Chapter

Medellin Air Quality Initiative (MAUI)

Andres Yarce Botero, Olga Lucia Quintero Montoya, Santiago Lopez-Restrepo, Nicolás Pinel, Jhon Edinson Hinestroza, Elias David Niño-Ruiz, Jimmy Anderson Flórez, Angela María Rendón, Monica Lucia Alvarez-Laínez, Andres Felipe Zapata-Gonzalez, Jose Fernando Duque Trujillo, Elena Montilla, Andres Pareja, Jean Paul Delgado, Jose Ignacio Marulanda Bernal, Jaime Andres Betancur, Alejandro Vélez, Arjo Segers, Arnold Heemink, Juan Ernesto Soto, Bibiana Esperanza Boada Sanabria and Sara Lorduy

Abstract

This chapter book presents Medellín Air qUality Initiative or MAUI Project; it tells a brief story of this teamwork, their scientific and technological directions. The modeling work focuses on the ecosystems and human health impact due to the exposition of several pollutants transported from long-range places and deposited. For this objective, the WRF and LOTOS-EUROS were configurated and implemented over the región of interest previously updating some input conditions like land use and orography. By other side, a spinoff initiative named SimpleSpace was also born during this time, developing, through this instrumentation branch a very compact and modular low-cost sensor to deploy in new air quality networks over the study domain. For testing this instrument and find an alternative way to measure pollutants in the vertical layers, the Helicopter In-Situ Pollution Assessment Experiment HIPAE misión was developed to take data through the overflight of a helicopter over Medellín. From the data obtained from the Simple units and other experiments in the payload, a citogenotoxicity analysis quantify the cellular damage caused by the exposition of the pollutants.

Keywords: Chemical Transport Model, LOTOS-EUROS, contaminant deposition, airborne measurenments, cellular damage, SimpleSpace

1. Introduction

1.1 Medellin air qUality initiative

Cyber-physical systems are concepts that have been positioned in the area of systems and control, such as the way to integrate different types of information sources in schemes that allow human interaction with machines for proper decision-making. From this perspective, many aspects of man's interaction with the environment in the era of the fourth revolution become a subject of study that must approach in an interdisciplinary way. Although they have been widely discussed worldwide, air pollution problems increasingly are appearing in people's daily lives with higher frequency than before, what has made this problem a center of public attention during the recent years.

This work has a public policy background on human and ecosystem health and its impacts aims to be on the science-based decision-making processes. In the framework of cyber-physical systems, mathematical models require not only initial and boundary conditions to represent the physical and chemical phenomena but the data and convert it into useful information that is reliably transmitted to the computers where these models live. The reduction of uncertainty in the representation of these phenomena, with the aim of control or mitigation of human actions, makes Bayesian data assimilation techniques play a fundamental role. When trying to attack the problem of the ability to make decisions based on mathematical models that accurately predict atmospheric pollutants' behavior in sources, a general approach is necessary to methodically and systematically address each of the issues questions and formalize the research questions.

1.1.1 A brief history

The project named Data Assimilation Schemes in Colombian Geodynamics - Cooperative Research Plan for 2017–2020 Between Universidad EAFIT in Colombia and TUDelft in the Netherlands started in 2016 to reduce uncertainty and incorporating data in large-scale mathematical models. In particular, the modeling of Colombian geodynamics using a chemistry and transport model responds to the complexities of atmospheric dynamics in the country due to its global location and the rugged terrain determined by the Andes mountain range system.

As in [1] The peculiar topography (such as abrupt elevation changes, with narrow inter-mountain valleys over 1000 meters deep, and transitions from sea level to over 5000 meters in less than 200 km), the environmental conditions of the region (such as the bi-annual transit of the Inter-Tropical Convergence Zone, and the irregular behavior of the El Niño Southern Oscillation) generate atmospheric conditions that impoverish air quality. The Tropical Andean Region (TAR) geographical singularities present unprecedented challenges for modeling atmospheric chemical dynamics.

However, this is not just a chemical modeling problem. The chemistry and transport models used to determine air quality aspects require meteorological (short term) and climatic (long time) information that allows them to reproduce the atmosphere's physics state. These numerical weather prediction (NWP) models are also problematic in terms of phenomenology, susceptible to initial and boundary conditions, and the effects of the numerical solution methods of these equations. This, without considering the difficulty of modeling the microphysics parametrization in terrain as complex as Colombia and neighboring countries in the TAR.

In this scenario, Bayesian data assimilation techniques for incorporating information into models play a fundamental role improving this atmosphere states. It is required to use different source of information such as satellite information for example GOES16, radar, metar, SYNOP, sounding probes, measurements on-site, and airborne measurements to complete the meteorology scenario in Colombia to achieve models with greater prediction capacity of meteorological phenomena that impact the chemistry representation of the atmosphere. The former questions arise and the research project called Sensitivity and uncertainty sources in numerical modeling to forecast atmospheric systems: High-resolution WRF model simulations in urban valleys applied to air quality issues. Was written in 2017 an effort to focus on the meteorological fields for the complex TAR.

The estimation of states and parameters represents mathematical challenges that must approach from the estimation theory, the numerical analysis, and control theory. It is here where not only technological and computational aspects give rise to questions that allow quantifying the uncertainty for applications not only of air quality in human health and ecosystems but also in factors such as navigation and air safety.

Speaking of atmospheric knowledge, in the effort to know and adequately model the country's meteorological conditions, a series of institutions whose mission is aligned must be incorporated. In terms of scientific research, university researchers tend to answer more fundamental questions regularly. Numerical models such as the WRF (Weather Research Forecast) and Chemical transport Model (LOTOS EUROS) can be coupled to use meteorology to improve the representation of the reality. Institutions such as the Colombian Air Force (FAC) daily solve high-value scientific problems in their mission of guaranteeing the safety of air navigation (Air navigation direction - Dirección de navegación aerea DINAV and the Centre of Technological Development for Defense CETAD). The data assimilation techniques in meteorological prediction models such as WRF vary from the variational in three dimensions to approximations using particle filters and location. None of them is cheap computationally and requires an infrastructure not only for computing but also data, information, and knowledge. Techniques of fusion of meteorological data and 3D variational assimilation in the WRF model existing in the FAC allowed the universities' researchers to pave the way to determining sources of inertness and quantification of the sensitivity of the models to focus efforts on modeling and parameterization of atmospheric phenomena.

Medellin Air Quality Initiative: MAUI aims to bring together local, regional, and international experts on subjects related to air quality and its impact on human and ecosystem health to establish a knowledge network, gather the available tools to tackle the problem, and identify knowledge gaps to contribute to a deeper understanding of the local and regional scale of the impact of air pollution, motivate research collaborations, and inform public policy [2].

Until now, several universities and the state institutions efforts began to align in search of the Colombian atmosphere's representation. The particularities of the country's principal cities and the vulnerability of Colombian biodiversity offer a field of research where the questions and the rigor they must be answered give rise to interdisciplinarity spaces. In MAUI, larger-scale aspects such as numerical models and the integration of satellite information and data from various sources are integrated, and research results at the micro and nanometric level are incorporated.

Chemistry and transport models require emissions inventories within their initial and boundary conditions regularly updated by environmental authorities. This statement is entirely proper for Europe and the United States, but in Latin America, some ethnographic and political factors mean that the agencies in charge of them cannot give prompt answers. The uncertainties in dedicated emissions inventories generate problems of over and underestimating the models. The assimilation of data from the high, medium, and low-cost sensor networks can help the models improve the representation of dynamics in various magnitude orders. However, the information on the concentration of pollutants such as 10 and 2.5-micron particulate matter or tropospheric ozone and nitrogenous is not complete.

The use of European emissions inventory leads to revising the biogenic and anthropogenic emissions and revisiting the current national emissions inventory. Several experts joined the effort, and some preliminary and results are close to being published. However, it is a reality that with the rapid growth of cities in Latin America and the poor planning of land use, an inventory regularly does not end up being updated on the date of its launch. Some modeling experiments showed how large Colombian cities behave like volcanoes that expel pollutants to the country's protected areas.

Other potential forms of emission modeling appear when using traffic information from large cities to estimate density, flow, velocity, and behavior models that allow the short, medium, and long term to understand the dynamics of emissions from traffic. This question is not easy to solve either and in the project Scale-FreeBack from the Research at the National Center for Scientific Research (CNRS) in France [3] aims to understand when and how a complex, large-scale network system can be represented by a scale-free (low complexity) model usable for control design, understanding how the internal states of a scale-free network system are monitored and estimated using information originating from sources of various kinds. This project aims to know how it will be possible to design scale-free control algorithms and make them resilient to changes of scale, node/link failures/disconnections/attacks, and how can those ideas be applied to large-scale road urban networks. MAUI initiative used their ideas and joined their team for the emission modeling and estimation research.

Using available mobility information and merging it with previous knowledge of the inventories of static emissions and other sources incorporates the ability to control within the extensive cyber-physical system the number of pollutants emitted into the atmosphere city and eventually mitigate its effect. The mathematical and control problems are not easy to solve, but the results of the beginning to bear fruit in the chain of description and modeling of air chemistry within and outside cities.

In 2016, simultaneous work was being done on the magnetic characterization of the particulate material of Medellín analyzed atmos9070283 via optical spectroscopy to determine the presence of ferromagnetic material in the 10 and 2.5-micron particulate. This research naturally raised more questions about the possibility of using analogous methods of validation of the results of the models and the potential quantification of exposure levels. The biosensors' findings allowed incorporating more advanced passive sensing techniques and subsequent analysis with optical spectroscopy. The PARTICLE VISION group joined the MAUI capabilities.

Particle Vision is a highly qualified team with long-standing experience in particle analysis, aims to develop innovative analytical methods for the characterization and quantification of particles and apply them to a wide variety of questions. With its technology and support from FAC SEM/EDX instruments, the project made progress in knowing the city's chemical and morphological characteristics of Medellin's particulate material. These investigations have potential impacts on public health issues but are beyond the scope of this book chapter.

Thus, the knowledge at the microscopic level of urban particles' components allows establishing models of validation of numerical results of environmental chemistry. At the local level, nanotechnology has the technical-scientific capacity to develop electrospinning polymeric nanofibers to capture finer particles and offer an additional ability to the analytical aspects of environmental pollutants. This ability represents a leap in scale in orders of magnitude and value since it is possible to obtain particulate material in nanofibers and generate a solution from them that allows evaluating their damage capacity at smaller scales.

The work team is recently completed with experts in in-vitro and in-vivo biological models that, from the nanofibers' material, can analyze and quantify cellular and molecular damage using state-of-the-art techniques.

Our curiosity and technical capacity then led us to advance in different sampling techniques, and in 2019 the first airborne pollutant measurement mission called Helicopter Insitu Pollution Acquisition Experiment HIPAE was carried out. In this mission, the counting instruments for particulate matter, nanofilters, measurement units (inertial, geoposition, meteorological, and gasses measurements) build by the EAFIT spinoff SimpleSpace, and passive samplers attached to air pumps to simulate the expected breath air flux through them. The helicopter with the instruments traveled through the Aburra Valley at different heights. In this aircraft of the Colombian Air Force (FAC), not only gases and meteorological variables were measured, but contamination profiles were established, and the experimental model's evaluation was carried out.

