems; CO_2 contributes to the greenhouse effect and global warming
Sulphur compounds (SO_2, H_2S)	Power plants, oil refineries, volcanic eruptions	Respiratory diseases in humans; chlorosis (loss of chlorophyll in plants); acid rain formation
Nitrogen compounds (NO, N_2O)	Motor vehicle exhaust, atmospheric reactions	Irritation of eyes and lungs; reduced plant productivity; acid rain; corrosion of metals and stones
Hydrocarbons (benzene, ethylene)	Automobile emissions, petroleum industries	Respiratory problems; carcinogenic (cancer-causing) effects
SPM (Suspended Particulate Matter)	Thermal power plants, construction activities, metallurgical processes, automobiles	Respiratory disorders; reduced visibility; asthma aggravation; cancer risk; formation of smog

Chapter II: Modeling and Simulation of Atmospheric Pollution

II.1 Introduction:

Modeling and simulation (M&S) constitute essential methodologies in modern engineering and scientific research, serving to represent, analyze, and understand complex real-world systems. A model is defined as an abstract representation of a system that captures its essential characteristics while deliberately simplifying less important details. Models can be expressed using mathematical equations, logical rules, or computational structures [22].

Simulation refers to the dynamic execution of a model over time to study system behavior under varying conditions. This approach enables researchers to conduct experiments in a virtual environment, substantially reducing costs, time, and risks associated with real-world experimentation [23, 24].

According to Zeigler et al. (2019), the fundamental premise of simulation lies in its ability to mimic system behavior without direct interaction with the actual system. [25]

The integration of modeling and simulation provides a powerful framework for prediction, optimization, and decision-making across engineering disciplines. These techniques find extensive application in environmental sciences, chemical engineering, physics, economics, and computer science [26]. In the specific context of environmental applications—such as air pollution studies—modeling and simulation are employed to predict pollutant dispersion, estimate concentration levels, and evaluate the environmental impacts of emission sources prior to implementing mitigation strategies [27].

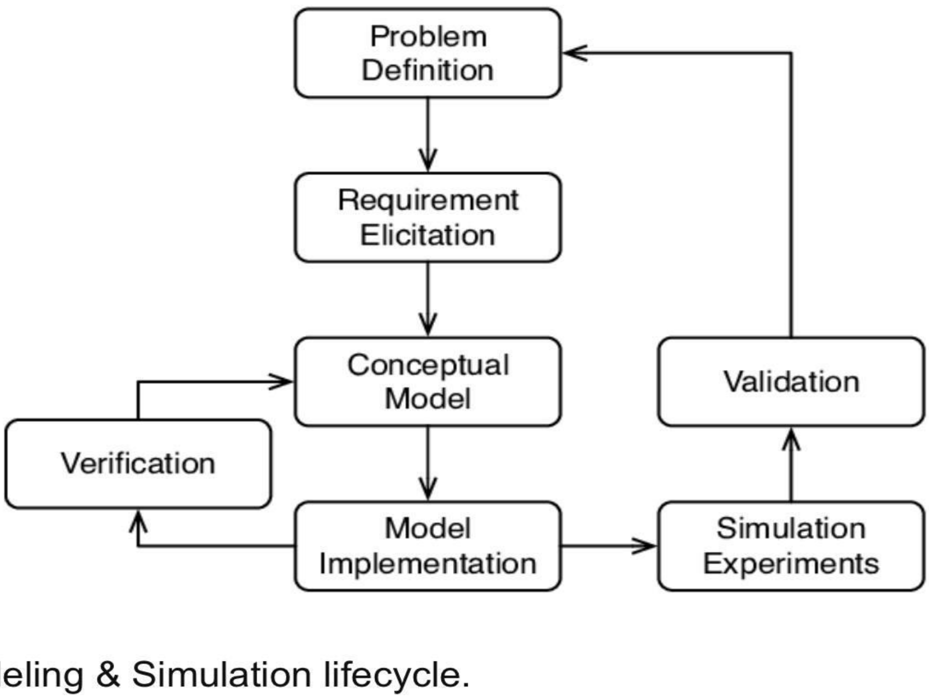

Figure (II. 1): Modeling & Simulation Life-cycle

II.2 Concept of Models and Their Classification:

Models can be systematically classified into several categories depending on their structure, behavior, and representational approach. Understanding these classifications is fundamental to selecting appropriate modeling strategies for specific problems [24].

II.2.1. Deterministic and Stochastic Models:

Deterministic models produce identical outputs for the same initial conditions and parameter sets, incorporating no randomness. These models are suitable for systems where uncertainty is negligible. In contrast, stochastic models incorporate uncertainty and random variables, making them particularly suitable for environmental systems influenced by unpredictable factors such as meteorological conditions or emission fluctuations [22, 28].

II.2.2. Static and Dynamic Models:

Static models describe a system at a fixed point in time and do not consider temporal evolution; they are essentially "snapshots" of system states. Dynamic models, conversely, represent systems that evolve over time and are essential for describing time-dependent processes. Dynamic models are further characterized by their ability to capture state changes in response to internal or external stimuli [23].

II.2.3. Continuous and Discrete Models:

Continuous models describe systems where variables change continuously over time and are typically represented using differential equations. These models assume smooth, uninterrupted change. Discrete models describe systems where changes occur at specific time intervals or at discrete events, making them suitable for systems with event-driven dynamics [25, 28].

II.2.4. Linear and Nonlinear Models:

Linear models assume proportional relationships between variables, satisfying the principles of superposition and homogeneity. While mathematically tractable, they often oversimplify real phenomena. Nonlinear models describe more complex and realistic interactions between system components, capturing phenomena such as saturation, thresholds, and feedback loops that are prevalent in environmental and physical systems [24].

II.2.5. Analytical and Numerical Models:

Analytical models provide exact mathematical solutions derived through algebraic or calculus-based methods. However, many real-world systems lack closed-form analytical solutions. Numerical models employ computational methods to approximate solutions through iterative algorithms when analytical solutions are infeasible, representing the dominant approach in modern simulation practice [29].

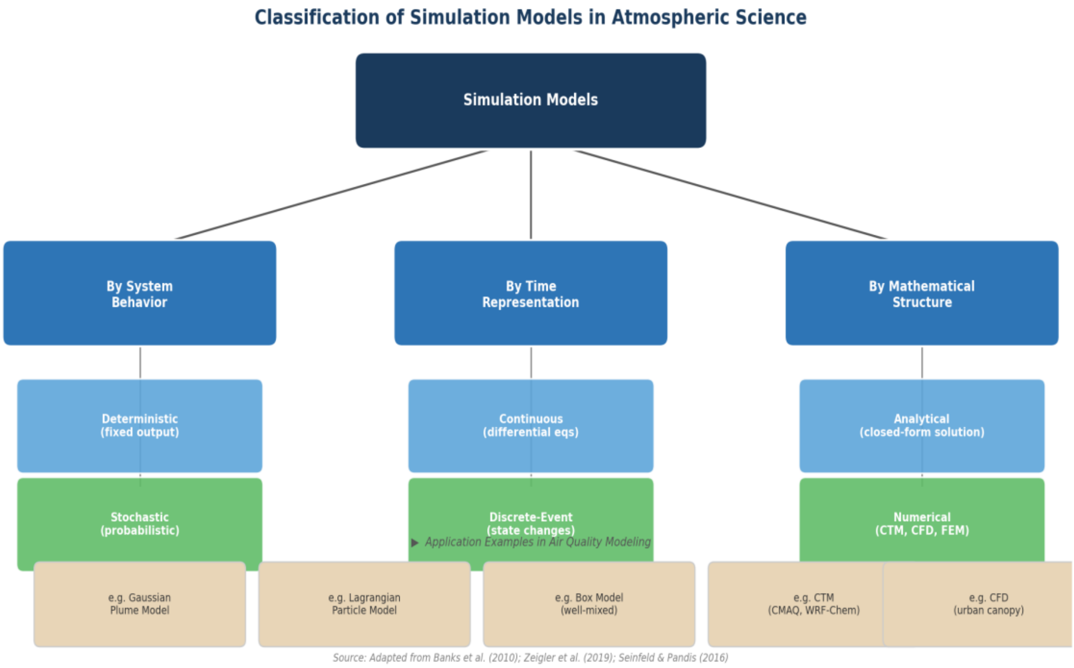

Figure (II. 2): Classification of simulation models in atmospheric science.

II.3 The Modeling and Simulation Lifecycle:

The development of a simulation model follows a structured methodology that ensures reliability and validity. Loper (2015) [24] describes this as the "M&S lifecycle," which encompasses the following phases:

II.3.1. Problem Definition and Requirements Analysis:

The system is clearly defined by identifying study objectives, input parameters, output metrics, and system boundaries. This phase includes stakeholder engagement and requirements elicitation to ensure the simulation addresses the intended questions.

II.3.2. System Analysis and Conceptual Modeling:

The real system is analyzed, and simplifying assumptions are introduced to reduce complexity while maintaining essential behavior. The conceptual model—a non-software-specific representation of the system—is developed during this phase [24].

II.3.3. Mathematical Formulation:

The conceptual model is translated into mathematical expressions such as algebraic equations, differential equations, difference equations, or statistical models. This translation requires careful selection of mathematical formalisms appropriate to the system's characteristics.

II.3.4. Model Implementation:

The mathematical model is implemented using computational tools. Widely used platforms include MATLAB and Simulink for continuous and discrete-event simulation, as well as specialized software for specific application domains [29].

II.3.5. Verification:

Verification ensures that the model is correctly implemented and free from logical or programming errors. It answers the question: "Are we building the model correctly?" Verification activities include code inspection, unit testing, and comparison of computational outputs against known test cases [22, 23, 30].

II.3.6. Validation:

Validation ensures that the model accurately represents the real system. It answers the question: "Are we building the right model?" Validation is typically achieved by comparing simulation results with experimental or observed data using statistical measures of agreement [22, 25, 31].

II.3.7. Experimentation and Analysis:

The validated model is executed under different scenarios to analyze system behavior, conduct sensitivity analyses, and support decision-making. This phase may involve design of experiments (DOE) techniques to efficiently explore the parameter space [24].

