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RESEARCH IN THE FIELD OF AIR QUALITY CONTROL. MEASURMENT VS. SIMULATION

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Abstract: Climate change is more than evident presently, and air quality is essential for both indoor and outdoor environments, playing a crucial role in human health and the overall ecosystem sustainable development. To protect the environment and slow down the phenomena generated by climate change, concrete legislative measures have been implemented, focusing on the main pollutants that can affect the quality of life and public health, and research activities are carried out in all countries. In Politehnica University of Timisoara (UPT) there is a tradition of about 25 years of RENAR-certified activity. The Fuel Analysis, Ecological Investigations and Noxious Dispersion Laboratory (LACIEDIN) carries out measurement and analysis activities of ambient air quality and determines the concentration of certain compounds in flue gases. Direct measurements of air quality parameters involve using instruments and sensors to quantify pollutants and other atmospheric conditions in real time. These measures are critical for assessing pollution levels, ensuring regulatory compliance, and protecting public health. Numerical simulation for air quality evaluation involves using mathematical models to predict the concentration and distribution of pollutants in the atmosphere. These simulations help understand the impact of various factors such as emissions, meteorology, and topography on air quality. By integrating both approaches, policymakers and researchers can gain a more robust and detailed understanding of air quality and make informed decisions to protect public health and the environment. Examples from the experience of the RENAR accredited laboratory LACIEDIN of Politehnica University of Timisoara will be given

Keywords: air quality, accreditation, numerical simulation, environmental measurements, measuring campaigns

1. ACCREDITATION ISSUES

An accredited laboratory is a testing facility that has undergone a formal assessment and evaluation process to ensure that it meets specific standards and requirements. Accreditation is a formal recognition of a laboratory's competence to perform certain types of testing, measurements, or calibrations. The process of accreditation is typically carried out by a national or international accreditation body, which is responsible for evaluating and confirming the laboratory's capabilities.

Figure 1. Interior of the Lab

The Fuel Analysis, Ecological Investigations and Noxious Dispersion Laboratory (www.mediu.ro), coordinated by Prof. Dr. Eng. Ioana IONEL, is holding a national trademark. The lab is an OECs (Conformity Assessment Bodies), and applies SR EN ISO/IEC 17025:2018 standard, by carrying out activities, generally contractual with the economic environment, supporting the functioning of a market oriented towards quality and competitiveness, but also the educational process (for master and PhD students), succeeding that, through technical competence, impartiality and integrity to gain the trust of partners and the awareness of the authorities, the business environment and civil society. Such a lab is necessary, in completion to the national monitoring grid of the Ministry for Environmental protection, as it is mobile, independent and based on modern policies and procedures, in accordance with national and European standards.

Figures 1 and 2 show images from the LACIEDIN laboratory. Figure 3 provides the latest RENAR Accreditation certificate for LACIEDIN, from 2025. Accredited laboratories are essential in various industries, including healthcare, manufacturing, environmental monitoring, and more, as they provide assurance of the reliability and accuracy of their test results or measurements.

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Figure 3. Present outfit of the mobile laboratory, including the truck

Some key characteristics of accredited laboratories include:

- Competence: Accredited laboratories have qualified personnel with the necessary expertise and training to perform specific tests or calibrations.
- Quality Assurance: They maintain rigorous quality control and quality assurance procedures to ensure the accuracy and consistency of their work.
- Valid Test Methods: Accredited laboratories use validated and recognized test methods and procedures, largely based on standardized methods
- Traceability: Measurements made by accredited laboratories are traceable to international standards or recognized references.
- Equipment and Facilities: Accredited labs have appropriate equipment and facilities to conduct their tests or calibrations.

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CERTIFICAT DE ACREDITARE
Nr. LI 1251

Asociaţia de Acreditare din România – RENAR, fiind recunoscută ca Organism Naţional de Acreditare prin OG 23/2009, prin prezentul certificat atestă că organizaţia:

Universitatea Politehnica Timişoara

Timişoara, P-ţa Victoriei nr. 2, judeţul Timiş

prin

Laborator de Analize de Combustibili, Investigaţii Ecologice şi Dispersia Noxelor

îndeplineşte cerinţele **SR EN ISO/IEC 17025:2018** şi este competentă să efectueze activităţi de **ÎNCERCĂRI/EŞANTIONĂRI**, aşa cum se detaliază în Anexa la prezentul certificat de acreditare.