The research groups, researchers, and students linked to this proposal compose an interdisciplinary group that has been working not only on the understanding of atmospheric phenomena, chemistry and transport of pollutants, assimilation of data, and artificial intelligence but also on studying the impact of anthropogenic activity on air pollution dynamics with effects on human health, ecosystems, and agriculture.

The result of this research history will be expanded a little more with the development of this chapter, sending the reader to the primary references of the works where they can obtain specific details of the principal methodologies, techniques, and findings of each area knowledge participating in MAUI.

Detailed review and explanation of some regional and worldwide initiatives similar to ours can be found in the critical review of QuinteroMontoya2020, and the recent paper of Advances in air quality modeling and forecasting BAKLANOV2020261. Some of the remarkably similar missions to HIPAE will be addressed in the following sections.

1.1.2 Scientific and technological directions

As a consequence of this interaction, much more specific goals are proposed in two directions: human health and ecosystem health. In the former direction, the research program called $ExPoR^2$ is proposed.

Exposure to Pollutants Regional Research $ExPoR^2$ aims to develop models of human exposure to air pollution in urban areas as a decision-making tool. Our purpose is to develop high-level scientific research that enables science-based decision-making and solutions to environmental and sustainability problems due to air pollution in human health, agriculture, and ecosystems. Three different research paths are going to be followed:

1. Ensemble of models to estimate human exposure to atmospheric pollutants. The General purpose is to develop an assembly of models to estimate human exposure to atmospheric pollutants in different areas of the Aburrá Valley. Specific objectives: Coupling the WRF model with the Open LOTOS-EUROS models at high resolution to simulate concentrations and dispersion of pollutants within the Aburrá Valley. Implement traffic models for the Aburrá Valley, to simulate the zonal contributions to atmospheric pollutant concentrations by the automotive fleet. Assimilate and merge data from various sources on concentrations of atmospheric pollutants. Coupling

high-resolution simulations of concentrations and dispersion of pollutants with data on human activity and occupation to estimate levels of human zonal exposure to air pollutants. Chemical and morphological profiles of the nano and microparticulate material present in the air of the Aburrá Valley. This research aims to establish the chemical and morphological profile of the nano and microparticulate material present in the Aburrá Valley air to establish its toxicological effect. Establish sampling areas and measurement periods to capture particulate matter of different sizes with the three filtration systems. Chemically and morphologically, characterize the particulate material present in the Aburrá Valley to identify the emission source and Manufacture nanofiber membranes from the selection of polymers with different surface energies to favor the capture of ultrafine particulate material.

2. Cytogenotoxicity of air pollutants. This research will particularly develop an in vitro evaluation model of the impact of particulate material on the health of the occupationally exposed population of the Aburrá Valley. Through this, build a zoned profile of the cytogenotoxic potential of particulate pollutants in the region. Specific objectives: To evaluate the sensitization, irritation and dermal corrosion of PM of different sizes collected with DRMPs, in 2D and 3D in vitro cell models. To evaluate the irritation and serious ocular damage of PM of different sizes collected with DRMPs, in 3D in vitro cell models. To evaluate PM's cytotoxicity and genotoxicity of different sizes collected in different city center areas in 2D and 3D in vitro cell models. To evaluate the mechanism of action of particulate matter in atmospheric pollutants on the distribution of cell cycle phases, mitochondrial activity, and the induction of senescence. Generate a Biosensor transgenic line by inserting the Hyper gene to detect intracellular ROS production after exposure to particulate matter from atmospheric pollutants. Relate the biological effects in vitro with the morphological and chemical composition of the particulate material collected in the different areas of the Aburrá Valley.

Focusing on the health of ecosystems and the various implications that cities can have on protected areas, the research program *3D + 1 Air Pollution Study: In situ, Surface, Remote Detection and Atmospheric Modeling Measurements" 4D Air - MISDAM*. The objectives of this research are oriented to develop remote laser and in situ detection technology to characterize pollutant particles and improve the precision of assimilation techniques in atmospheric modeling.

Some main goals of our current research directions are:

1. Design and implement a multi-channel laser remote detection system to obtain in real time the volumetric concentration of atmospheric aerosols.

2. Design and implement network sensors for in situ and surface monitoring of particulate matter, NO2 and O3 with aerospace technology.

3. Develop and implement the signal inversion algorithm backscattering of atmospheric aerosols.

4. Develop and implement the experimental model and the depolarization signal calibration algorithm for tropospheric aerosols.

5. Estimate the operating parameters of the HSI-DOAS instrument for its operation in the geomorphological and climatic conditions of northwestern South America.

6. Carry out joint measurement campaigns of remote and in situ detection systems on the surface to obtain the microphysical and radiative properties of the atmospheric components (gases and particles) in the Aburrá Valley.

7. Demonstrate the scientific relevance of determining the chemical and morphological characteristics of particulate matter as a differentiating element in determining sources of pollutants.

8. Compositionally and morphologically characterize the coarse particulate material (PM10) and (PM2.5) present in the city of Medellín through the use of SEMEDX techniques, in order to carry out a categorization of sources corresponding to the production of this particulate material.

9. Study the regional dynamics of emission and deposition of pollutants and their effect on protected areas, ecosystems and agriculture and their impact on biodiversity, its evolution and conservation.

10. Develop large-scale model evaluation techniques using robust functional data analysis techniques applied to modeling pollutant transport at high spatial resolutions within the Aburrá Valley.

11. Develop new and better data assimilation schemes in complex systems studying the problems of uncertainty, not Gaussianity, taking into account the problems of spatially dispersed data. With applications in the study of the dispersion of pollutants in the Aburrá Valley.

Additionally, MAUI's research path will allow obtaining results that extend not only to society in matters of public health but also to become antecedents of regional positioning in science and technology and aerospace technology's knowledge.

The confluence of public and private universities with the Colombian state through the Colombian Air Force and the Ministry of Sciences allows the work's speed to be doubled. The results also led to improved quality of life and the protection of biodiversity and economic growth.

At the national level, our purpose is to scale our research to the entire territory. Expand our goals to human and ecosystem health to guarantee our national resources and proper land use. To achieve this, it is evident that meteorological modeling and data incorporation to the models via assimilation must be carried out.

Colombian Air Force system for meteorological information (in Spanish, Sistema de Información meteorológica de la Fuerza Aerea Colombiana -SIMFAC) is the integrated and operational system for meteorological information for military forces and public state aviation. SIMFAC operates with the Weather Research and Forecasting (WRF) model version 4.1 under the 3DVar data assimilation scheme. Our multidisciplinary team seeks to review and test the performance of the current implementation of the data assimilation techniques on the WRF model, looking to understand the technique's results in 3DVar implementations for a known micro-physics. In order to achieve this, we use the micro-physics parameterization of the SIMFAC to generate a background on the WRF model and, via comparison against the 3DVar implementation using satellite, radar, and in-situ observations, Potential improvements of the 3DVar implementation were verified, looking for an accurate assessment and determining the potential risks for air navigation. Our main goal is to scale the operational set up to 4DVar implementation to enhance the Colombian Air Force's capabilities.

Observational and model weather records are a source of valuable data since hydro climatological variables like precipitation are recorded through time. Functional data analysis (FDA) encompasses different numerical and statistical methodologies that could help separate climate variability aspects and explore their consequences, improving the system understanding. These methodologies seek to represent the data in ways that aid additional analysis, highlighting different data characteristics. Further, a comparison between observational and model functional data analyses would serve as a model evaluation technique. FDA is used to compare two or more sets of data concerning certain types of variation, where two sets of data can contain different sets of replicates of the same functions or different functions for a standard set of replicates.

The FDA seeks to group multivariate functional data, identifying homogeneous groups without using any additional label to the model's records. The objective is to promote a classy and compare it with a natural and intuitive geographical classification offering a basis for the correction of biases.

With the achievement of a correct and precise representation of the national meteorology at different time scales, different objectives are achieved that are fundamental for studies of climate change, air pollution, and protection of Colombian biodiversity. Additionally, the national airspace's flight safety standards increase with information from different sources via data assimilation and deep learning techniques. Significant improvements on command and control for national security are part of the non-predicted results of our joint effort.

It is undeniable that thanks to the concern to attend to human health and ecosystems' relevant problems, it has been possible to articulate a network of knowledge that can also leverage Colombia's aerospace development. This is based on the development capacity of low-cost sensors with CanSat technology developed from the Spinoff SimpleSpace, which, due to their versatility in modularity and adaptive communications for different scenarios, allows the completion of the temporal space measurements, reducing the covariance of the state matrices and measurements in the assimilation of large scale models. Additionally, some preliminary results of the work team's ability to measure over the airspace with SimpleSpace units aboard Colombian Air Force aircraft show how data use can lead to precise knowledge and strategies for making environmental decisions matters.

Regarding human health, in a section, we will present some results obtained in the HIPAE mission where analysis of the particulate material captured with polymer nanofibers was carried out through cellular and molecular analyzes.

The Tropical Andean countries (Venezuela, Colombia, Ecuador, Peru, and Bolivia) face deteriorating air quality. When thinking about the assimilation of data and intelligent systems for data fusion or automatic learning, the quantity and quality of the sources begin to be a concern.

If a complete understanding of TAR's atmospheric dynamics is desired, satellite information on land use and chemical species combined with images of unmanned aerial vehicles is becoming a viable option for developing land-use models.

In the subsequent sections, the reader will find some scientific and technical details of the activities carried out by MAUI. In particular, we have selected some sections that are not published. In them, aspects of ecosystem health and the influence of the correct estimation of land use parameters to determine deposits of species such as nitrogenous are discussed. Also, the models with which our team has been advancing data assimilation techniques, artificial intelligence, and coupling are presented. We mention some hypothetical modeling scenarios where meteorological information can give relevant clues about the influence of cities' emissions and their impact on surrounding areas such as water sources.

Factors such as reducing uncertainty in the topographic representations and land cover in the tropicalization of models developed in other latitudes are briefly mentioned. The need to know and make this type of knowledge technologically independent has led to the emergence and potentiation of several technological developments such as SimpleSpace units and LIDAR 4D systems that are not specifically mentioned due to their current state design.

It is expected to advance in the development of more frequent measurement campaigns, but during 2020 they have been suspended as MAUI researchers overturn our ability to respond with science for the country in the situation of COVID-19. Our computing, nanomaterials, and cellular and molecular biology laboratories had to slow down the expected results. However, the design of additional sampling mechanisms means that in 2021 we announce a new airborne measurenment platform dedicated to meteorology and air quality.

Finally, concrete examples of the data assimilation for applying contamination by the particulate matter of 10 and 2.5 microns are presented in the second chapter of this book. These sections will be partially published in magazines on the subject in a short time.

We hope that our work experience, scientific findings, technological developments, and research directions allow the reader to define the strategy that best suits him for the correct knowledge of the surrounding systems, however, even more so for developing strategic decision-making tools in public health, environment, biodiversity, air safety, and national security. None of the above can be achieved without a network that involves actors from different sectors and researchers from many specialties.