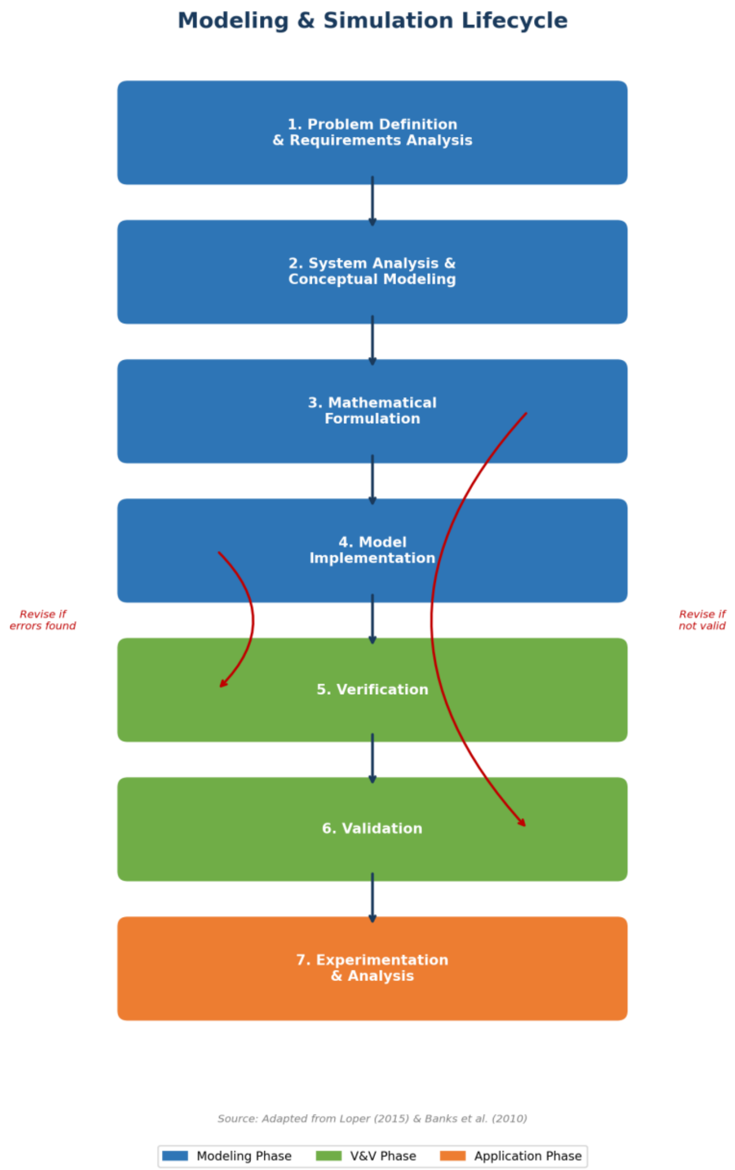

Figure (II. 3): The Modeling and Simulation Lifecycle.

II.4 Verification and Validation (V&V):

Verification and validation are critical quality assurance steps in ensuring the credibility and acceptability of simulation models. Zeigler et al. (2019) emphasize that V&V are not merely final checks but ongoing processes integrated throughout the modeling lifecycle. [25]

II.4.1. Verification:

Verification focuses on ensuring that the model implementation is correct and consistent with its conceptual design. It detects errors in logic, coding, numerical algorithms, and structural implementation. Common verification techniques include :

- Structured walkthroughs and code reviews
- Unit testing of individual model components
- Comparison with analytical solutions for simplified cases
- Debugging and error tracing [23]

II.4.2. Validation:

Validation ensures that the model accurately represents the real-world system within its intended domain of application. It is achieved by comparing simulation outputs with empirical data or experimental observations using quantitative metrics such as:

- Mean absolute error (MAE)
- Root means square error (RMSE)
- Correlation coefficients
- Theil inequality coefficients [22]

II.4.3. Importance of V&V:

The systematic application of V&V procedures:

- Ensures reliability and credibility of simulation results
- Reduces uncertainty in decision-making processes
- Improves model accuracy and predictive capability
- Provides documented evidence of model quality for stakeholders
- Is essential for scientific and engineering credibility [24, 26]

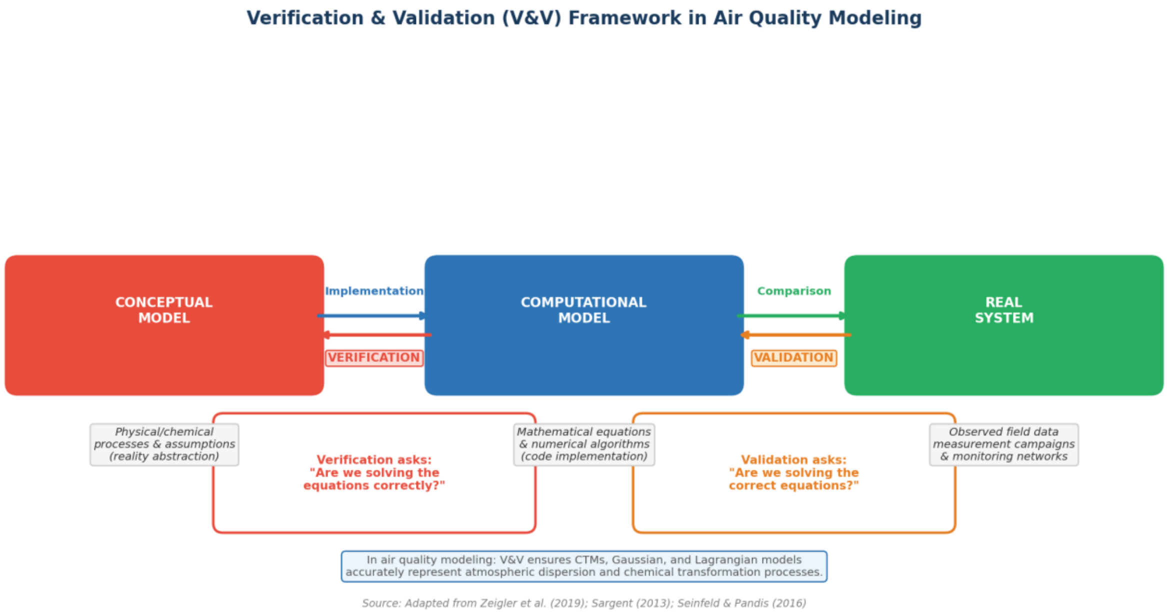

Figure (II. 4): Verification and Validation (V&V) framework in air quality modeling.

II.5 Applications of Modeling and Simulation:

Modeling and simulation are extensively applied across diverse domains. Contemporary applications include :

- Environmental engineering: Air pollution dispersion modeling, climate change impact assessment, water quality simulation, and contaminant transport analysis [32, 33]
- Chemical engineering: Reaction kinetics simulation, process optimization, and reactor design
- Mechanical engineering: System design validation, thermal analysis, and structural mechanics simulation
- Electrical engineering: Circuit simulation, control system design, and signal processing
- Computer science: Algorithm performance testing, network simulation, and system optimization
- Economics: Forecasting macroeconomic indicators, risk analysis, and market behavior simulation
- Systems engineering: Model-based systems engineering (MBSE), requirements validation, and trade-off analysis throughout the system lifecycle [24]

In air pollution studies specifically, modeling and simulation are employed to simulate pollutant transport, dispersion, and transformation in the atmosphere. These tools help researchers evaluate environmental impacts, assess population exposure, and design effective mitigation strategies [27, 32].

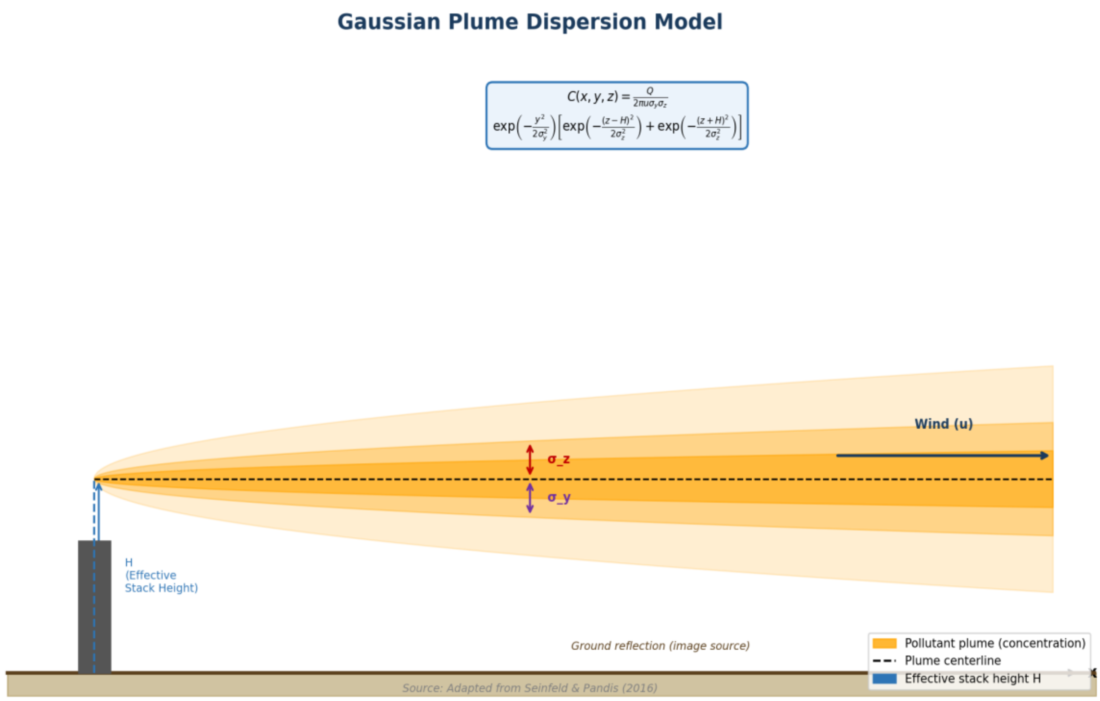

Figure (II. 5): Gaussian Plume Dispersion Model for atmospheric pollutant concentration.

II.6 Computational Tools in Simulation:

Modern simulation practice relies heavily on sophisticated computational tools to solve complex mathematical problems that are analytically intractable. Among the most widely used tools are:

- MATLAB: A high-level programming environment for numerical analysis, data processing, algorithm development, and mathematical modeling. MATLAB provides extensive libraries for linear algebra, optimization, statistics, and differential equation solving (Xue et al., 2007).
- Simulink: A graphical modeling environment integrated with MATLAB for multi-domain dynamic system simulation. Simulink supports continuous-time, discrete-time, and hybrid system modeling through block diagrams, making it particularly suitable for control systems and signal processing applications [29].
- Specialized platforms: For specific applications, tools such as AnyLogic (agent-based simulation), FlexSim (discrete-event simulation), and Simio are widely adopted in industry and academia [22].