Această acreditare este menţinută cu condiţia îndeplinirii în mod continuu a criteriilor de acreditare stabilite de Asociaţia de Acreditare din România - RENAR.

Prezentul certificat este însoţit de Anexa nr. 1/24.03.2025 (2 pagini), parte integrantă a acestuia.

Certificatul de acreditare este un document de acreditare esenţial, care poate fi revizuit şi emis periodic de către RENAR. Cea mai recentă versiune a certificatului de acreditare este disponibilă pe website-ul RENAR, www.renar.ro.

Data acreditării iniţiale: 27.10.2021
Data actualizarii: 24.03.2025
Data expirării acreditării: 26.10.2025

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Alina Elena TAINĂ

PREŞEDINTE AL CONSILIULUI DE ACREDITARE
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Certificatul de acreditare nu exonerează OEC de obligaţia de a obţine toate aprobările şi autorizaţiile necesare pentru funcţionarea sa conform legii.

Reproducerea parţială a prezentului certificat este interzisă.

Figure 2. RENAR Accreditation Certificate

- Impartiality: Accredited laboratories operate independently and are free from conflicts of interest that could affect the integrity of their results.
- Regular Assessment: They undergo regular assessments and audits to ensure that they continue to meet the accreditation standards.

Accreditation can vary depending on the field of work. For example, a medical laboratory might seek accreditation from a healthcare accreditation body, while a materials testing laboratory might seek accreditation from a materials testing accreditation body.

Accreditation provides confidence to customers, regulatory bodies, and the public that the laboratory's results are reliable and meet established quality standards. It is important for laboratories to play a critical role in product quality, safety, and compliance with regulations.

Teamwork in an accredited laboratory is essential for the effective and efficient operation of the facility, ensuring accurate and reliable testing, measurements, and calibrations. Here are some key aspects of teamwork in an accredited laboratory:

- Roles and Responsibilities: Clearly define the roles and responsibilities of each team member. This includes laboratory managers, scientists, technicians, quality assurance personnel, and support staff. Having well-defined job descriptions and expectations is crucial for smooth operations.
- Communication: Effective communication is critical in a laboratory setting. Team members can communicate clearly with each other, share information, and discuss test procedures, results, and any issues that may arise. Regular meetings and a culture of open communication help maintain a collaborative environment.

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- Training and Skill Development: Ensure that all team members receive proper training and have the necessary skills to perform their tasks. This includes ongoing professional development and staying up to date with the latest techniques, equipment, and standards.
- Cross-Training: Cross-training team members in different areas of the laboratory can be valuable. This ensures that there is redundancy in skill sets and that team members can support each other during peak workloads or in the absence of a colleague.
- Quality Assurance: Quality control and quality assurance measures are integrated into the laboratory's processes. Team members understand and adhere to these procedures to maintain the accuracy and reliability of test results.
- Standard Operating Procedures (SOPs): The laboratory has well-documented SOPs for all testing and calibration processes. These SOPs are followed by all team members to maintain consistency and reliability.
- Equipment and Maintenance: The laboratory team works together to ensure that the equipment is properly maintained and calibrated. Regular checks and maintenance schedules are in place to prevent instrument failures and inaccuracies.
- Sample Handling: Proper sample handling is crucial to prevent contamination or errors. Team members are trained in sample collection, storage, and transportation procedures.
- Problem Solving: Team members collaborate to solve problems and address unexpected issues. This may involve troubleshooting equipment, resolving discrepancies in test results, or investigating incidents of non-conformity.
- Continuous Improvement: Team members are motivated to identify opportunities for enhancing laboratory processes, reducing errors, and improving efficiency. This encourages a culture of continuous improvement.
- Documentation and Records: Thorough and accurate record-keeping is essential; therefore, all team members maintain detailed records of their work, test results, and any deviations from standard procedures.
- Ethical Conduct: Upholding ethical standards in the laboratory, including honesty, integrity, and impartiality is particularly important when dealing with sensitive or regulated materials.
- Safety: To ensure a strong safety culture within the laboratory, team members are trained in safety protocols and follow them rigorously to prevent accidents and exposure to hazardous materials.