2. Modeling pollution for health: human and ecosystems

2.1 Ecosystem health

This work presents the implementation of the LOTOS-EUROS regional atmospheric Chemical Transport Model (CTM) on Northwestern South America. The impact of land use and orography update in the model was analyzed to identify potential vulnerable natural areas by quantifying atmospheric deposition pollutants. CTMs allow simulating the physical dynamics of trace gasses and aerosols, including processes such as emission, chemical reactions, transport, and deposition. The deposition of atmospheric contaminants like nitrogen dioxide (NO_2) and ammonia (NH_3) induces chemical fluxes in natural ecosystems, with potential subsequent severe impacts like biodiversity loss. Due to the vast geographical diversity present in the study area, the LOTOS-EUROS model was updated for the land and topography inputs to simulate more representative conditions for the study region. Depositions were very sensitive for the change of land cover maps used in the model, and on the other side, topography update impacts more in the high layer of the model above harsh terrain. Additional simulations for the updated scenario using point sources were performed to identify the deposition area's spatial extent for the principal Colombian cities.

Through atmospheric transport and deposition, emitted pollutants from different anthropogenic and natural sources can alter remote ecosystems' dynamics [4, 5]. Atmospheric deposition is described as the mechanism that induces a flux of gasses and particles to the land surface due to meteorological, chemical, and biological phenomena [6] which is responsible for the balance concentration change of the different soil components.

Anthropogenic activities are significant sources of reactive nitrogen (N_r) to the atmosphere [7]. Photochemical reactions of NO_x and NH_3 create secondary inorganic aerosols [8] that can be transported over large distances [9]. Long-distance transport of secondary inorganic aerosol accounts for over 8% of the planet's reactive nitrogen flow in terrestrial ecosystems [7], and a significant source of Nr to the ocean [10]. Deposition of atmospheric N_r alters oligotrophic ecosystems [8, 11], affecting the distribution of communities of species [12–16] and ecosystem stability [17]. NO_2 is a gas emitted by anthropogenic and natural sources as part of the family of the nitrogen oxides $NO_x(NO+NO_2)$. NO_2 is emitted from anthropogenic (industrial activity, transport, and biomass burning) and natural (NO_x soil emissions and lighting) sources. Agricultural activities and livestock feedlot operations are the primary sources of atmospheric NH_3, followed by wood-burning (including forest fires) and to a lesser degree fossil fuel combustion. Acute exposures to NH_3 near its origin (4–5 km) can lead to substantial foliar damage to the plant, growth and productivity decrease [18].

Atmospheric ozone exposure can cause ecological and agricultural harm (e.g., [19] and references therein), so it also poses a risk to protected areas. The identification of natural and agricultural areas that may be excessively exposed to ground-level ozone will allow us to estimate the detrimental impact that urban pollution may be having on our protection and agricultural efforts.

Páramos are high-altitude ecosystems that serve as water supplies for a large part of Colombia and as suppliers of critical ecosystem services, they are protected under Colombian law. The following picture shows a quantification analysis of the paramos ecosystems (**Figure 1(a)**) and natural protected areas (**Figure 1(b)**) delimitation, quantifying the model output and the total deposition those areas are receiving.

The Paramo de Las Baldias was the paramo zone with greater exposure to atmospheric pollutants. It receives 14 kg/(ha yr), above the standard critical load of Nr, and above 60 kg/(ha yr) of ozone. The paramos of western Antioquia receive 5–6 kg/(ha yr), while the Sonson Paramos are identified as those with the lowest exposure to atmospheric pollutants (2.2–2.6 kg/(ha yr) Nr; 35–40 kg/(ha yr) ozone). The west of the Caribbean coast ecosystems receives the highest ozone load nationwide (50–100 kg/(ha yr)).

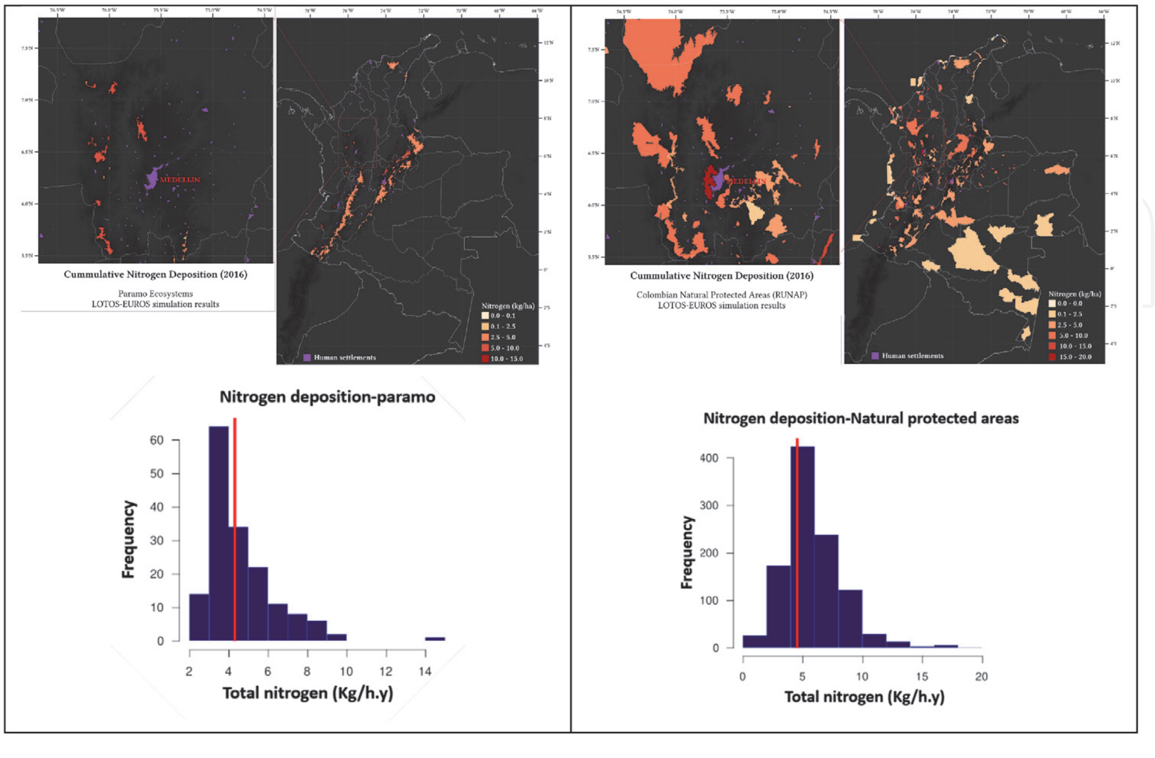

Figure 1.
Simulated calculation of annual (2016) deposited nitrogen budget for natural protected areas and paramo ecosystem.

Figure 1 shows a histogram quantification over the natural protected areas and paramo ecosystems to identify the critical deposition load of NO_2 in ecosystems and how many areas are at higher risk for the transport of pollutants. The critical load in a tropical ecosystem is not very well determine, and probably, due to the high biodiversity index in this region, the critical load should be less.

2.1.1 The WRF (weather research and forecasting) model

The WRF (Weather Research and Forecasting) model is a numerical weather prediction and atmospheric simulation system designed for research and operational applications. This model tries to advance the understanding and prediction of mesoscale weather and accelerate the transfer of research advances into operations. This model mainly is the result of the effort of the National Center for Atmospheric Research (NCAR) which is operated by the University Corporation for Atmospheric Research (UCAR), but, have contributions of many other sources, like Mesoscale and Microscale Meteorology (MMM) Division, the National Oceanic and Atmospheric Administration's (NOAA) National Centers for Environmental Prediction (NCEP) and Earth System Research Laboratory (ESRL), the Department of Defense's Air Force Weather Agency (AFWA) and Naval Research Laboratory (NRL), the Center for Analysis and Prediction of Storms (CAPS) at the University of Oklahoma, and the Federal Aviation Administration (FAA), so like contributions of researchers and Universities [20].

It's worth pointing out that for the operations of a model like WRF is necessary to set aspects like parameterizations, boundary and initial conditions. So, usually, if it desires to evaluate the performance of a model like WRF in a domain, different configurations are used, for example, changing parameters the initial and boundary conditions [21], doing online modeled [21, 22], modified the planetary boundary layer schemes, micro-physics, land-surface models, radiation schemes, sea surface temperature and 4-dimensional data assimilation [23] or to integrate new methodologies such as data assimilation [23, 24]. This aspect correspond to the physic options of the ARW, grouped in the micro-physics, cumulus parameterization, planetary boundary layer (PBL), land-surface model and radiation [20]. These options are important because they let obtaining a solution that according to the particularities of the work domain. It important to say that an important research for us is developed in Cauca river valley-Colombia, by [25], where the topography is similar to Aburrá Valley. This team try with convective parameterization schemes KF, BMJ, and G3D and show that the best is schemes KF.

With WRF model is possible to understand the behavior of a meteorological variable set through simulations, where the parameters of the model are configured in relation with the domain [21, 22, 26–29] of study like the Aburrá Valley that is our interest. However, here the intention is to understand initially the behavior of the model to alteration or modification in the information that received, particularity, the initial conditions.

One part from WRF model is its solver, ARW module or the Advanced Research WRF (ARW). Through this module is possible to producing a simulation [20]. The ARW is really important in the representations of the modeled in WRF. this component is composed by several programs for the idealized, and real simulations, as like as numerical integration program[1]. As ARW is the solver of WRF, this one have the mathematical representation of the physic and/or meteorological process, in

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[1] http://www2.mmm.ucar.edu/wrf/users/docs/user_guide_V4/WRFUsersGuide.pdf, Consulted: September 10 2018.

general this is represented by a set of partial differential equations obtained of the flux-form Euler equations.

The WRF (Weather Research and Forecasting) model is a numerical weather prediction and atmospheric simulation system designed for research and operational applications. However, this model's behavior depends on domain configuration, physic parameterizations, boundary and initial conditions, and terrain characteristics. The model has to be configured according to the researchers' interest or particularities characteristic of the domain of interest and the information available for assimilation purposes. For this reason, one way to improve the model's performance is to use data assimilation for integrating additional information to understand the dynamics in an irregular territory like Colombian geography.

The accuracy of the numerical weather prediction is limited by the precision of the mathematical and physical representations of reality, bringing uncertainty from the initial and boundary conditions incorporated into a numerical model.

In WRF, the implementations of data assimilation cover since hybrid method as ensemble transform Kalman filter–three-dimensional variational data assimilation (ETKF–3DVAR) system [30], three dimensional variational data assimilation 3DVAR, four-dimensional variational data assimilation (4Dvar) [31–33], or ensemble methods as [34–38].

2.1.2 The LOTOS-EUROS model

The LOTOS-EUROS (LOng Term Ozone Simulation- EURopean Operational Smog model) [39] is a chemical transport model that models in three dimensions different species in the lower troposphere. This model was developed in 2004 by TNO and RIVM/MNP organizations, in The Netherlands, unifying the previously developed LOTOS and EUROS models. At the beginning it was developed as a model focused on ozone, but currently, the LOTOS-EUROS calculates concentrations of ozone, particulate matter, nitrogen dioxide, heavy metals and organic components [40]. LOTOS-EUROS has been widely used in different projects around the world, demonstrating the capacity of the model [41]. The dynamics of pollutants in LOTOS-EUROS is regulated by processes of chemical reactions, diffusion, drag, dry and wet deposition, emissions and aversion [42]. The LOTOS-EUROS dynamics are given by:

$$
\begin{aligned}
\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} + V\frac{\partial C}{\partial y} + W\frac{\partial C}{\partial z} &= \frac{\partial}{\partial x}\left(K_h\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_h\frac{\partial C}{\partial y}\right) \\
&\quad + \frac{\partial}{\partial z}\left(K_z\frac{\partial C}{\partial z}\right) + E + R + Q - D - W
\end{aligned} \tag{1}
$$

where C is the concentration of a specie; U, V and W, are wind components in West–East, South–North direction and vertical direction, respectively; K_h and K_z are horizontal and vertical coefficients of diffusion by turbulenc; E represents the entrainment or detrainment due to variations in layer height; R represents generation and consumption rates of pollutant by chemical reactions; Q is contribution by emissions and D and W are loss by dry and wet deposition process, respectively.