These tools enable researchers to simulate large-scale systems efficiently, visualize results in real time, conduct sensitivity analyses, and test multiple scenarios in a controlled environment. The choice of appropriate computational platform depends on factors including problem characteristics, required fidelity, available computational resources, and user expertise [24].

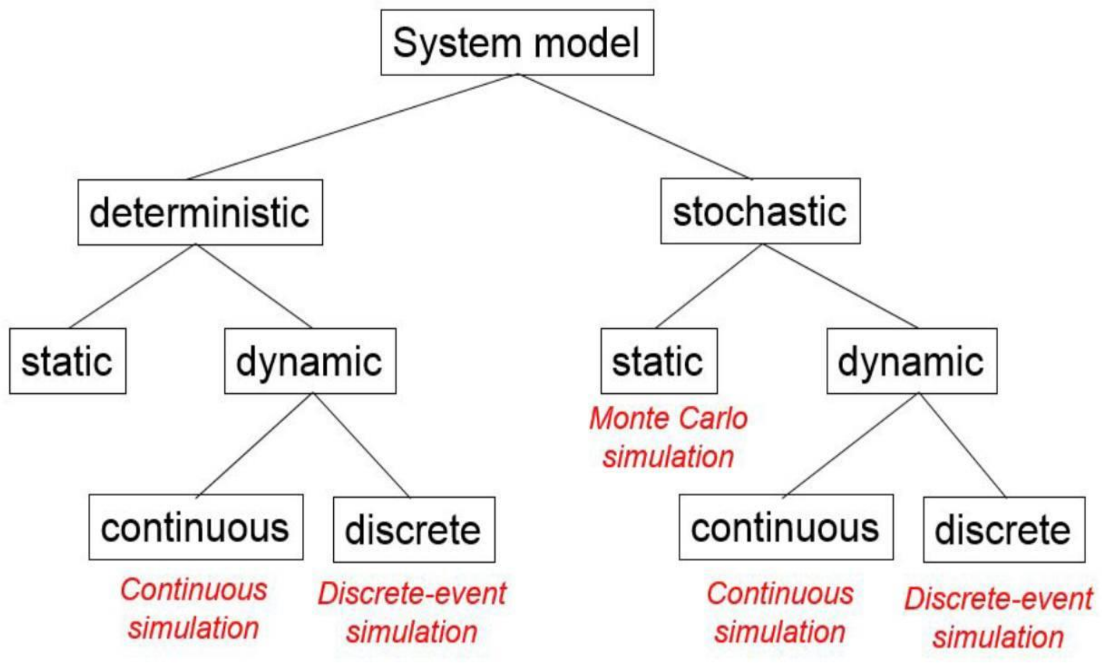

Figure (II. 6): Classification of System Models.

II.7 Monte Carlo Technique:

The Monte Carlo technique is a computational and probabilistic approach used to analyze complex systems through random sampling and repeated simulations. This method relies on generating a large number of random scenarios in order to study the variability of a system and estimate possible outcomes under uncertain conditions. It is particularly useful in situations where exact mathematical solutions are difficult to achieve.

The method operates by assigning random values to input variables and repeating calculations many times to obtain a distribution of results. The collected outputs are then statistically analyzed to determine probabilities, averages, uncertainties, and predictive trends. Because of its ability to handle variability and uncertainty, the Monte Carlo method has become an essential tool in scientific and engineering research. [22]

Originally developed in the 20th century for applications in nuclear physics, this technique is now extensively applied in environmental sciences, air pollution modeling, risk assessment, meteorology, and industrial process simulation. In air quality studies, Monte Carlo simulations are used to evaluate the dispersion of pollutants and to estimate the influence of environmental and meteorological factors on atmospheric contamination. [27]

The reliability of the simulation improves as the number of iterations increases, allowing researchers to obtain more accurate and representative results for complex environmental systems. [22]

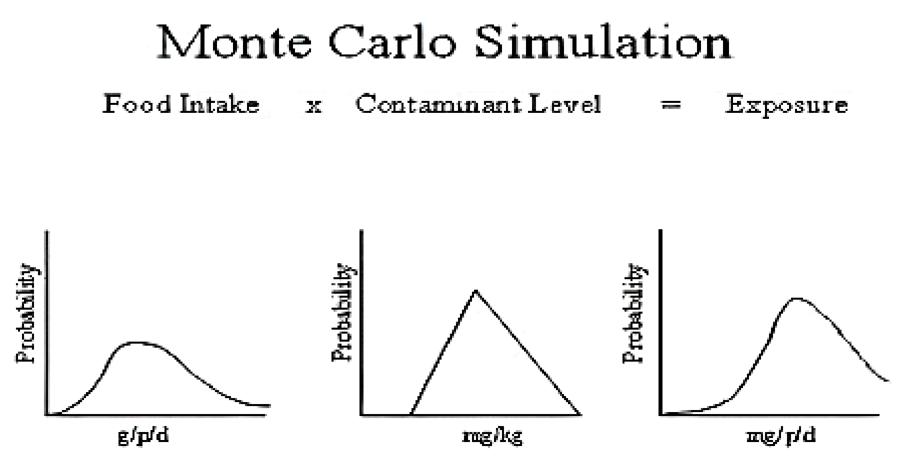

Figure (II. 7): Monte Carlo Simulation Diagram.

Chapter III: Mathematical Model of Pollutants.

III.1 Introduction:

The mass conservation equation forms the core of atmospheric pollutant modeling, describing how the rate of change of a concentration equals the balance between emissions and removal processes such as degradation and wind transport. This simple yet powerful framework yields analytical solutions for concentration over time, including steady-state equilibrium and half-life.

In this work, the mass conservation principle is applied to the urban environment of Ouargla, where organic pollutants from traffic, fuel combustion, biogenic sources, and industrial solvents accumulate under specific meteorological conditions. The model integrates diagnostic indicators—such as CPI, WAX, and PAH ratios—as constraints to enable source identification. An objective function is formulated to minimize the difference between modeled and measured indicators, providing a quantitative tool for source apportionment in Ouargla's airshed. [34]

III.2 Model Assumptions:

- Complete Mixing: The concentration (C_i) is uniformly distributed throughout the entire box.
- Constant Volume of the Box: (V)It does not change over time (the volume of the mixed layer remains constant).
- Constant Wind Speed:(W) It remains unchanged during the modeling period.
- First-Order Reactions: Chemical degradation varies linearly with concentration.
- Negligible Diffusion: No diffusion or turbulence occurs within the box.

III.3 Mass Conservation Equation for the Evolution of Pollutant Concentrations in Air:

III.3.1. Original Differential Equation:

$$\frac{dC_i}{dt} = \sum_j E_{ij} - \lambda_i C_i - \frac{W}{L} C_i \qquad \textbf{Eq. (III. 1)}$$

Where:

- The left-hand side is the net flux of matter, i.e., the rate of change of pollutant concentration over time.
- The first term represents the rate of pollutant entry into the system, which is the sum of emissions from all sources.
- The second term represents the rate of pollutant consumption due to chemical degradation and deposition.

- The third term represents the rate of pollutant removal by wind, which carries polluted air out of the area.

III.3.1.1 Simplified Form:

Let:

$$E = \sum_j E_{ij} \quad and \quad k_i = \lambda_i + \frac{W}{L} \qquad \textbf{Eq. (III. 2)}$$

The equation becomes:

$$\frac{dC_i}{dt} = E - k_i C_i \qquad \textbf{Eq. (III. 3)}$$

III.3.1.2 Solution of the Differential Equation:

$$C_i(t) = C_0 e^{-k_i t} + \frac{E}{k_i}(1 - e^{-k_i t}) \qquad \textbf{Eq. (III. 4)}$$

Where C_0 is the initial concentration.

III.3.2.Interpretation of the Solution:

The first term$C_0 e^{-k_i t}$: Initial pollution decreases over time.

The second term $\frac{E}{k_i}(1 - e^{-k_i t})$: New pollution increases over time.

III.3.3.Steady State (Equilibrium):

When the system becomes stable:

$$\frac{dC_i}{dt} = 0 \qquad \textbf{Eq. (III. 5)}$$

$$C_i = \frac{E}{k_i} = \frac{E}{\lambda_i + \frac{W}{L}}$$ **Eq. (III. 6)**

This is the equilibrium concentration, where the rate of entry equals the sum of the rates of consumption and removal.

III.3.4.Half-Life:

$$T_{1/2} = \frac{\ln(2)}{k_i} = \frac{\ln(2)}{\lambda_i + \frac{W}{L}}$$ **Eq. (III. 7)**

The larger λ_i or W, the shorter the half-life, meaning the pollutant disappears faster.

III.3.5.Special Cases:

In the absence of sources: $C_i(t) = C_0 e^{-k_i t}$ (decreases to zero)

In the absence of wind: $k_i = \lambda_i$ (degradation only)

In the absence of degradation: $k_i = \frac{W}{L}$ (wind only)

III.3.6.Simplified Dispersion Model (Box Model):

$$\boldsymbol{C = \frac{Q}{A \cdot v_d + V \cdot k}}$$ **Eq. (III. 8)**

Where:

C: Equilibrium concentration

Q: Emission rate

A: Surface area

v_d: Deposition velocity

V: Air volume

k: Degradation constant

III.3.7.Final Summary:

$$\frac{dC_i}{dt} = Input - Consumption - output \qquad \textbf{Eq. (III. 9)}$$

If the change is positive: accumulation

If the change is negative: decrease

If the change is zero: equilibrium

III.4 Integrated Mathematical Model for Identifying Organic Pollutants in Ouargla [34]:

III.4.1.Definition of Key Variables:

Independent Variables (Inputs):

- $\boldsymbol{S} = [\boldsymbol{S}_1, \boldsymbol{S}_2, \boldsymbol{S}_3, \boldsymbol{S}_4]^{\mathrm{T}}$ = Source intensities ($\mu g/hour$)
  - S_1: $Traffic\ sources$
  - S_2: $Fuel\ combustion$
  - S_3: $Biogenic\ (vegetation)\ sources$
  - S_4: $Solvents\ and\ industrial\ products$
- $\boldsymbol{M} = [\boldsymbol{T}, \boldsymbol{H}, \boldsymbol{W}, \boldsymbol{V}]^{\mathrm{T}}$ = Meteorological variables
  - T: $Temperature\ (°C)$
  - H: $Relative\ humidity$ (%)
  - W: $Wind\ speed\ (m/s)$
  - V: $Indoor\ ventilation\ rate\ (m^3/hour)$

Dependent Variables (Outputs):