Effective teamwork in an accredited laboratory is crucial for maintaining the quality, reliability, and reputation of the lab's services. It also helps meet the requirements set by accreditation bodies and regulatory agencies.

2. MEASURMENT VS. SIMULATION

Both direct measurements and numerical simulations are essential for comprehensive air quality evaluation. When specific pollutant information is needed, the best approach is to use direct measurements. For broad spatial coverage, scenario analysis, and understanding complex atmospheric processes, the numerical simulation is recommended. Integrating both approaches iteratively ensures comprehensive and accurate air quality evaluation.

Direct measurements and numerical simulations both have their strengths and weaknesses in the context of air quality evaluation. The choice between simulation and measuring (direct measurements) for air quality evaluation depends on the specific context, objectives, and resources available.

Both methods have their unique advantages and can be used complementarily to achieve the best results. A common and effective approach is to begin with direct measurements and then use numerical simulations to extend and enhance the insights gained from those measurements.

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3. DIRECT MEASUREMENTS

Direct measurements meet several essential conditions, considered as strengths:

- Accuracy and reliability, as they provide real-time data that accurately reflects current air quality conditions.
- Validation, because they are crucial for validating and calibrating numerical models and ensuring their reliability.
- Specificity, as they can detect and quantify specific pollutants with high precision.
- Temporal resolution, because high-frequency measurements can capture rapid changes in pollutant concentrations.

However, direct measurements also bring with them a few disadvantages, among the most significant of which are:

- Spatial coverage, because measurements are typically limited to specific locations, which may not represent broader regional or global conditions.
- Cost and maintenance, as installing and maintaining monitoring stations is expensive and labor-intensive.
- Data gaps, resulting in bad data coverage due to equipment malfunctions or maintenance.
- Limited scope, because direct measurements alone cannot provide insight into future scenarios or the effects of potential policy changes.

Next, Figure 4 shows some equipment used within LACIEDIN for measuring atmospheric emissions, and Figure 5 shows the mobile laboratory used for air quality monitoring.

Figure 4. Some emission control equipment of LACIEDIN

Figure 5. Mobile laboratory for Air quality control of LACIEDIN

4. NUMERICAL SIMULATION

Overall, numerical simulation is a powerful tool for understanding and managing air quality, providing critical insights that help protect public health and the environment.

Several models are commonly used in air quality simulations:

- Gaussian Dispersion Models: Assumes normal distribution of pollutants. It is used for point source pollution (e.g., factories, power plants). Examples include ADMS for local assessments and EMEP model for transboundary pollution.
- Eulerian Grid Models: Fixed grid system, used for regional to global simulations, solving advection-diffusion-reaction equations on a grid. Examples include CMAQ (Community Multiscale Air Quality), CAMx (Comprehensive Air quality Model with extensions), and WRF-Chem (Weather Research and Forecasting model coupled with Chemistry).
- Lagrangian Particle Models: Track the movement of pollutant particles over time. Examples include HYSPLIT (Hybrid Single-Particle Lagrangian Integrated Trajectory) and FLEXPART.

Numerical simulations require extensive input data, such as emissions data (industrial emissions, traffic emissions, and natural sources), meteorological data (wind speed and direction, temperature, humidity, and solar radiation), topographical data (terrain features which can affect the dispersion and transport of pollutants), and chemical data (reactions and transformations of pollutants in the atmosphere).

The process of numerical simulation typically involves data collection (gathering all necessary input data), pre-processing (converting raw data into a format suitable for the model, model execution (running the model using the pre-processed data), post-processing (analyzing the model outputs, which might involve visualization and statistical analysis), and validation (comparing the simulation results with observed data to assess accuracy).