The main equation of LOTOS-EUROS dynamics is composed of different operators. Each one models different components of pollutants behavior. The operators that compose the LOTOS-EUROS are: i) the transport operator, ii) the chemistry operator, iii) the dry deposition operator, and iv) the wet deposition operator. Emissions and values related to meteorology are directly taken as input data. The transport operator consists of the dynamics of advection in three dimensions, diffusion and entrainment. The chemistry operator models everything related to the production and consumption of components by different chemical reactions in the atmosphere. The dry deposition is divided in two phases, the dry deposition of gases and the dry deposition of particles. The dry deposition of gases is modeled through the transfer of gases between the land surface and the atmosphere, result of the difference in concentrations and resistance between them. In the dry deposition of particles the scheme used depends on the given land use over the analysis region. The operator of wet deposition is modeled through the below cloud scavenging process. The below cloud scavenging process uses a sweep coefficient that describes the mass transfer speed of a pollutant from the air to the raindrops.

The LOTOS-EUROS model as other CTMs, is considered a high-uncertainty system due to the large number of uncertainty sources like meteorology, emissions, depositions parameters, among others. Additionally it is a high-dimensional system since the solution of Equation (1) is executed for different components and in each point belonging to a grid on the region of analysis. Due to this process, the state vector has a dimension in the order of millions.

The simulation of the deposition of atmospheric species is a challenging task highly dependent on whether the phenomena are modeled in the near, local or long-field range. Near-field deposition is dominated by larger particles. Local field events occur in the portion of the plume dominated by the wind-driven trajectory where the peak-to-mean concentration ratios are much smaller than closer to the source, resulting in more uniform deposition patterns. In long-range fields the larger particles have been removed so smaller particles are the main concern of the modeling [43]. The parameters that describe the deposition phenomena are highly uncertain, especially when land use and vegetation type data are low in detail or spatial resolution. Existing models of atmospheric deposition might not be appropriate for simulating deposition fluxes around urbanized environments, which present varied and rapidly changing forms of land use [44]. This study focuses on the impact of updating the land use data on the estimates of nitrogen deposition in Colombia. Whereas previous studies were limited by the use of rather coarse spatial resolutions [45, 46], here a resolution of 0.09° x 0.09° was used to increase the level of detail in the simulations. The sensitivity to input (land use and topography) modifications was studied to determine the impacts on the model deposition predictions. Additionally, point source experiments were conducted to start to understand the spatial deposition dynamics of N_r emanating from the principal urban areas of Country. This work contributes in assessing the performance of the LOTOS-EUROS CTM in NW South America.

In order to have a model that represents the principal meteorological, chemical and transport dynamics over a region is important first to improve as much as is possible the input information. Two input information were updated for the LOTOS-EUROS implementation over the northwest-southamerica region, the orography and the land use information.

The default elevation model for LOTOS-EUROS is obtained from the ECMWF meteorological data, which has a resolution of 0.07° (≈ 7 km). An updated elevation model used for the region was obtained from the Global Multi resolution Terrain Elevation Data (GMTED 2010) [47], with a resolution of 0.002° (≈ 220 m). **Figure 2** shows a comparison between the default (**Figure 2(A)**) and the updated elevation model (**Figure 2(A)**). The inset zoomed in around the Aburrá Valley (Medellín and neighboring munici-palities) demonstrates how the valley is entirely absent in the default elevation model (**Figure 2(A)**).

LOTOS-EUROS interpolates the input elevation data within each grid cell according to the resolution of the simulation. Changing the input elevation model can generate changes in the outcome of variables such as the temperature profiles of

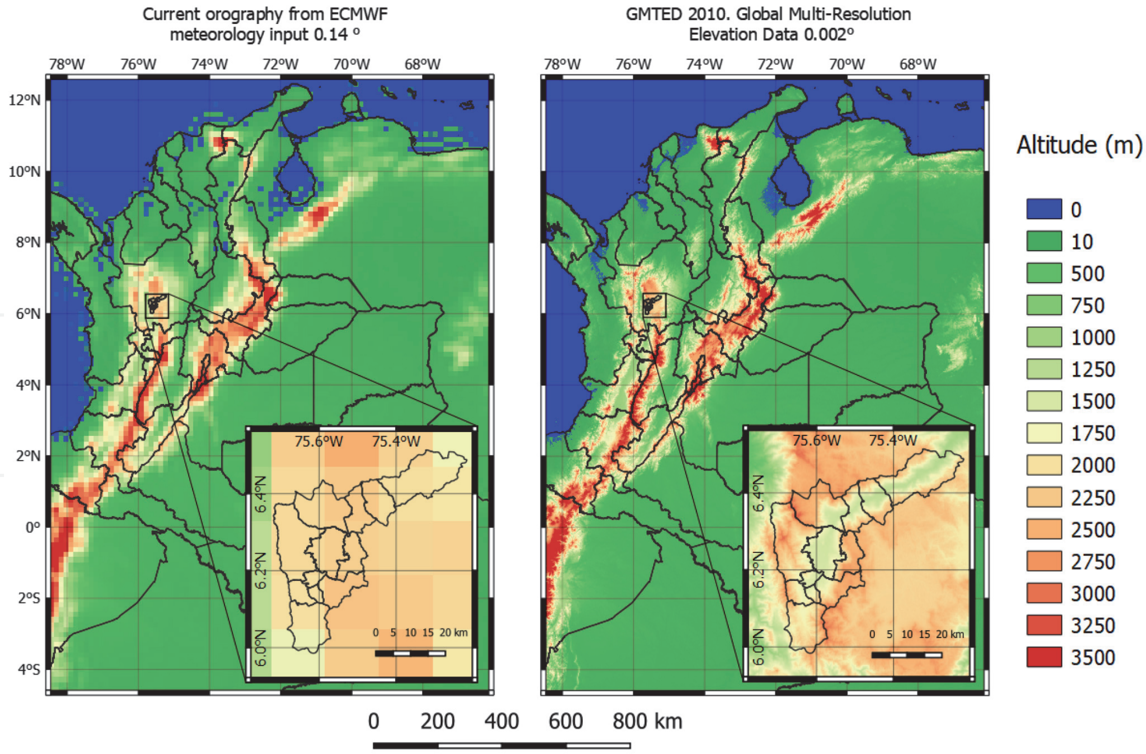

Figure 2.
(Comparison between the default elevation model for LOTOS-EUROS (A) and the updated elevation model derived from the GMTED 2010 data (B). The insets illustrate the differences in elevation representation for the Aburrá Valley.

the vertical layers. The effect of an updated elevation model depends on the desired simulation grid resolution. **Figure 3** shows a transverse cut at a latitude of 6.6°North for the simulation at a horizontal resolution of 0.09° x 0.09°, illustrating the impact of the change through the Aburrá Valley. The most significant changes in temperature occurred in the upper layers, reaching differences of up to 5°C degrees in top layers.

For modeling the deposition dynamics LOTOS-EUROS requires a map with deposition properties per grid cell. Land use characteristics are relevant for the deposition dynamics of a CTM because they define the parameters of the terrain roughness and canopy altitude of each category that determine the velocity at which the component is going to be deposited dependent on the vegetation type. The default land use/land cover (LU/LC) input data for LOTOS-EUROS were derived from the Global Land Cover (GLC2000) project [48], which includes 23 categories consistent with the Land Cover Classification System of the Food and Agriculture

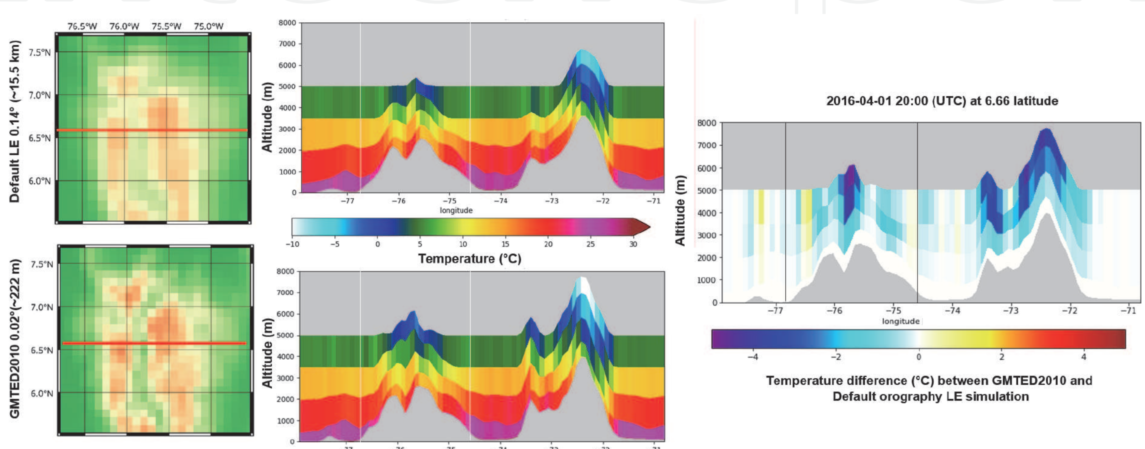

Figure 3.
Transversal cut at 6.6°N for vertical temperature profile comparison.