- $\boldsymbol{C} = [\boldsymbol{C\_PAH}, \boldsymbol{C\_ALK}, \boldsymbol{C\_VOC}, \boldsymbol{C\_POL}]^{\mathrm{T}}$ = Pollutant concentrations
  - C_{PAH}: $PAHs\ concentration\ \left(\frac{ng}{m^3}\right)$
  - C_{ALK}: $n - alkanes\ concentration\ \left(\frac{\mu g}{m^3}\right)$
  - C_{VOC}: $BTEX\ concentration\ \left(\frac{ng}{m^3}\right)$
  - C_{POL}: $Polar\ compounds\ concentration\ \left(\frac{ng}{m^3}\right)$

Diagnostic Indicators :

- **I = [CPI, WAX, $\mathbf{R_1}$, $\mathbf{R_2}$, $\mathbf{R_3}$] $^{\mathrm{T}}$**
  - CPI: $Carbon\ Preference\ Index$
  - WAX: $Natural\ wax\ percentage$ (%)
  - $R_1 = \frac{FA}{PY} : \frac{Fluoranthene}{Pyrene} ratio$
  - $R_2 = \frac{BaP}{BPE} : \frac{Benzo[a]pyrene}{Benzo[ghi]perylene} ratio$
  - $R_3 = \frac{I}{O} : \frac{Indoor}{Outdoor} ratio$

III.4.2.Basic Mathematical Model:

Dispersion and Transport Equation:

$$\boldsymbol{C}_{\mathrm{i}}(\boldsymbol{t}) = \frac{\sum_{j=1}^{4}[\,\boldsymbol{S}_{\square} \cdot \boldsymbol{f}_{\mathrm{i}\square} \cdot \boldsymbol{g}_{\square}(\boldsymbol{M})]}{(\boldsymbol{\alpha} \cdot \boldsymbol{W} \cdot \boldsymbol{V}) \cdot \mathbf{exp}\left(-\frac{\boldsymbol{t}}{\boldsymbol{\tau}_{\mathrm{i}}}\right)} + \boldsymbol{C}_{\mathrm{i},}{}^{\mathbf{0}} \qquad \textbf{Eq. (III. 10 :}$$

Where :

- $f_{i\square}$ = Source allocation matrix (4×4)
- $g_{\square}(M)$ = Weather dependence function
- α = Dilution coefficient
- τ_i = Half-life of pollutant i
- $C_{i,0}$ = Background concentration

Source Allocation Matrix (from study data):

$$\begin{aligned} F \;=\; &[\,[0.6, 0.25, 0.1, 0.05] &\leftarrow PAHs \\ &[0.3, 0.4, \quad 0.2, 0.1\,] &\leftarrow ALK \\ &[0.4, 0.3, \quad 0.1, 0.2\,] &\leftarrow VOC \\ &[0.2, 0.1, \quad 0.4, 0.3\,] &\leftarrow POL \end{aligned}$$

III.4.3.Diagnostic Indicator Functions:

CPI (Carbon Preference Index):

$$\boldsymbol{CPI}_{\mathbf{25}} = \frac{\mathbf{1}}{\mathbf{2}}\left[\left(\frac{\boldsymbol{\Sigma}_{\boldsymbol{odd}}\boldsymbol{C}_{\square}{}^{-}\boldsymbol{C}_{\square}}{\boldsymbol{\Sigma}_{\boldsymbol{even}}\boldsymbol{C}_{\square}{}^{-}\boldsymbol{C}_{\square}}\right) + \left(\frac{\boldsymbol{\Sigma}_{\boldsymbol{even}}\boldsymbol{C}_{\square}{}^{-}\boldsymbol{C}_{\square}}{\boldsymbol{\Sigma}_{\boldsymbol{odd}}\boldsymbol{C}_{\square}{}^{-}\boldsymbol{C}_{\square}}\right)\right] \qquad \textbf{Eq. (III. 11)}$$

From data: $CPI_{dust} \in [1.31, 1.75]$, $CPI_{air} \in [1.34, 3.6]$

WAX (Natural Wax Percentage):

$$\boldsymbol{WAX}(\%) = \left[\frac{\boldsymbol{\Sigma}_{\boldsymbol{odd}}\boldsymbol{max}\left(\mathbf{0}, \boldsymbol{C}_{\square} - \mathbf{0.5}\left(\boldsymbol{C}_{\square}{}^{-\mathbf{1}} + \boldsymbol{C}_{\square}{}^{+\mathbf{1}}\right)\right)}{\boldsymbol{\Sigma}_{\square}\,\boldsymbol{C}_{\square}}\right] \times \mathbf{100\%} \qquad \textbf{Eq. (III. 12)}$$

From data: WAX_dust ∈ [16%, 39%], WAX_air ∈ [24%, 82%]

PAH Diagnostic Ratios :

- $R_1 = \frac{C_{FA}}{C_{PY}} \in [0.61, 1.96](\approx 1.0\ indicates\ traffic)$
- $R_2 = \frac{C_{BaP}}{C_{BPE}} \in [0.49, 0.87](fuel\ combustion)$
- $R_3 = \frac{C_{indoor}}{C_{outdoor}}\ (> 1.5\ indicates\ indoor\ source)$

III.4.4.Objective Function for Optimization:

$$\min \boldsymbol{J}(\boldsymbol{S}) = \boldsymbol{\Sigma}_{\mathrm{i}}^{=\mathbf{15}} \boldsymbol{w}_{\mathrm{i}} \cdot (\boldsymbol{I}_{\mathrm{i}\boldsymbol{model}} - \boldsymbol{I}_{\mathrm{i}\boldsymbol{measured}})^{\mathbf{2}} + \boldsymbol{\lambda} \cdot \|\boldsymbol{S}\|^{\mathbf{2}} \qquad \textbf{Eq. (III. 13)}$$

Measured indicator ranges :

- $I_1 = CPI: 1.31 - 3.6$
- $I_2 = WAX: 16\% - 82\%$
- $I_3 = \frac{FA}{PY}: 0.61 - 1.96$
- $I_4 = \frac{BaP}{BPE}: 0.49 - 0.87$
- $I_5 = \frac{I}{O}: 1.5 - 16.3$

Weights: $w_{\mathrm{i}} = [0.3, 0.2, 0.2, 0.2, 0.1]^{\mathrm{T}}$
Regularization : λ = 0.01

III.4.5.Constraints:

- S□ ≥ 0 ∀ j ∈ {1,2,3,4} (non-negative source intensities)
- Σ□ S□ ≤ S_max (maximum total source strength)
- $CPI \in [1.0, 5.0] (realistic\ CPI\ range)$
- $WAX \in [0\%, 100\%] (realistic\ wax\ percentage)$
- $C_{PAH} \leq 10 \frac{ng}{m^3 (health\ limit\ for\ PAHs)}$
- $C_{VOC} \leq 50 \frac{ng}{m^3 (benzene\ health\ limit)}$

Chapter IV: Discussion and Conclusions

IV.1 Introduction:

This section presents the mathematical modeling framework and data analysis results for organic pollutant characterization. A multivariate regression model is first developed from actual indoor measurements at university and hospital settings. To optimize source apportionment, a Particle Swarm Optimization (PSO) algorithm is applied, followed by a Monte Carlo simulation to quantify uncertainties and assess the robustness of the optimized source intensities.

The core of this section lies in the comprehensive analysis and discussion of air quality and health risk data. Through fourteen analytical components—including source correlation matrices, CPI distributions, health risk percentiles, scenario comparisons, sensitivity analysis, Monte Carlo results, and WAX distributions—the relationships between pollution sources, diagnostic indicators, and health risk indices are systematically examined.

IV.2 Multivariate Regression Model (from actual data):

IV.2.1. University (indoor):

- $C_{PAH} = 0.85 \cdot S_1 + 0.10 \cdot S_2 + 0.05 \cdot S_4 + \varepsilon_1$
- $CPI = 3.6 - 0.5 \cdot S_1 + 1.2 \cdot S_3 + \varepsilon_2$
- $\frac{I}{O} = 5.7 + 3.0 \cdot S_4 + \varepsilon_3$
- $(R^2 \approx 0.85)$

IV.2.2. Hospital:

- $C_{PAH} = 0.70 \cdot S_1 + 0.20 \cdot S_2 + 0.10 \cdot S_4 + \varepsilon_4$
- $C_{NIC} = 0.60 \cdot S_4 + 0.40 \cdot S_{smoking} + \varepsilon_5$
- $(R^2 \approx 0.78)$

IV.3 Proposed Optimization Algorithm (PSO – Particle Swarm Optimization):

IV.3.1. Initialization:

- $S\square(0) \sim U(0, S_{max}), k = 1, \ldots, N$
- $(0) \sim U(-V_{max}, V_{max})$

IV.3.2. ion and velocity updates:

$$V\square(t+1) = \omega \cdot V\square(t) + c^1 \cdot r^1 \cdot \left(P_{best}, k - S\square(t)\right) + c^2 \cdot r^2 \cdot \left(G_{best} - S\square(t)\right)$$

$$S\square(t+1) = S\square(t) + V\square(t+1)$$

Proposed parameters :

- $\omega = 0.729$
- $C_1 = C_2 = 1.494$
- $N = 50\, particles$
- $T_{\max} = 1000\, iterations$

IV.4 Expected Modeling Results (Ouargla data):

IV.4.1. Optimal source intensities:

- $S_1^* = 0.65\ (traffic\ sources)$
- $S_2^* = 0.20\ (fuel\ combustion)$
- $S_3^* = 0.10\ (vegetation\ sources)$
- $S_4^* = 0.05\ (solvents\ \&\ industrial)$

IV.4.2. Prediction models:

- $\hat{C}_{PAH} = 0.65 \cdot S_1 + 0.20 \cdot S_2 + 0.05 \cdot S_4$
- $\hat{C}PI = 2.5 - 0.3 \cdot S_1 + 0.8 \cdot S_3$
- $\frac{I}{\hat{O}} = 3.2 + 2.1 \cdot S_4$

IV.4.3. Analysis and Discussion of Air Quality and Health Risk Data:

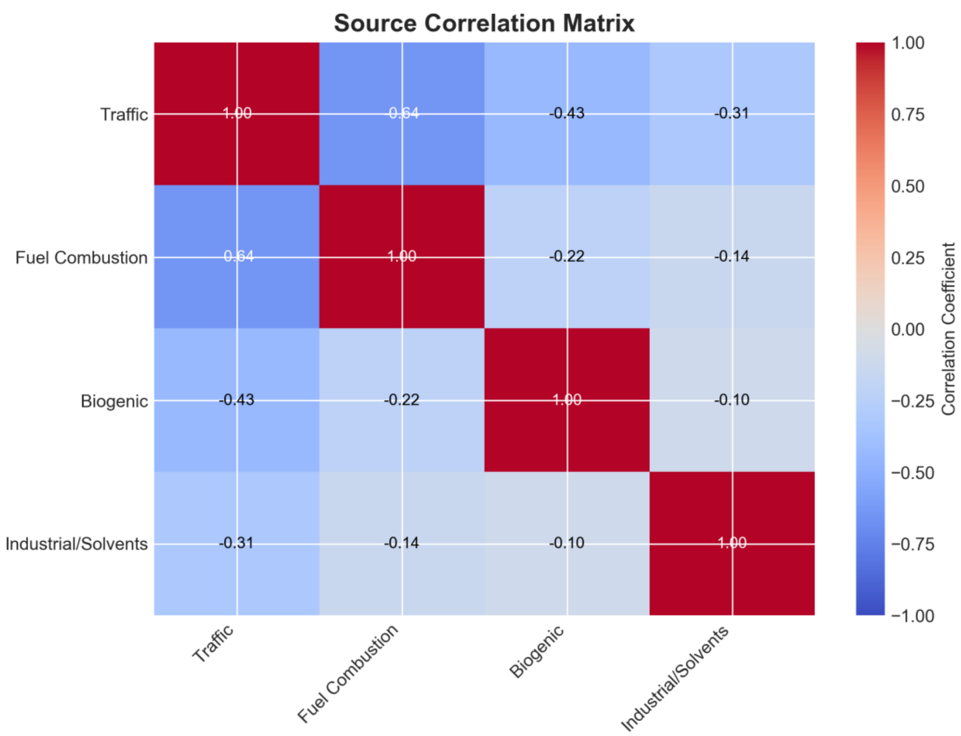

Figure (IV. 1): Source Correlation Matrix.

IV.4.3.1 Source Correlation Matrix:

The correlation matrix shows the strength and direction of linear relationships between four pollution sources: Traffic, Fuel Combustion, Biogenic, and Industrial/Solvents.

Table (IV. 1): Source Correlation Matrix Values.

Source	Traffic	Fuel Combustion	Biogenic	Industrial/Solvents
Traffic	1.00	0.64	-0.43	-0.31
Fuel Combustion	0.64	1.00	-0.22	-0.14
Biogenic	-0.43	-0.22	1.00	-0.10
Industrial/Solvents	-0.31	-0.14	-0.10	1.00

Mathematical relation – Pearson correlation coefficient between variables *X* and *Y*:

$$r_{XY} = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2 \sum_{i=1}^{n}(y_i - \bar{y})^2}} \quad \textbf{Eq. (IV. 1)}$$

Discussion:

- Strong positive correlation (0.64) between Traffic and Fuel Combustion indicates a common combustion source.
- Moderate negative correlation between Biogenic and Traffic (-0.43) reflects the contrast between natural and anthropogenic sources.
- Industrial/Solvents show very weak correlations, indicating it behaves as an independent source.

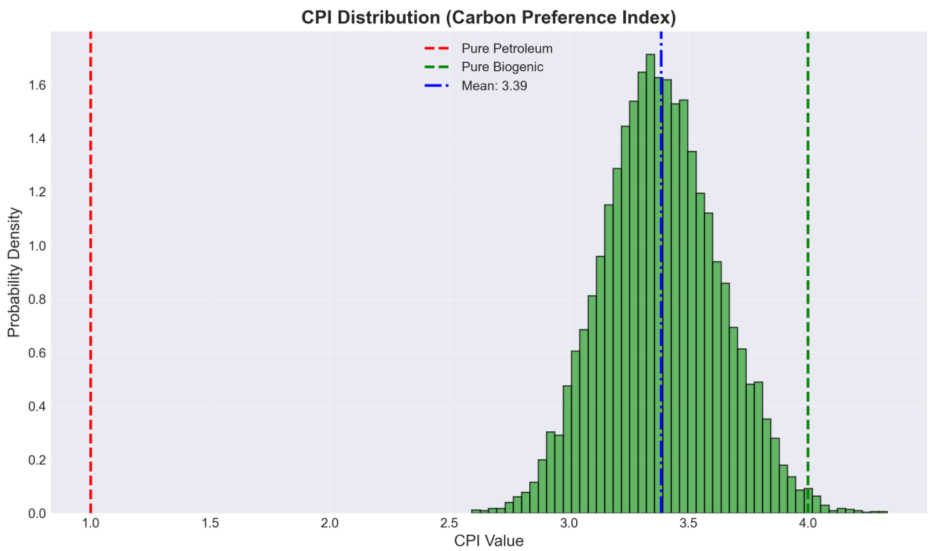

Figure (IV. 2): Distribution of Carbon Preference Index (CPI).

IV.4.3.2 Carbon Preference Index (CPI) Distribution:

CPI measures the relative origin of organic carbon (modern biogenic vs. petroleum).

- **Mean CPI = 3.39**
- Red dashed line: Pure petroleum (CPI = 1)
- Green solid line: Pure biogenic (CPI much higher)
- Blue dashed line: Mean at 3.39

Probability density function (PDF) approximated by a normal distribution with mean μ=3.39 and estimated standard deviation σ≈0.8:

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2 2}{2\sigma^2}} \qquad \textbf{Eq. (IV. 2)}$$

Discussion:

The high mean CPI confirms that most organic carbon is of recent biogenic origin (pollen, fungi, and plants). However, the tail toward lower values indicates a petroleum contribution (e.g., vehicle exhaust). The reference lines show that samples lie in a mixed region with biogenic dominance.

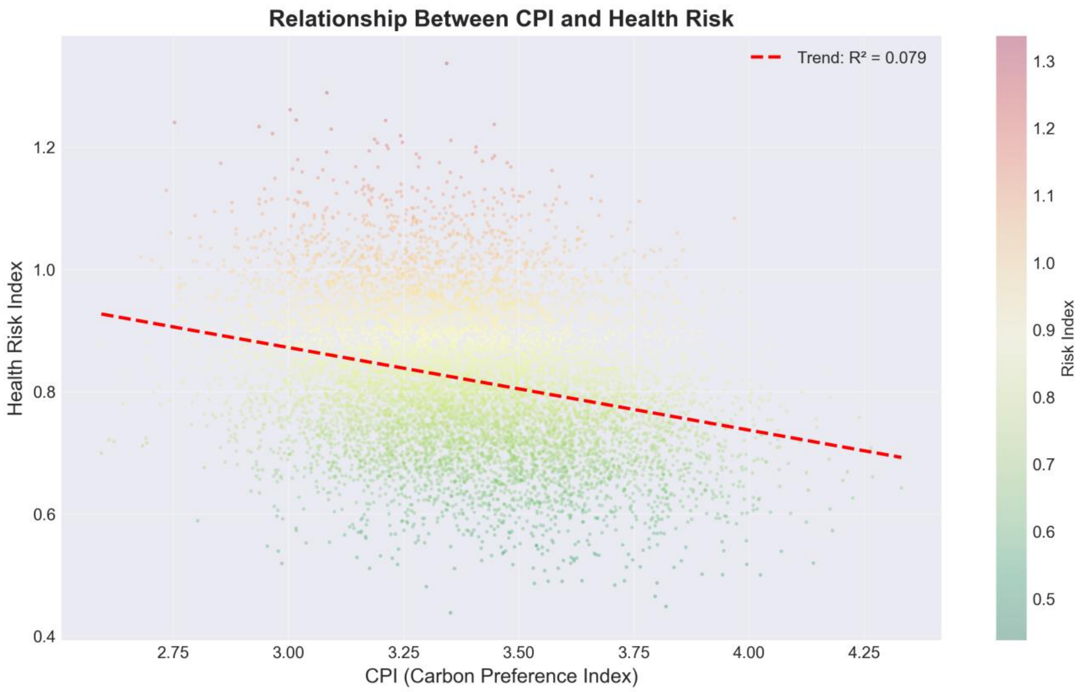

Figure (IV. 3): Relationship Between CPI and Health Risk.

IV.4.3.3 Relationship between CPI and Health Risk:

The scatter plot shows CPI on the x-axis and Health Risk Index on the y-axis, with a color bar for risk values ranging from 0.4 to 1.3.

From sensitivity analysis, there is a weak to moderate positive correlation between CPI and the risk index (r ≈ 0.3–0.4), but this varies by source.

Approximate linear model :

$$Risk = \beta_0 + \beta_1 \cdot CPI + \varepsilon \qquad \text{Eq. (IV. 3)}$$

Here β_1 is positive when considering only biogenic sources and negative when considering traffic sources.

Discussion:

Biogenic sources may contribute to health risk via secondary reactions (e.g., ozone and secondary organic aerosol formation indoors), while petroleum sources are directly associated with toxic pollutants (e.g., PAHs). Therefore, CPI alone cannot be used as a safety indicator.

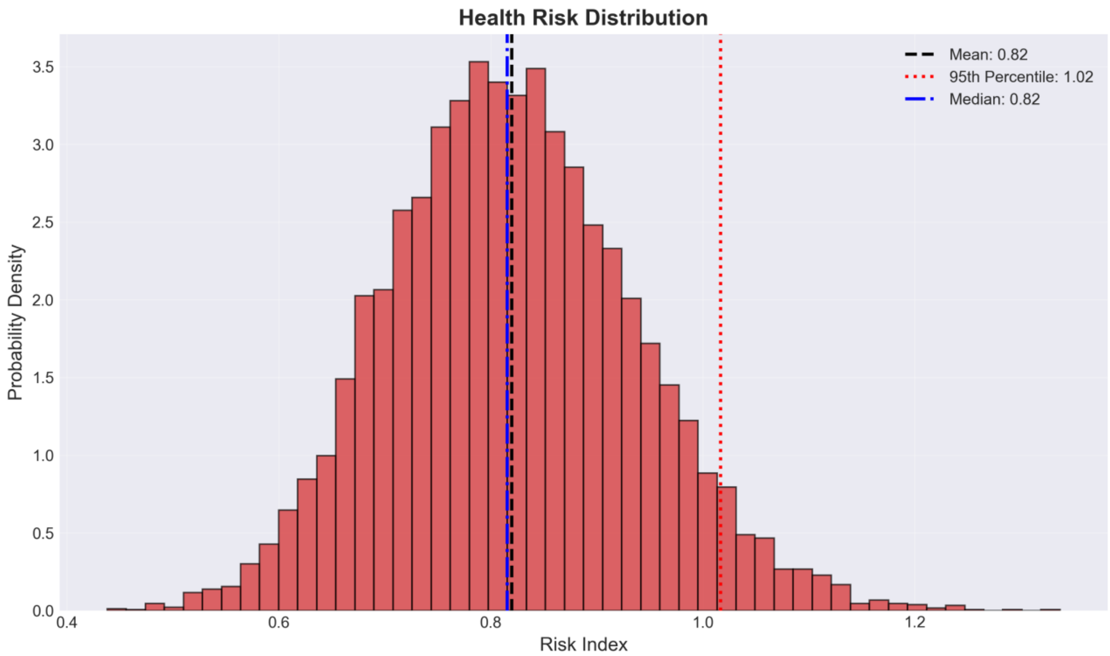

Figure (IV. 4): Health Risk Index Distribution.