Numerical simulations are used in various applications:

- Air Quality Forecasting: Predicting pollution levels to inform the public and authorities.
- Policy and Regulation: Assisting in the development of air quality standards and regulations.
- Health Impact Studies: Assessing the potential health impacts of different pollution scenarios.
- Environmental Impact Assessments: Evaluating the air quality impacts of new projects or developments.

Despite their usefulness, numerical simulations face several challenges, such as uncertainty in input data (inaccuracies in emissions inventories or meteorological data can lead to errors in predictions), significant computational resources, complexity of chemical reactions in the atmosphere, making it difficult to model all relevant processes accurately.

5. DIRECT MEASUREMENTS VS. NUMERICAL SIMULATION

Direct measurements and numerical simulations are not mutually exclusive; rather, they are complementary, measurements validate simulations, providing the ground truth necessary for validating and improving numerical models, and simulations fill spatial and temporal gaps in measurement data, providing a more complete picture of air quality. While measurements provide

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current and historical data, simulations can predict future conditions and evaluate potential impacts of changes in emissions or policies.
The approach with the best and most complete results is the one that is based on both approaches and integrates them into a complex system. Thus, the following steps should be followed:

1. STARTING WITH DIRECT MEASUREMENTS:
— Establishing Monitoring Stations: Set up air quality monitoring stations at key locations to gather accurate and reliable data on pollutant concentrations.
— Collecting Baseline Data: Gather baseline data over a significant period to understand the current air quality conditions and identify any trends or patterns.
— Validating and Calibrating: Use the measurement data to validate and calibrate numerical models. Ensure that the models accurately reflect the observed conditions.
2. USING NUMERICAL SIMULATIONS:
— Expanding Spatial and Temporal Coverage: Use numerical simulations to cover areas beyond the monitoring stations and to project future air quality scenarios.
— Scenario Analysis: Simulate various scenarios, such as changes in emissions, weather patterns, or policy interventions, to predict their impact on air quality.
— Understanding Complex Interactions: Use models to analyze the interactions between different pollutants and atmospheric processes, which may be difficult to capture with measurements alone.
3. INTEGRATING AND ITERATING:
— Iterative Process: Continuously refine models using new measurement data, improving their accuracy and reliability over time.
— Integrated Analysis: Combine insights from both direct measurements and numerical simulations to provide a comprehensive assessment of air quality.
— Informing Decision-Making: Use the integrated data to inform policy decisions, public health recommendations, and environmental management strategies.

The following table (Table 1) summarizes the major differences between the two types of approaches in terms of air quality monitoring.

Table 1. Differences between direct measurements and numerical simulations

Aspect	Direct Measurements	Numerical Simulations
Data Type	Real-world observations	Computer-generated predictions
Spatial Coverage	Point locations (limited)	Regional/global (wide)
Temporal Resolution	Real-time/historic	Past, present, and future
Accuracy	High (if calibrated)	Depends on model & inputs
Cost	Expensive (equipment)	Lower (after setup)
Maintenance	High (sensor upkeep)	Low (software updates)
Use Case	Compliance, alerts	Forecasting, policy planning

For an informed and conscious choice of a particular approach to air quality monitoring, it is necessary to think about its purpose: if a measurement campaign is desired that aims to comply with legal regulations and alerts regarding exceeding limit values, which may affect public health, then use the approach based on direct measurements.
If the purpose of the air quality measurement campaign is to develop a pollution forecast, to develop more concrete and targeted public policies, then both approaches will be used, initially the one based on direct measurements, then the one based on numerical modeling, i.e. a hybrid approach.
By combining both approaches, you can achieve a more robust and comprehensive air quality evaluation, leveraging the strengths of each method.

6. DISPERSION MODELING

Dispersion modeling is a computational approach to predict how air pollutants disperse in the atmosphere after being emitted from various sources. These models are essential tools for environmental impact assessments, regulatory compliance, and urban air quality management.