Organization (FAO) classification. For South America, the mapping of these categories at spatial resolutions of 1 km x 1 km was done in [49], with contributions from some regional experts based on multi-resolution satellite data. In this work, the LU/LC data was updated with the 2009 Land Cover Climate Change Initiative (CCI) dataset [50], with 38 categories at a horizontal resolution of 300 m x 300 m. **Figure 4** compares the default and updated LU/LC models for Aburrá Valley. The mapping of the 39 (CCI) and 23 (GLC) LU/LC categories to the 9 classes of the DEPAC deposition model is illustrated in **Figure 5**. The descriptions of each category are presented in **Table 1**. The mapping from GLC to DEPAC is the standard scheme constructed for LOTOS EUROS. The mapping from CCI to GLC

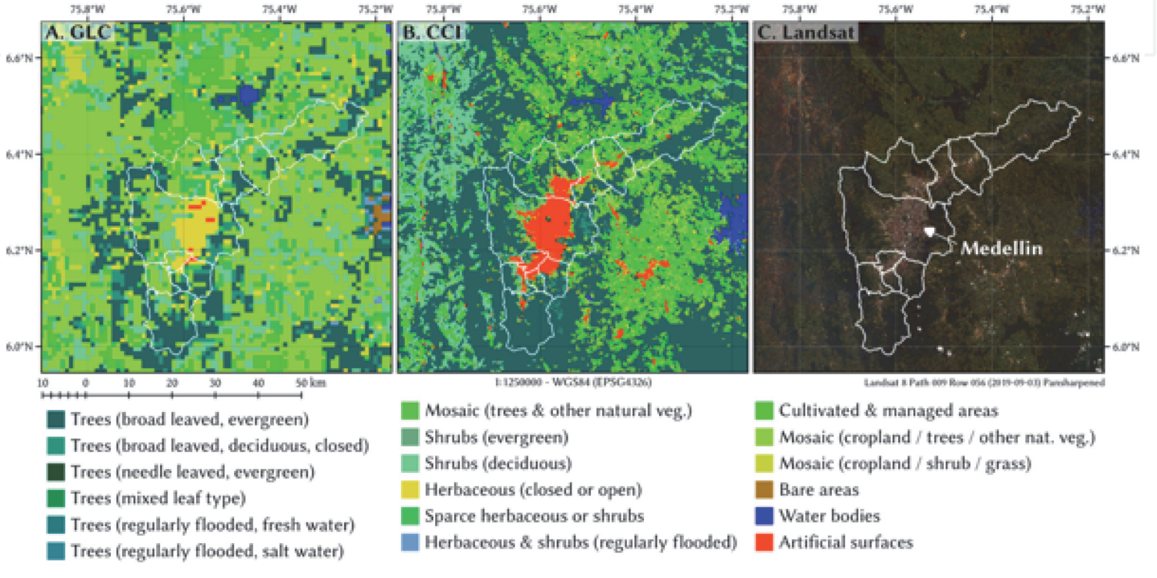

Figure 4.
Comparison between (A) the LOTOS-EUROS's original land cover model (global land cover, with resolution of 1 km x 1 km.) and (B) the updated land cover scheme (land cover from the climate change initiative, with resolution 0.3 km x 0.3 km). Real color Landsat cloudless imagery for the date 2019-09-03 is included in (C) as a reference for the artificial surfaces from the city infrastructure. The political boundaries correspond to the municipality of Medellín and the other nine municipalities that constitute the Aburrá Valley metropolitan area conurbation.

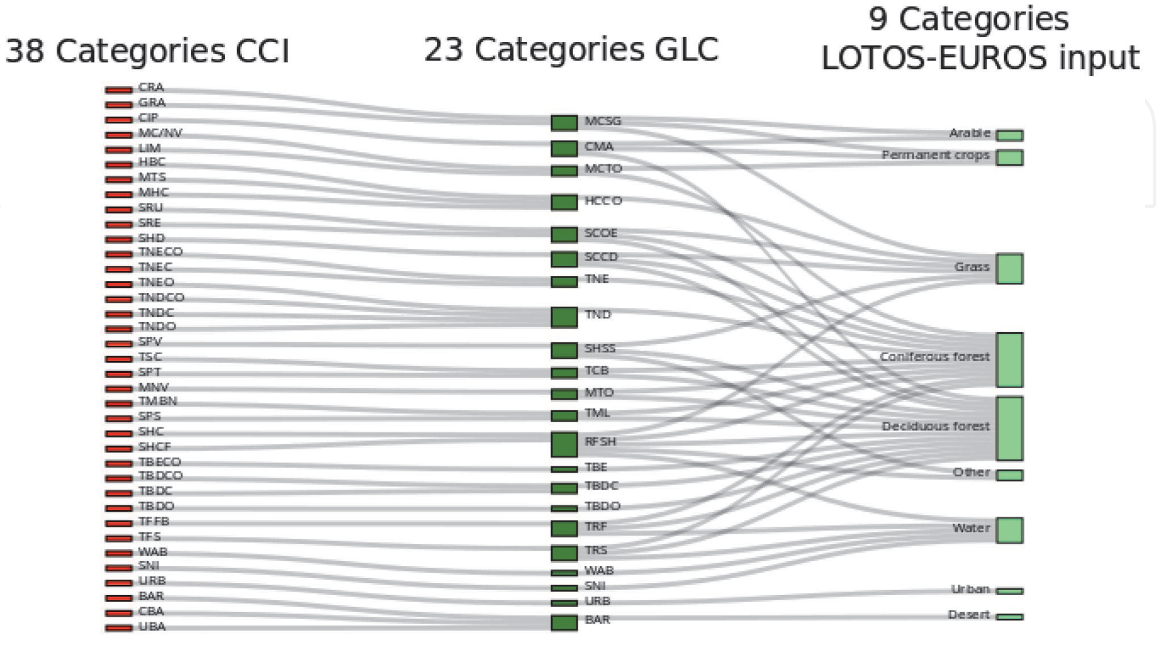

Figure 5.
Climate change initiative (CCI) land cover data categories mapped to the global land cover (GLC). The GLC categories are in turned mapped to the model's equivalencies. The category's codes are as in ***Table 1****.*

Number	Land Cover Climate Change Initiative (CCI) label	Code CCI	Number	Global Land Cover (GLC) label	Code CORINE
0	No data	ND	1	Tree Cover, broadleaved, evergreen	TBE
10	Cropland, rainfed	CRA	2	Tree Cover, broadleved, deciduous, closed	TBDC
11	Herbaceous cover	HBC	3	Tree Cover, broadleaved, deciduous, open	TBDO
12	Tree or shrub cover	TSC	4	Tree Cover, needle-leaved, evergreen	TNE
20	Cropland, irrigated or post-flooding	CIP	5	Tree Cover, needle-leaved, deciduous	TND
30	Mosaic cropland (>50%)/natural vegetation (tree, shrub, herbaceous cover) (<50%)	MC/NV	6	Tree Cover, mixed leaf type	TML
40	Mosaic natural vegetation (tree, shrub, herbaceous cover) (>50%)/ cropland (<50%)	MNV	7	Tree Cover, regularly flooded, fresh water	TRF
50	Tree cover, broadleaved, evergreen, closed to open (>15%)	TBECO	8	Tree Cover, regularly flooded, saline water	TRS
60	Tree cover, broadleaved, deciduous, closed to open (>15%)	TBDCO	9	Mosaic: Tree Cover/ Other natural vegetation	MTO
61	Tree cover, broadleaved, deciduous, closed (>40%)	TBDC	10	Tree Cover, burnt	TCB
62	Tree cover, broadleaved, deciduous, open (15–40%)	TBDO	11	Shrub Cover, closed-open, evergreen	SCOE
70	Tree cover, needleleaved, evergreen, closed to open (>15%)	TNECO	12	Shrub Cover, closed-open, deciduous	SCCD
71	Tree cover, needleleaved, evergreen, closed (>40%)	TNEC	13	Herbaceous Cover, closed-open	HCCO
72	Tree cover, needleleaved, evergreen, open (15–40%)	TNEO	14	Sparse herbaceous or sparse shrub cover	SHSS
80	Tree cover, needleleaved, deciduous, closed to open (>15%)	TNDCO	15	Regularly flooded shrub and/or herbaceous cover	RFSH
81	Tree cover, needleleaved, deciduous, closed (>40%)	TNDC	16	Cultivated and managed areas	CMA
82	Tree cover, needleleaved, deciduous, open (15–40%)	TNDO	17	Mosaic: Cropland/ Tree Cover / Other natural vege	MCTO
90	Tree cover, mixed leaf type (broadleaved and needleleaved)	TMBN	18	Mosaic: Cropland/ Shrub and/or grass cover	CSG
100	Mosaic tree and shrub (>50%)/ herbaceous cover (<50%)	MTS	19	Bare areas	BAR
110	Mosaic herbaceous cover (>50%)/ tree and shrub (<50%)	MHC	20	Water bodies	WAB

Number	Land Cover Climate Change Initiative (CCI) label	Code CCI	Number	Global Land Cover (GLC) label	Code CORINE
120	Shrubland	SRU	21	Snow an Ice	SNI
121	Shrubland evergreen	SRE	22	Artificial surfaces and associated areas	URB
122	Shrubland deciduous	SHD	23	No Data	ND
130	Grassland	GRA	**Number**	**LOTOS-EUROS fractional categories**	**LE-fract-code**
140	Lichens and mosses	LIM	1	Arable	ARA
150	Sparse vegetation (tree, shrub, herbaceous cover) (<15%)	SPV	2	Permanent crops	CRP
151	Sparse tree (<15%)	SPT	3	Grass	GRS
152	Sparse shrub (<15%)	SPS	4	Coniferous forest	CNF
153	Sparse herbaceous cover (<15%)	SHC	5	Decidious forest	DEC
160	Tree cover, flooded, fresh or brackish water	TFFB	6	Other	OTH
170	Tree cover, flooded, saline water	TFS	7	Water	WAT
180	Shrub or herbaceous cover, flooded, fresh/saline/brackish water	SHCF	8	Urban	NO2
190	Urban areas	URB	9	Desert	DSR
200	Bare areas	BAR			
201	Consolidated bare areas	CBA			
202	Unconsolidated bare areas	UBA			
210	Water bodies	WAB			
220	Permanent snow and ice	SNI			

Table 1.
Land use/land cover categories for the two sources of data used in this study and for the DEPAC module.

took into account the similar morphological characteristics between categories, and the aseasonality in this tropical region. The model defines for each grid cell the fraction covered by each one of the LU/LC classes used by the DEPAC module, and calculates the deposition over each fractions.

Deposition depends on land-use changes. It was essential to analyze the temporal behavior of the area of interest to identify zones with over and subs estimation comparing with the early reference. Natural protected areas with notable changes in deposition between the default and updated input data were identified, emphasizing the importance of using up-to-date and accurate land cover data in the simulation model. Vulnerable areas like natural protected areas and paramos ecosystems may require more than a local conservation effort for the preservation of their ecological functions.

To explore the fate of nitrogenous atmospheric species emitted from the main Colombian cities, the grid cells housing the centroids of the urban area for Bogotá, Medellín, Cali, and Barranquilla were assumed as artificial point sources of emissions. The simulations were conducted with the updated elevation model and updated LU/LC scheme detailed above, for a total of 10 days in four different times of the year: March 1–10, June 1–10, September 1–10, and December 1–10. After a

2-day model spin up, the point source was from 08:00–18:00 of day 3 of the simulation, emitting a total of 1000 kg/hour NO_2, which is the amount of daily NO_2 emissions reported for Medellń [51]. The artificial emissions were monitored during seven additional days, during which time all of the emitted species had either deposited or transformed. Similar simulations were conducted but without the activation of the point source in order to estimate the background deposition values for each grid cell.

A second experiment was conducted as above, but focusing on either Medellín or Rionegro. The latter city is located to the East of the Aburrá Valley, near the international airport that serves Medellín and the immediate region. Rionegro is the largest and fastest growing city in the Valley of San Nicolás. The urban growth in this region is being fueled in part by the migration of people from the Aburrá Valley. Many residents in the Valley of San Nicolás hold jobs inside the Aburrá Valley, and many schools that serve middle and upper income families from the Aburrá Valley are located in the Valley of San Nicolás. The second experiment was aimed at understanding the potential implications for regional Nr deposition derived from increase urban develpment in the Valley of San Nicolás.