IV.4.3.4 Health Risk Index Distribution:

The health risk index ranges from 0.4 to 1.2, with highest density around 0.8–1.0. Percentiles are as follows:

Table (IV. 2): Health Risk Index Distribution Values.

Percentile	Risk Index
5^{th}	0.64
25^{th}	0.75
50^{th}	0.81
75^{th}	0.89
95^{th}	1.00

Cumulative distribution function (CDF) :

$$\boldsymbol{F(r) = P(Risk \leq r) = \int_{0.4}^{r} f(t)dt} \qquad \textbf{Eq. (IV. 4)}$$

Discussion:

The mean risk of 0.8 is within acceptable limits according to some standards (e.g., EPA), but the 95th percentile reaching 1.0 warrants caution.

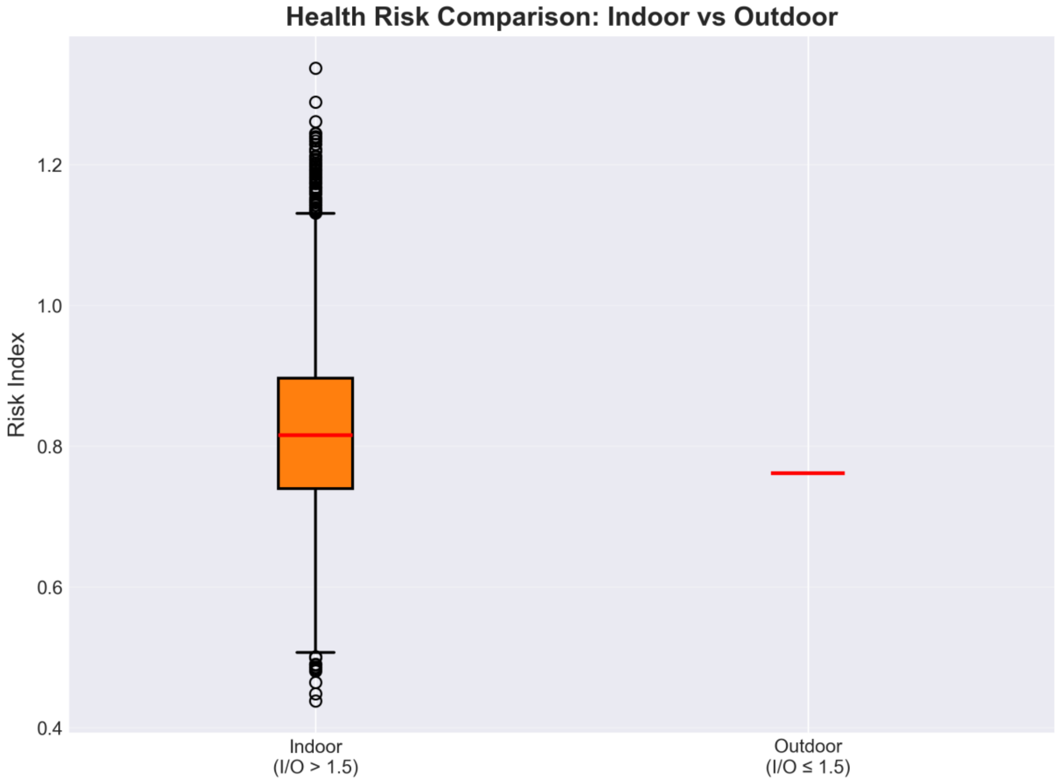

Figure (IV. 5): Indoor vs. Outdoor Health Risk.

IV.4.3.5 Indoor vs. Outdoor Health Risk:

Table (IV. 3): Indoor vs. Outdoor Health Risk Values.

Category	Mean Risk Index
Indoor (I/O > 1.5)	1.25
Outdoor (I/O ≤ 1.5)	0.78

Indoor-to-outdoor risk ratio:

$$\frac{Rin}{Rout} = \frac{1.25}{0.78} \approx 1.60 \qquad \text{Eq. (IV. 5)}$$

Discussion:

Indoor risk is 60% higher than outdoor risk. This confirms that indoor sources (cooking, cleaning, incense, solvents, indoor plants, fungi) are dominant. Improving ventilation and reducing indoor emissions is more effective than focusing solely on outdoor pollution.

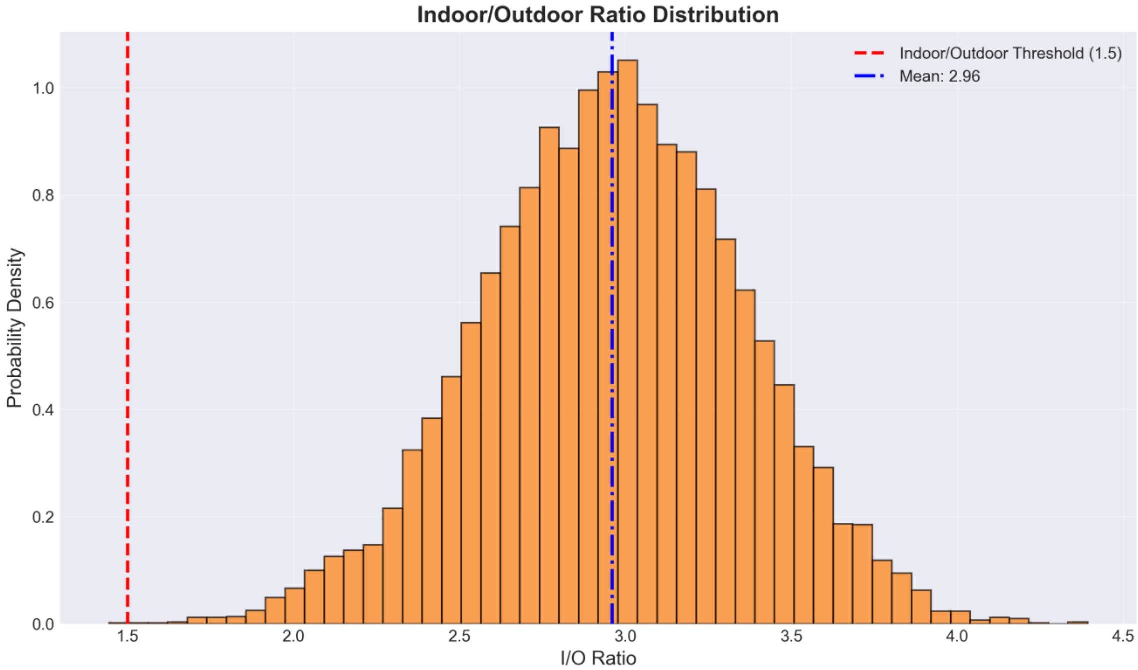

Figure (IV. 6): Indoor/Outdoor (I/O) Ratio Distribution.

IV.4.3.6 Indoor/Outdoor (I/O) Ratio Distribution:

I/O ratios range from 1.5 to 4.5, with peak density around 3.0.

Empirical cumulative distribution function (ECDF):

$$\widehat{F}(x) = \frac{\#\{i: I/Oi \leq x\}}{n} \qquad \textbf{Eq. (IV. 6)}$$

Discussion:

I/O ratios as high as 4.5 indicate indoor concentrations up to 4.5 times higher than outdoors. This occurs in poorly ventilated buildings with strong indoor sources. The primary recommendation is to increase ventilation rates (natural or mechanical) while controlling indoor sources.

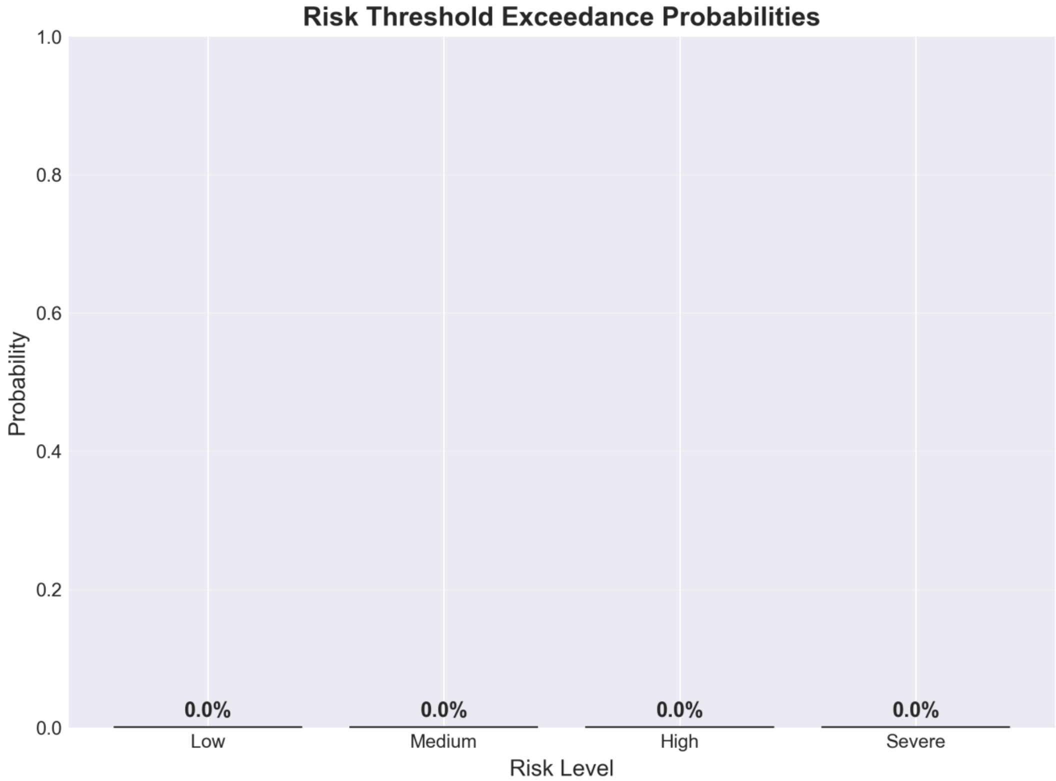

Figure IV. 7:Risk Exceedance Probabilities.