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Overall, dispersion modeling of air quality can be ethical when conducted transparently, with accuracy and accountability, and with the intention of protecting public health and the environment. However, it's essential to remain vigilant about potential biases, ensure equity, and involve affected communities in decision-making processes. The ethics of dispersion modeling for air quality assessment depend on how it's used and the context in which it's applied. In many cases, dispersion modeling is used to assess the potential impact of industrial emissions, traffic pollution, or other sources on air quality.

Table 2. Example of dispersion modeling

Strategy	1 MWth	No of sources	Position of emissions
A (centralized heat system)	Coal with 10 % oil support	1	Outside the city
B (District heating)	Gas	1	In the city, old Power plant
C (individual heating with gas)	Gas	100	100 individual houses heated by individual stoves (gas), on 1000 m x 1000 m

By understanding these impacts, policymakers and regulators can make informed decisions to protect public health and the environment (public benefit). It's important for dispersion modeling to be transparent and accurate.

Ethical considerations should include ensuring that dispersion modeling protects vulnerable populations (equity and environmental justice). People have the right to know how their health and well-being may be affected by air quality and to participate in decisions that impact them (informed consent). The following table (Table 2) presents an example of dispersion modeling, carried out by our laboratory in Timisoara.

Values of air quality (CO), measured in the same central area of Timisoara, used for comparison between the three strategies (A, B, C), are: 1,52/2,99/12,976 μg/Nm^3. The dispersion modeling for these three strategies are presented below, in Figures 6-8.

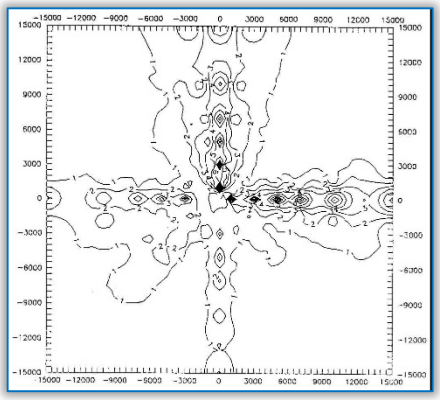

Figure 6. Centralized heat system (strategy A)

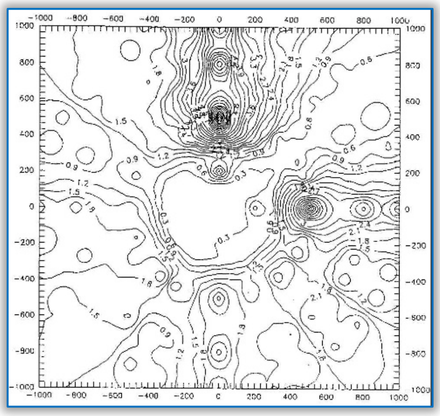

Figure 7. District heating (strategy B)

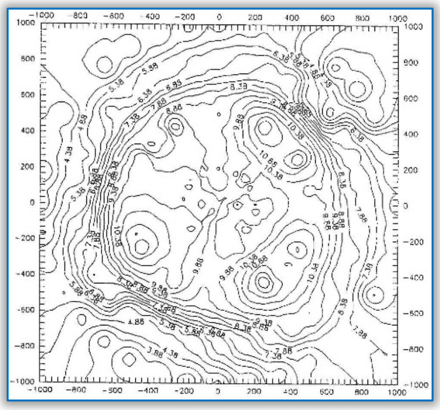

Figure 8. Individual heating with gas (strategy C)

7. CONCLUSIONS

Politehnica University of Timisoara is offering through the Lab for environmental control (LACIEDIN) a real support to the civil, university and economic society in the region, fulfilling its scope, as mentioned by King Ferdinand, by 1920, when signed the legal decree for establishing the Politehnica School in Timisoara, to serve the regional development of the society.

The results of direct measurements carried out within our accredited RENAR laboratory, as well as the inclusion of the numerical simulation approach, by dispersion modeling, ensure the obtaining of valid and sustainable data, which can form the basis for establishing local policies regarding the improvement of air quality.

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