The LOTOS-EUROS emission module explains the discharge of tracers and aerosols from various sources (anthropogenic, biogenic, marine, airborne dust, fires) that can be configured to define emissions in specific point sources to simulate scenarios. **Figure 6(A)** shows the simulation of the total deposition (dry and wet) for Nitrogen taking into account the emission of the four principal cities in Colombia. Cities here were assumed to be point emission sources, which works to determine the influence area of this city. **Figure 6(A)** shows the contours generated

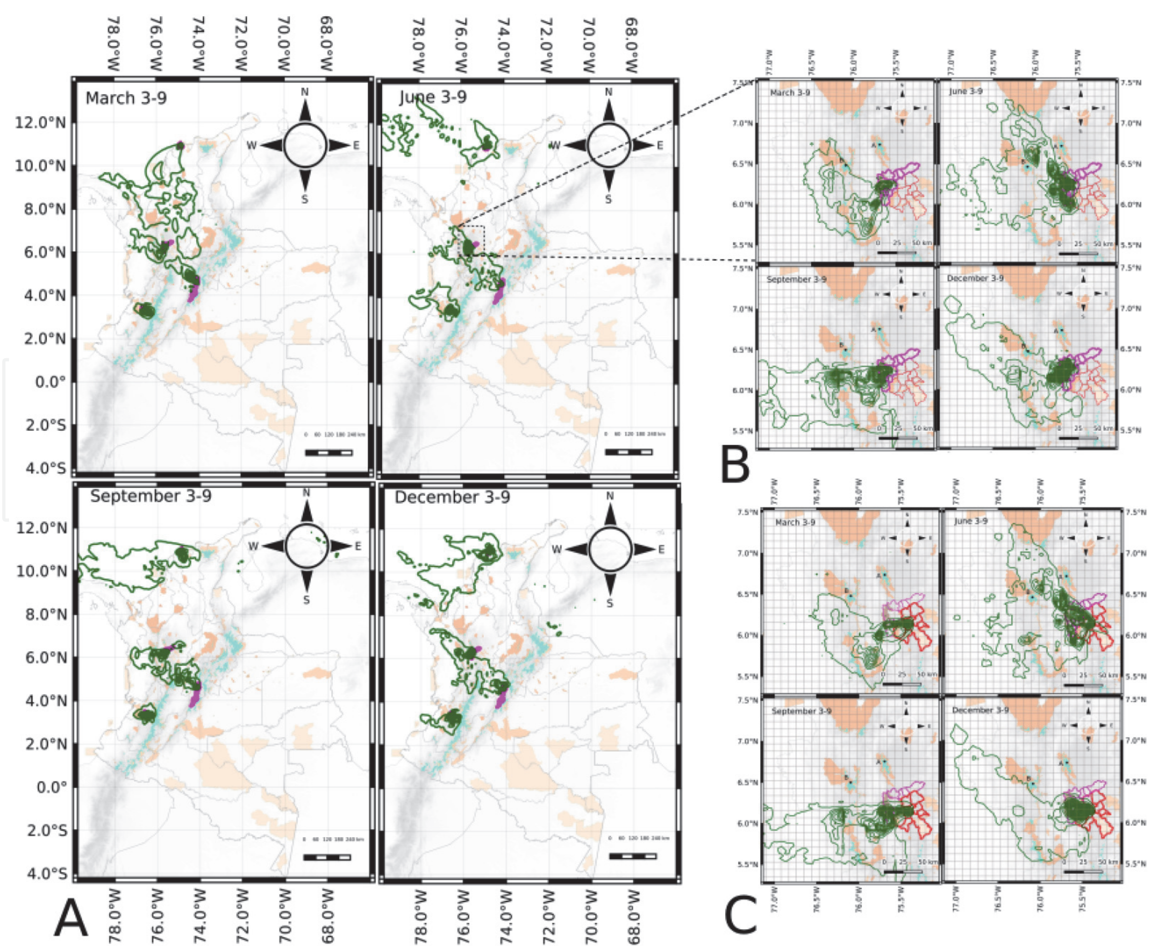

Figure 6.
Point source contour experiment for the 4 biggest cities in the country and contour limitation of the influence area.

with an increment of $5\,g/ha$ between contour level and bias correction of $+2\,g/ha$ to avoid negative values that appears as a numerical noise from the rest of the reference run minus the punctual perturbed emission run for the city of Medellín as a point source in the **Figure 6(B)** this same magnitude contour levels but in this case having the emission source located in Rionegro city. The more rounded contour delimits the impact zone for each of the cities.

It is possible to identify some trends in the wind direction for the four different times of the year, for which was performed simulations for the 1–9 days of March, June, September, and December. The influence of Barranquilla to faraway zones is perceivable due to the near location of this city to the Caribbean coast, where intense wind conditions exist as well as flat topography that drives the transport dynamics far away. More of the depositions from Barranquilla is going to the ocean direction and, in other time of the year to the southwest of the city reaching inclusive the other cities deposition areas. For the other cities, the impact area is more limited but with higher deposition values due to the roughness of the mountainous terrain and the less magnitude of the wind patterns presented. It is also interesting to see that the deposition from Bogotá could reach other cities as Medellín at some times of the year.

Figure 6(B) shows a simulation for what happens with Medellín for increase simulation resolution to 0.03x0.03°, conceiving the point source concentrated in a grid cell in the middle of the metropolitan area. The results of simulations indicate that the northwest-west area of the Aburra Valley (Medellín and municipalities of the metropolitan area) are the most affected, which could be seen in how paramos ecosystems located in the points a and B in the map receive nitrogen that was emitted from the cities. In the mosaic in the right part of **Figure 6(C)** a detailed simulation, conceiving the point source concentrated now in a grid cell in the middle of the metropolitan Rionegro area. It is important to notice during some parts of the year that Rionegro influences Medellín in terms of the deposition of its emissions. It means there is a transport dynamic of contaminants that should be studied from more detail because of the increasing Rionegro area for the industrial and urban setting.

Simulations with point sources identified the transport patterns in the territory, and showed the regional influence of the major cities in base of qualitative and quantitative results to understand the dynamics of emission and deposition of contaminants for the principal cities of Colombia which consist in an attractive information supply to start understanding the transport of atmospheric contaminants over this territory. The atmospheric transport and deposition of pollutants present ecosystem risk factors that require an evaluation of impacts directly in the field based on the reported results, and their inclusion in conservation strategies.

2.1.3 Technological development: SimpleSpace

A Simple module is a "CanSat" form factor measurement device with a standard for pico-satellites (0.1–1 kg). It has a mass of 0.4 kg and a volume of approximately 330 *ml*. It is a product of SimpleSpace, a spin-off program started at Universidad EAFIT since the early 2020 (**Figure 7**). Its aerospace design is versatile, and it does not represent a heavy load for any possible airborne campaign. As the module has already been measured at a stratospheric level in different High Altitude Balloon activities in the country, the sensors' robustness is guaranteed. Two simple modules inside and outside the aircraft provided an exciting framework for distributing pollutants outside and inside the urban area.

A Simple module is depicted in **Figure 8**, showing that it contains the necessary subsystems that a satellite architecture requires: an energy power supply, a

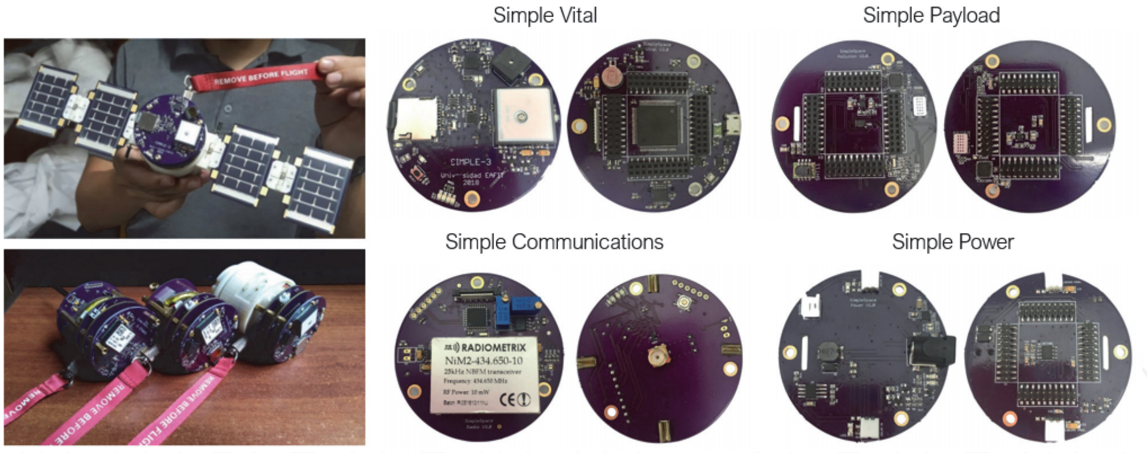

Figure 7.
Low-cost sensing solution from SimpleSpace. The simple unit is divided in subsystems which can be adapted into a vertical bus which allows the insertion of new pcb layers with new measurement instruments.

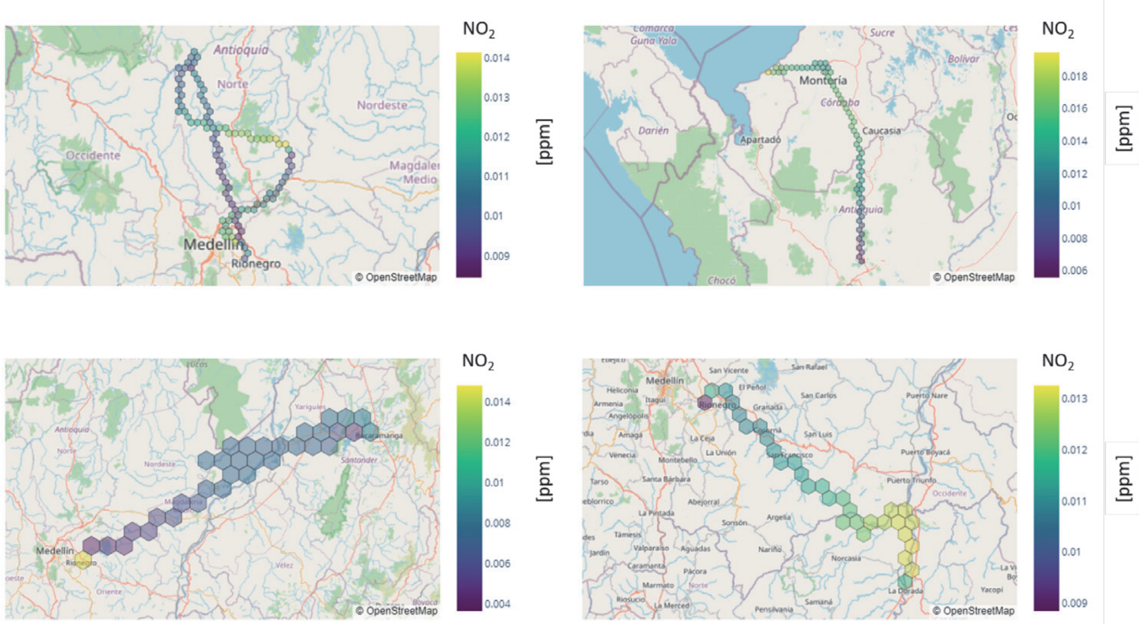

Figure 8.
Airborne measurements from the simple module for four days in our national territory for nitrogenous species taken from the airborne air quality platform (https://space-1516288940015.uc.r.appspot.com/).

communications subsystem, an on-board command data-handling subsystem, and a payload subsystem and a communication bus through all this subsystems.