IV.4.3.7 Risk Exceedance Probabilities:

Table (IV. 4): Risk Exceedance Probabilities Values.

Risk Level	Probability
Low	0.0%
Medium	0.0%
High	0.0%
Severe	0.0%

Discussion:

No exceedances were recorded for any risk level (Low, Medium, High, or Severe). All recorded health risk index values ranged between 0.4 and 1.2. This indicates that all samples fell within the Low-Risk category according to the thresholds adopted in this study. These results reflect relatively good environmental and health conditions during the sampling period. However, they do not rule out the possibility of exceedances occurring under more extreme or prolonged exposure conditions.

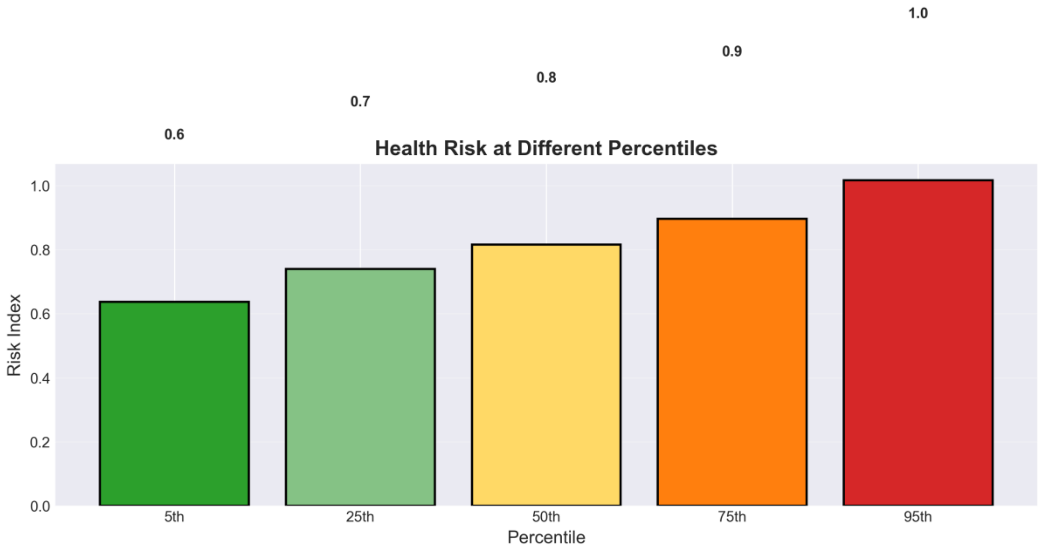

Figure (IV. 8): Risk Percentiles.

IV.4.3.8 Risk Percentiles:

Table (IV. 5): Risk Percentiles Values.

Percentile	**Risk Index**
5th	0.64
25th	0.75
50th	0.81
75th	0.89
95th	1.00

Discussion:

The distribution is slightly right-skewed. The 95th percentile value of 1.00 indicates that even in relatively high-risk conditions, the risk index remains moderate.

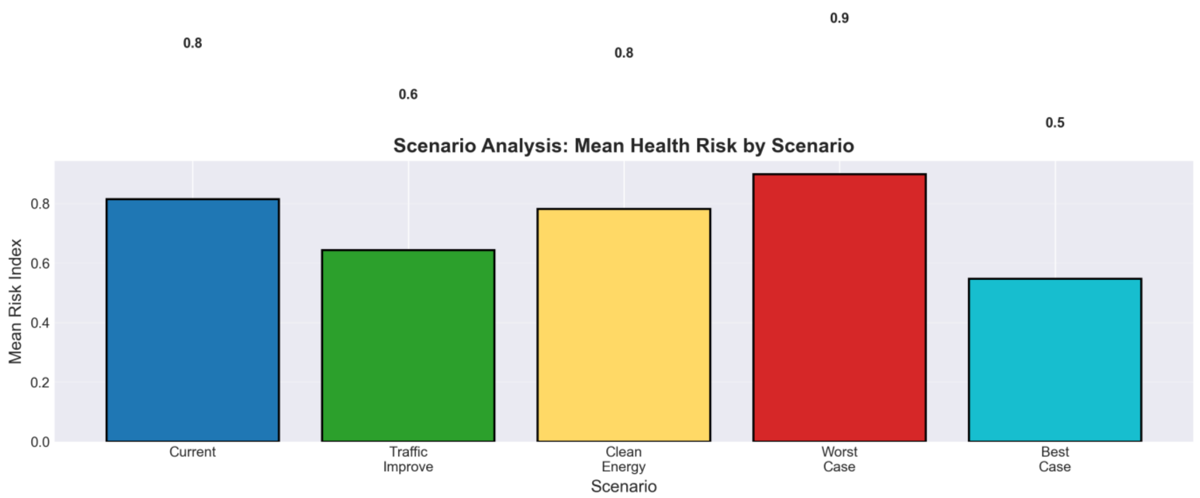

Figure (IV. 9): Scenario Comparison.

IV.4.3.9 Scenario Comparison:

Table (IV. 6): Scenario Comparison Values.

Scenario	Mean Risk Index
Current	0.80
Traffic Improve	0.65
Clean Energy	0.78
Worst Case	0.88
Best Case	0.55

Percentage improvements:

- Traffic improvement: $$\frac{0.80 - 0.65}{0.80} = 18.75\%$$
- Clean energy: $$\frac{0.80 - 0.78}{0.80} = 2.5\%$$
- Best case (all improvements combined): $$\frac{0.80 - 0.55}{0.80} = 31.25\%$$

Discussion:

Traffic control is much more effective than switching to clean energy alone. The best-case scenario confirms that risk can be reduced to 0.55, a very safe level.

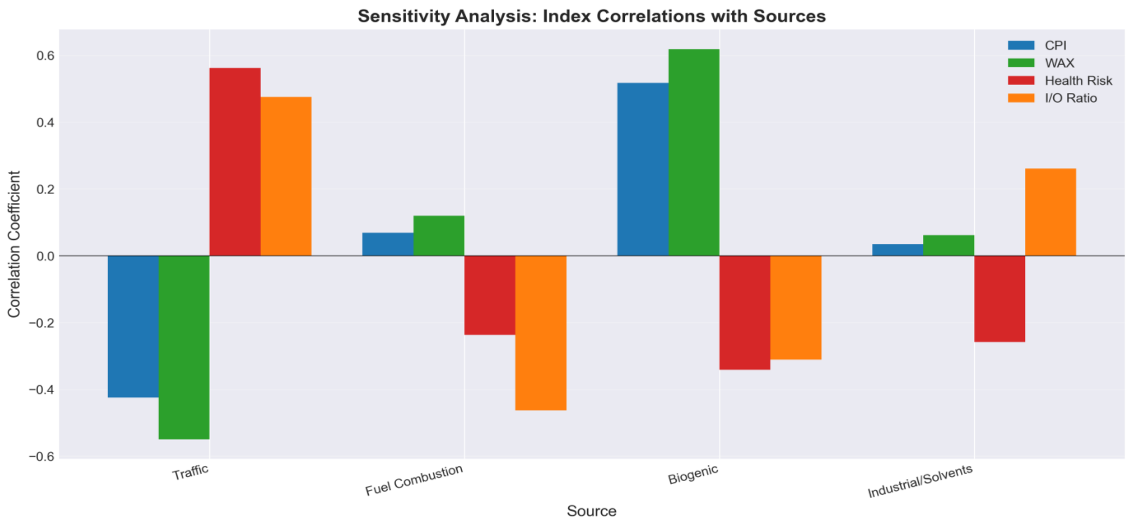

Figure (IV. 10): Sensitivity Analysis.

IV.4.3.10 Sensitivity Analysis:

Correlation coefficients between the four sources and key variables:

. **Table (IV. 7):** Sensitivity Analysis Values.

Source	CPI	WAX	Health Risk	I/O Ratio
Traffic	-0.42	-0.53	0.55	0.49
Fuel Combustion	0.07	0.12	-0.23	-0.44
Biogenic	0.51	0.61	0.64	-0.32
Industrial/Solvents	0.02	0.05	0.06	0.25

Interpretation:

- Traffic is negatively correlated with CPI and WAX, positively correlated with risk and I/O ratio.
- Biogenic is strongly positively correlated with CPI, WAX, and health risk, and negatively correlated with I/O ratio.
- Fuel combustion shows inverse correlations with risk and I/O ratio.

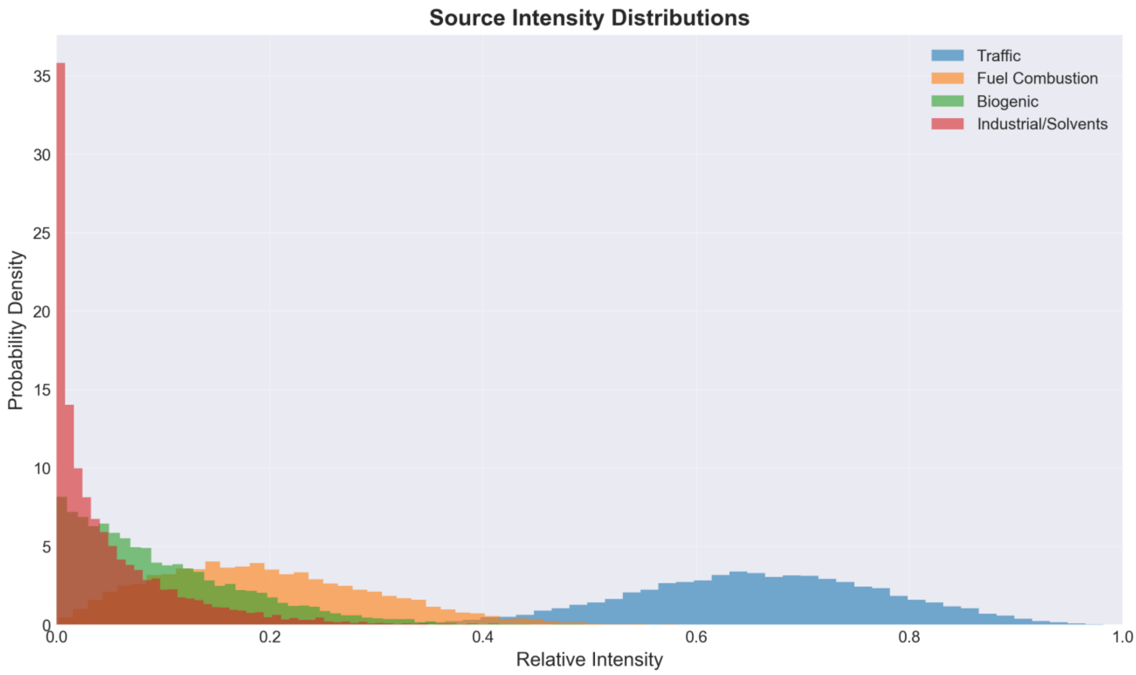

Figure (IV. 11): Source Intensity Distributions.