The gases that were measured by the SimpleSpace modules for measurement in vertical layers in the HIPAE missio were: Carbon monoxide CO (1–1000 ppm), Nitrogen dioxide NO_2 (0.05–10 ppm), Ethanol C_2H_6OH (10–500 ppm), Hydrogen H_2 (1–1000 ppm), Ammonia NH_3 (1–500 ppm), Methane CH_4 (¿1000 ppm), Propane C_3H_8 (¿1000 ppm), Iso-butane C_4H_10 (¿1000 ppm), altitude, pressure and temperature using a CMOS based sensor. Additional sensor like the meteorology (Pressure, Humidity, Temperature, Wind direction and magnitude) and inertial sensor (accelerometers and magnetometers).

The previous figure shows the single units' observations onboard a non-pressurized aircraft of the Colombian Air Force for airspace protection. Valuable information is obtained in this research study regarding dynamics over the sensor devices and data assimilation experiments with the LOTOS-EUROS and WRF models. Scientists use numerical models that consider emissions and depositions of pollutants such as nitrogenous species and ozone in ecosystems to calculate these pollutants' transport and chemical reaction. The value of this lies in the possibility of defining courses of action to protect them because, in natural protected areas, the long-range transport pollution problem has not been extensively studying.

2.2 Human health

Behind many of the efforts of MAUI lies the intention to contribute to improving the environmental health in our region. Poor breathing air quality is amply recognized as a major environmental cause of morbidity and mortality [52], with global estimates suggesting nearly 9 million annual deaths being related to exposure to outdoor air pollution [53]. The National Institutes of Health in Colombia estimates that poor air quality is annually responsible for nearly 16,000 deaths representing the leading detriment to the national environmental health [54]. In Medellín and two other large Colombian cities, exposure of industrial air pollution has been associated with clusters of Acute Childhood Leukemia [55]. As has been repeatedly observed around the globe (e.g., [56]), urban exposure to air pollution has been found to be associated with increased rates of hospital visits related to respiratory and circulatory conditions in Medellín and other three large Colombian cities [57], and impact seemingly dominates by the effect of atmospheric NO_2 and its synergistic effect with other contaminants [58]. Atmospheric contaminants represent a threat to the health of Colombian people not only through their respiratory and mucosal exposure to polluted air, but also to surface-deposited contaminants [59].

The dynamics and spatial patterns of pollutant emissions in urban settings accentuate economic disparities with marked inequities in exposure to pollution [60]. Despite the reductions in air pollution resulting from total and partial lock downs in response to the COVID-19 pandemic [61], long-term exposure to poor air quality has been observed to exacerbate the manifestations of COVID-19 and increase its mortality rate [62]. Curiously, this effect was not apparent in Colombia, where sociodemographic differences appeared to be the leading factor influencing the dynamics of SARS-CoV-2 infections in the country [63]. Nevertheless, the cited authors suggest that ample errors affect the strength of the conclusions related to air pollution, and given the dearth of exposure models or assessments at sufficiently high spatial resolution available for Colombian cities, these results are indeed preliminary.

The development of mathematical models that could help us estimate the human exposure levels was one of the early goals at the outset of MAUI. With the research program ExPoR^2 we have been given the opportunity to finally pursue that goal.

2.2.1 HIPAE Mission

Research into nitrogenous species, ozone, and marine aerosols faces a common challenge posed by a scarcity of *in situ* measurements [8, 64]. Ideally, additional research infrastructure and sensors would be installed in the regions of interest. In the meantime, however, researchers will need to maximize the usefulness of satellite data, which is already available [11, 65] and alternative measurements sources as the airborne measurenment campaigns.

Airborne measurements constitute complementary *in situ* information for the vast array of measurements that may be collected from the atmosphere. To this end, HIPAE proves the viability of a measurement concept mission performed inside the

Colombian UH-60 L "Black Hawk" aircraft FAC4121, with the support of two groups within the Colombian Air Force: the fifth Air combat command -Comando aereo de combate N5 (CACOM5)- and Center for the technological development for defense -Centro de desarrollo tecnológico aeroespacial para la defensa (CETAD). This is the first time that this kind of measurement has been performed over Colombian territory.

Some references of airborne measuring campaigns come from the European project IAGOS (In-service Aircraft for a Global Observing System), a project that combines the expertise of two successful European research projects [66], MOZAIC (Measurements of OZone, water vapor, CO, NO_x by in service AIrbus airCraft) [67] and CARIBIC (Civil Aircraft for the Regular Investigation of the atmosphere Based on an Instrument Container) used in different scenarios to study the atmosphere composition [68]. The work of (Anthony et al., 2018) [69] used helicopter-borne electromagnetic measurements to derive a 3D resistivity model to study the permafrost carbon emission and compare a chemical transport model. One example from North America is the project from NOAA-ESRL named Tropospheric Aircraft Ozone Measurement Program focused on O_3 measurements [70]. Other project focused on aircraft measurements is called EMeRGe (Effect of Megacities on the transport and transformation of pollutants in the Regional and Global scales) which exploits the unique capabilities of the HALO (High Altitude and Long-Range aircraft) to investigate the impact of major population centers emissions on air pollution (Griffing et al., 2019).

In the mission HIPAE, we have the possibility of experimenting on topics such as nanomaterials, applied electromagnetism, atmospheric optics, environmental magnetism, biodiversity and conservation, mathematical modeling and meteorology [71]. This paper is the detailed extension of the work of [71]. The data assessed constitute a valuable source necessary for data assimilation experiments with the LOTOS EUROS to understand the dynamic of transport of contaminants in the region. The optical particle count and information retrieved from the 8 aerosol compounds of the Simple modules will allow valuable annotations to be used for the design of Lidar 4D systems; that will complement the TROPOMI ground and satellite measurements for the assimilation of data from the LOTOS-EUROS model at high and low resolution, increasing the impact from local to national in terms of the capacity to forecast the transport of pollutants (**Figure 9**).

The results of this experiment will not only validate the use of nanomaterials to capture particulate material, but will also offer valuable information on its composition, morphology, and chemistry via scanning electron microscopy (SEM) with energy-dispersive X-ray (EDX) analysis. These results are not going to be discussed in this paper and are considered under review on different journals. On the other hand, we address studies of cytogenotoxicity of pollutants in vertical columns of the atmosphere will provide valuable information to be used in human health risk assessments.

2.2.2 Preliminary results

From *in situ* aerosol measurements performed by HIPAE, a very clear picture emerged about the volumetric distribution of urban and rural pollutants in the Aburrá Valley. These data achieved good temporal and spatial resolutions. Direct analysis of numerous gases supported several decision-relevant findings, including spatial dynamics and source apportionment. This data will be assimilated into models in order to provide accurate dispersion scenarios and forecasting. Collected data by the OPC-N2 for PM 1.0, 2.5 and 10 match with those reported for the government services for the air quality monitoring. This demonstrates the reliability of the method.

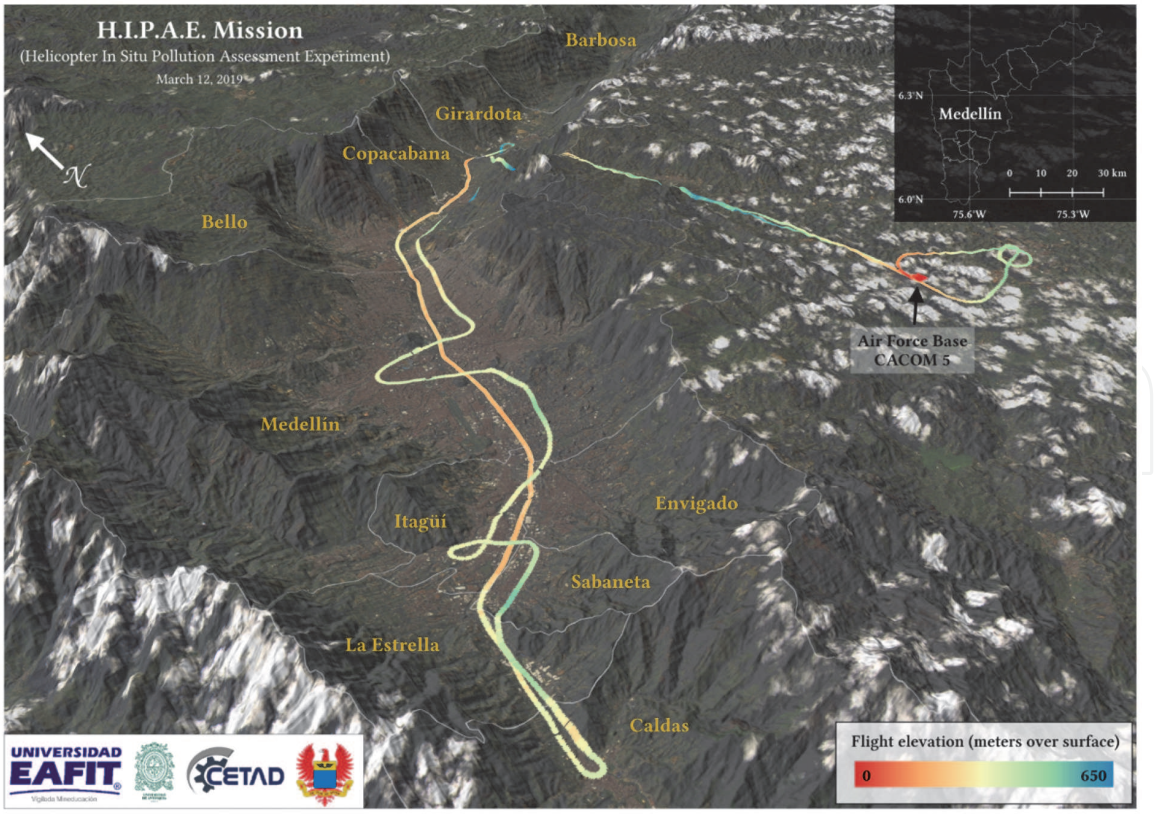

Figure 9.
Flight above the Aburrá Valley entering from the north and flying to the south and return at two different heights.

From a simple inspection of the comparison between the altimeter from the Simple device and the PM counters, several urban atmosphere dynamics were revealed. The concentrations of the two measures (PM10 and PM2.5) increased as the helicopter descended through the valley. Concentration data is useful for assimilation in a chemical transport models. The assimilated LE model was able to represent the concentrations of PM10 at low altitudes, as can be corroborated by ground stations; however, the model tends to underestimate concentrations proportional to the target altitude.

A remote laser detection device for research will be designed taking into account this information to define the physical design and its portability and of course, define the optimal channels to measure key particles i.e. wavelengths to detect, depolarization or Raman channels.

An automatized system for particulate matter collection is also needed to be designed, in order to have the possibility to capture particulate matter at different flying altitudes or city zones. This system also prevents to incorporate particle matter during take-off, landing and external load hooking maneuvers. Detailed information must be found in [71].