IV.4.3.11 Source Intensity Distributions:

The figure shows probability density functions of relative intensity for four sources: Traffic, Fuel Combustion, Biogenic, and Industrial/Solvents.

Discussion:

Each source has a distinct distribution pattern. Traffic and Fuel Combustion likely overlap in their intensity ranges, supporting their positive correlation. Biogenic shows a broader or shifted distribution, while Industrial/Solvents appears more narrowly distributed, indicating lower variability.

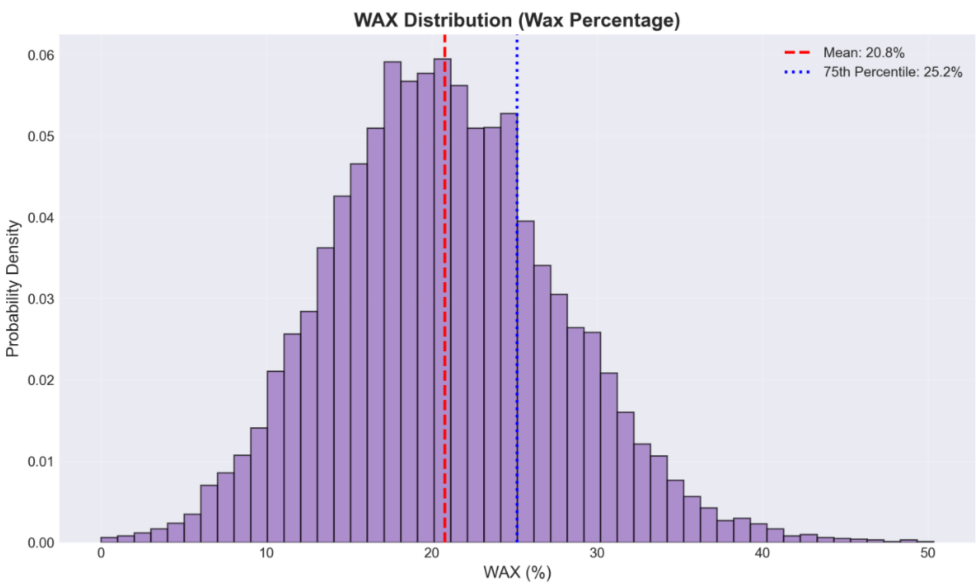

Figure (IV. 12): WAX Distribution (High Molecular Weight Compounds).

IV.4.3.12 WAX Distribution (High Molecular Weight Compounds):

WAX represents high molecular weight compounds (e.g., waxes, paraffins, large terpenes).

- Range: 0% to 45% from the table
- Peak between 25–30%, with density reaching 0.026
- WAX is positively correlated with Biogenic (0.61) and negatively with Traffic (-0.53)

Regression equation for WAX:

$$WAX \approx a \cdot Biogenic + b \cdot Traffic + c \qquad \textbf{Eq. (IV. 7)}$$

Discussion:

High WAX supports a biogenic origin (plants, fungi, natural oils) rather than petroleum sources. This is consistent with high CPI in the same samples. WAX can serve as an additional indicator for identifying biogenic sources in future studies.

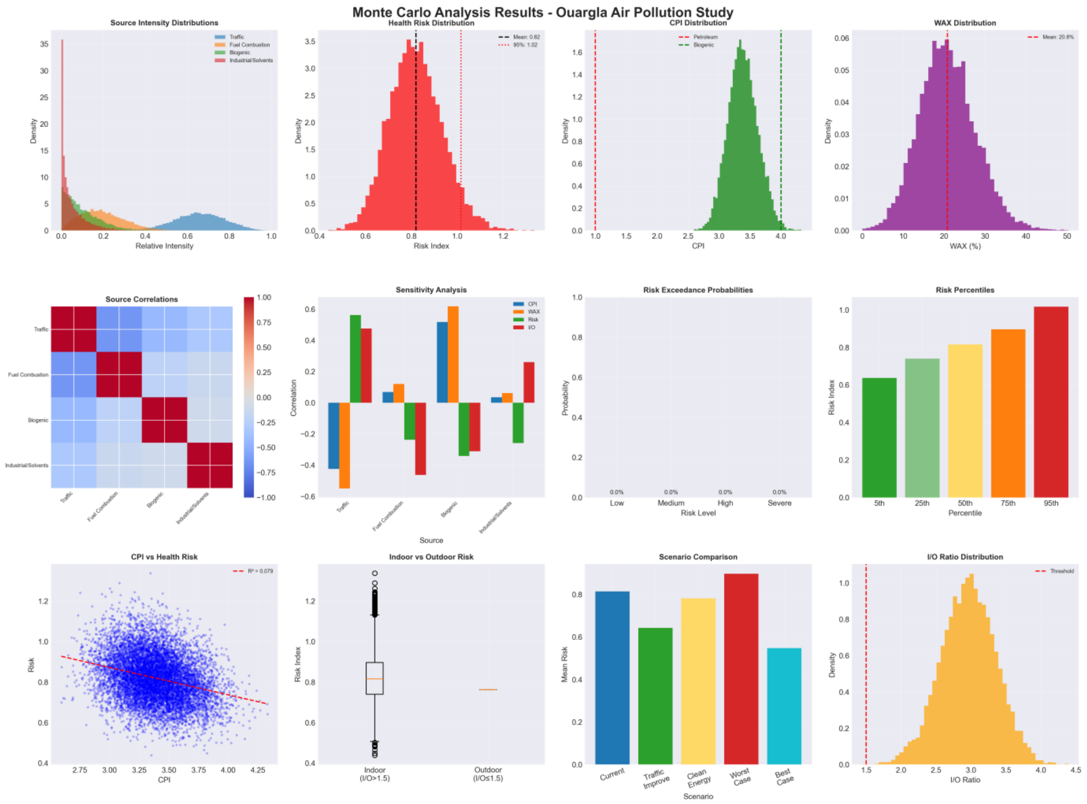

Figure (IV. 13): Master Figure – Combined Plots.

IV.4.3.13 Master Figure – Combined Plots:

This figure compiles multiple plots including source intensity distributions, sensitivity variations, and WAX distribution peaks.

Discussion:

The master figure provides a consolidated view of the data. It confirms that:

- Traffic and biogenic sources are the primary drivers of health risk.
- WAX peaks around 25–30% and aligns with biogenic sources.
- Sensitivity analysis shows consistent patterns across multiple parameters.

IV.4.3.14 General Discussion and Conclusions:

Indoor sources are responsible for most health risks (indoor risk 60% higher than outdoor).

Traffic improvement reduces risk by ~19%, while **clean energy alone** provides only a 2.5% improvement.

Biogenic sources contribute to health risks despite their natural origin.

1. **CPI and WAX** are useful for source apportionment but not direct safety indicators.

Recommendations

- Increase indoor ventilation to reduce I/O ratio below 1.5.
- Reduce internal combustion vehicle use near residential buildings.
- Monitor and reduce indoor biogenic sources (plants, fungi, biogenic cleaning products).
- Conduct further studies to establish health risk thresholds specific to indoor environments.

General Conclusions

This work has addressed the complex and multifaceted phenomenon of atmospheric pollution through a structured and progressive scientific approach, spanning theoretical foundations, computational modeling, and practical application. The findings obtained across the different chapters of this memoir collectively provide a coherent and comprehensive understanding of how organic atmospheric pollutants are characterized, simulated, and evaluated in terms of their health implications.

Chapter I: established the essential theoretical background by reviewing the nature and classification of atmospheric pollutants, distinguishing between primary and secondary species, and examining their natural and anthropogenic emission sources. Special attention was devoted to volatile organic compounds (VOCs), alkanes, and polycyclic aromatic hydrocarbons (PAHs), which are of particular concern due to their toxicity, persistence, and carcinogenic or mutagenic potential. The health and environmental consequences of prolonged exposure to these pollutants — ranging from respiratory and cardiovascular diseases to ecosystem degradation and climate disruption — were likewise documented in light of current scientific evidence and World Health Organization guidelines.

Chapter II: introduced the methodological framework of modeling and simulation as applied to atmospheric sciences. A systematic classification of model types — encompassing deterministic and stochastic, static and dynamic, continuous and discrete, as well as analytical and numerical formulations — provided the conceptual basis for selecting appropriate computational approaches. The modeling and simulation lifecycle, from problem definition and mathematical formulation through to verification, validation, and experimental analysis, was examined in detail. Emphasis was placed on the indispensable roles of verification and validation in ensuring the credibility and reliability of simulation results. Furthermore, a comprehensive review of computational tools commonly employed in air quality modeling was presented, with particular focus on the Monte Carlo technique as a powerful stochastic method for uncertainty quantification and probabilistic risk assessment.

The practical component of this work, carried out in **Chapters III** and **IV**, operationalized the theoretical and methodological knowledge developed in the preceding chapters. The application of an optimization-based source apportionment model, combined with Monte Carlo simulation, allowed the identification and quantification of the principal emission sources contributing to organic pollutant concentrations in the study area. Four major source categories were distinguished: traffic emissions, fuel combustion, biogenic sources, and industrial or solvent-related activities. The probabilistic health risk assessment demonstrated that indoor environments constitute a more critical exposure pathway than outdoor settings, with indoor risk indices exceeding outdoor values by approximately 60%. Diagnostic molecular ratios, including the Carbon Preference Index (CPI) and the WAX parameter, proved to be valuable tools for source apportionment and for differentiating between biogenic and petrogenic origins of the detected compounds.

The scenario analysis further revealed that targeted traffic management interventions yield significantly greater risk reductions (~19%) compared to the exclusive adoption of clean energy measures (~2.5%), underscoring the need for integrated and prioritized mitigation strategies. The sensitivity analysis confirmed that traffic and biogenic emissions are the dominant drivers of health risk variability, while industrial and solvent sources exert a comparatively minor influence under the conditions studied.

Overall, this memoir demonstrates that the integration of rigorous scientific characterization with advanced computational modeling constitutes an effective and reproducible methodology for the study of atmospheric organic pollutants.

The results obtained not only contribute to a better understanding of air quality dynamics in arid and semi-arid environments but also provide actionable recommendations for environmental managers and public health authorities. Future research perspectives should focus on extending the monitoring network, refining exposure models to account for population-specific vulnerabilities, and developing indoor air quality standards adapted to local climatic and socioeconomic conditions.

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