2.2.2.1 Polymer nanofibers for capture of particulate matter

In order to determine the capability of a novel nanofiber filter design, two types of filters were used in this study: one manufactured at Universidad EAFIT, based on PolyAcryloNitrile (PAN) nanofibers; and the other a commercial filter based on glass microfibers (GMF) [71].

The nanofilters were manufactured by an electrospinning technique. A high voltage was applied to a polymer solution in a syringe so that the polymer formed a small filament that traveled to a collection system. To manufacture the nanofilters, a concentration of 12 wt% of PAN, a voltage of 8 kV, and a 12-cm needle-collector were used.

Each fiber diameter was 560 +/− 130 nm, with a length of 50 +/− 5um.

The commercial filters were obtained from Electron Microscopy Sciences (Hatfield, PA). The assembly of the filters was done using air cassettes and GilAir 3 air sampling pumps (Sensidyne, USA).

The cassettes were connected by hoses to the pumps, which were programmed to intake 3 L/min. The filters were massed in a microbalance prior to installation (Mettler Toledo, USA) and were massed again at the end of the test [71]. The filtration efficiency of the particulate matter was determined in this way by gravimetry.

2.2.2.2 Celular and molecular damage quantification

2.2.2.2.1 Particulate matter extraction

The PAN and GMF filters were suspended in dichloro-methane (DCM) and stored at 20°C until extraction. The organic fraction of the PM was extracted with DCM in a sonicator for 45 min, broken into 15-min periods. The supernatant was rotavaporated at 35°C until the extract reached 0.5 mL. The extracts were then placed in amber bottles and left to dehydrate overnight. The PM extracts obtained from both filters were dissolved in 1 mL of dimethyl sulfoxide (DMSO).

2.2.2.2.2 Cell cultures

HaCaT cells were grown in Dulbecco's Modified Eagle's Medium (DMEM), which was supplemented with 5% fetal calf serum (Sigma, USA), 100 μg/mL penicillin, and 100 μg/mL streptomycin, in a humidified atmosphere of 5% CO2/95% air at 37°C. Exponentially growing cultures were used in all experiments.

2.2.2.2.3 Cytotoxicity assay

Cytotoxic evaluations of particulate matter captured with PAN and GMF filters were performed using MTT (3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide) assays, according to ISO/EN10993–5. Proliferating HaCaT cell lines were seeded in 96 well plates at a density of 10 cells/well in 100 mL of DMEM medium. Three concentrations of PM extract were tested: 25, 50, and 75 mg/mL. A positive control (methyl methanesulfonate, MMS, 100 mg/mL) and a negative control (DMSO, 1%) were implemented. Cells were incubated for 24 h with test extract concentrations, and all tests were carried out in triplicate. After the treatment, MTT (1 mg/mL) was added to each well and incubated for an additional 3 h. The performance of each well was quantified by measuring the spectral absorbance of the solution at 540 nm, using a microplate spectrophotometer.

2.2.2.2.4 Alkaline comet assay

Comet assays were performed with minor modifications, according to Sing et al. (1988). Briefly, HaCaT cells were seeded in each of 24 well plates, and exposed to 25, 50, 75 mg/mL PM solutions, and negative (DMSO 2%) and positive (50 mM H2O2) controls, for 1 hour. Cells were then trypsinized. Cell suspensions were mixed with low-melting-point agarose (0.75%), and immediately spread onto a microscope slide precoated with normal-melting-point agarose. Slides were then incubated in an ice-cold lysis solution (2.5 M NaCl, 10 mM Tris, 100 mM EDTA, 1%

Triton X-100, and 10% DMSO, at a pH of 10.0) at 4°C for 1 h. For the alkaline comet assay, slides were placed in an electrophoresis chamber containing freshly prepared alkaline buffer (300 mM NaOH and 1 mM EDTA, pH > 13.0) at 4°C for 20 min. After that a 300-mA and 25-V electric current was applied for 20 min to perform DNA electrophoresis. Slides were then neutralized (0.4 MTris, pH 7.5) and stained using 2% ethidium bromide solution. For the analysis, 200 randomly selected cells from each treatment were measured for DNA damage (% tail DNA). The tests were carried out in triplicate.

2.2.2.2.5 Cell cycle analysis

After 24 h of treatment, cell samples were fixed in 70% ethanol and subsequently incubated with 5 g/mL R5000 RNase (Sigma, USA), stained with 5 g/mL P4170 propidium iodide (Sigma, USA) for 30 min, and then analyzed for propidium iodide fluorescence using a BD LSRFortessa flow cytometer (BD Biosciences, USA). Percentages of cells in each phase were calculated using the FlowJo software package (FlowJo LLC, USA).

2.2.2.3 Cytogenotoxicity and genotoxicity analysis

2.2.2.3.1 Statistics on the data

As usual in biological sciences, a statistical analysis was carried out. Unless stated to the contrary, all data presented in this report represent results obtained from three independent experiments. Analysis of variance tests were performed with GraphPad Prism or Statview software, with post-hoc comparisons carried out by Fisher's protected least significant difference tests.

The cell viability examined by MTT assay showed that, compared with the unexposed control cells, there was statistically significant ($p < 0.05$) reduction in relative viability as the PM extract concentration increased from 25 to 50 to 75 mg/mL of PM. At the highest tested concentration, the cells reached a reduction of 25% of relative viability (**Figure 10**).

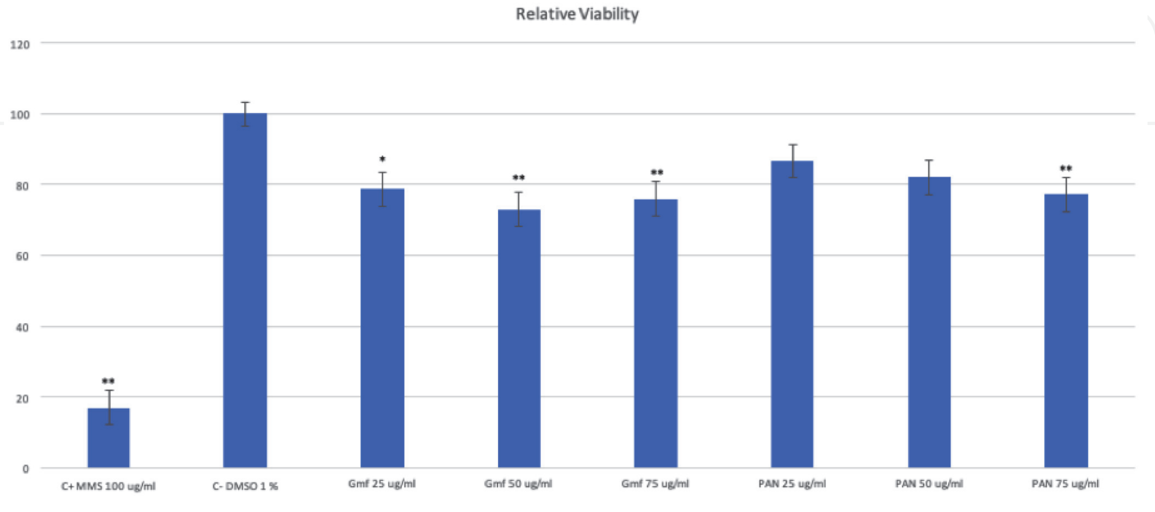

Figure 10.
*Cytotoxicity determined by relative viability, as measured by MTT assay of different concentrations of particulate matter extract obtained from GMF and PAN filters (25, 50, and 75 mg/mL). Positive control (C+; MMS 100 ug/mL) and negative control (C+; DMSO 1%) results are also depicted. The results are expressed as mean ± SE. Asterisks indicate statistical significance: * = (p ¡ 0.05), ** = (p < 0.01).*

2.2.2.3.2 Alkaline comet assay

As shown in **Figure 11**, the alkaline comet assay identified no significant statistical difference between the negative control (DMSO 2%) and the different concentrations of PM evaluated (25, 50, or 75 mg/mL).

2.2.2.3.3 Cell cycle analysis

Flow cytometry analysis indicated that, relative to control cells, the particulates captured by both GMF and PAN filters had no effect on the DNA content or the cell cycle phase distribution (**Figure 12**). The histograms in **Figure 13** show a slight population increase in the S phase, but without a significant statistical difference.

The cytotoxicity results show a clear reduction in the real viability related to the increase in the concentration of MP. The cytotoxicity results obtained in this work are in accordance with what was reported in other research papers that report cytotoxicity caused by PM after exposure to concentrations above 25 g/ml, for periods longer than 24 hours. (D. On the other hand, no evidence of genotoxicity or effects on the cell cycle of HaCaT cells was found at the concentrations evaluated. Which differs from the results reported by other researchers at similar concentrations of PM. These results may be related to the chemical composition of the PM at the sampling height.

Our analysis of the performance of PolyAcryloNitrile nanofibers in the capture and chemical and morphological analysis of particulate matter were promising. The designed nanomaterials outperformed the commercial filters at efficiently capturing particulate matter and in a way that was accessible for analysis.

Cell cycle analysis carried out on the particulate matter captured by the PAN nanofibers and GMF revealed lower rates of cellular damage compared with previous analysis on the surface. In addition, the comet assay identified no statistically significant difference between the negative control and the different concentrations of PM evaluated. The chemical composition of nano- or microscale particulate matter will determine the validity the hypothesis that cellular and genetic damage can be caused by human exposure to heavy particulate matter trapped near the surface in urban areas. Despite non-significative results on DNA damage and cell cycle analyses. We do strongly recommend taking into account these tests for future

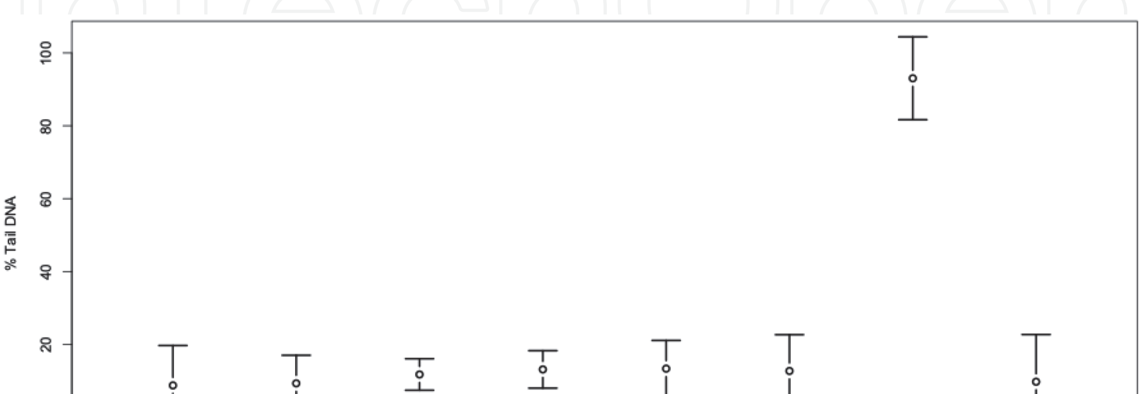

Figure 11.
Alkaline comet assay based on DNA breakage induced by different concentrations of PM extract obtained from GMF and PAN filters (25, 50, and 75 mg/mL). Positive control (C+; H2O2 50 mM) and negative control (C; DMSO 2%) results are also depicted. The results are expressed as mean ± SE.

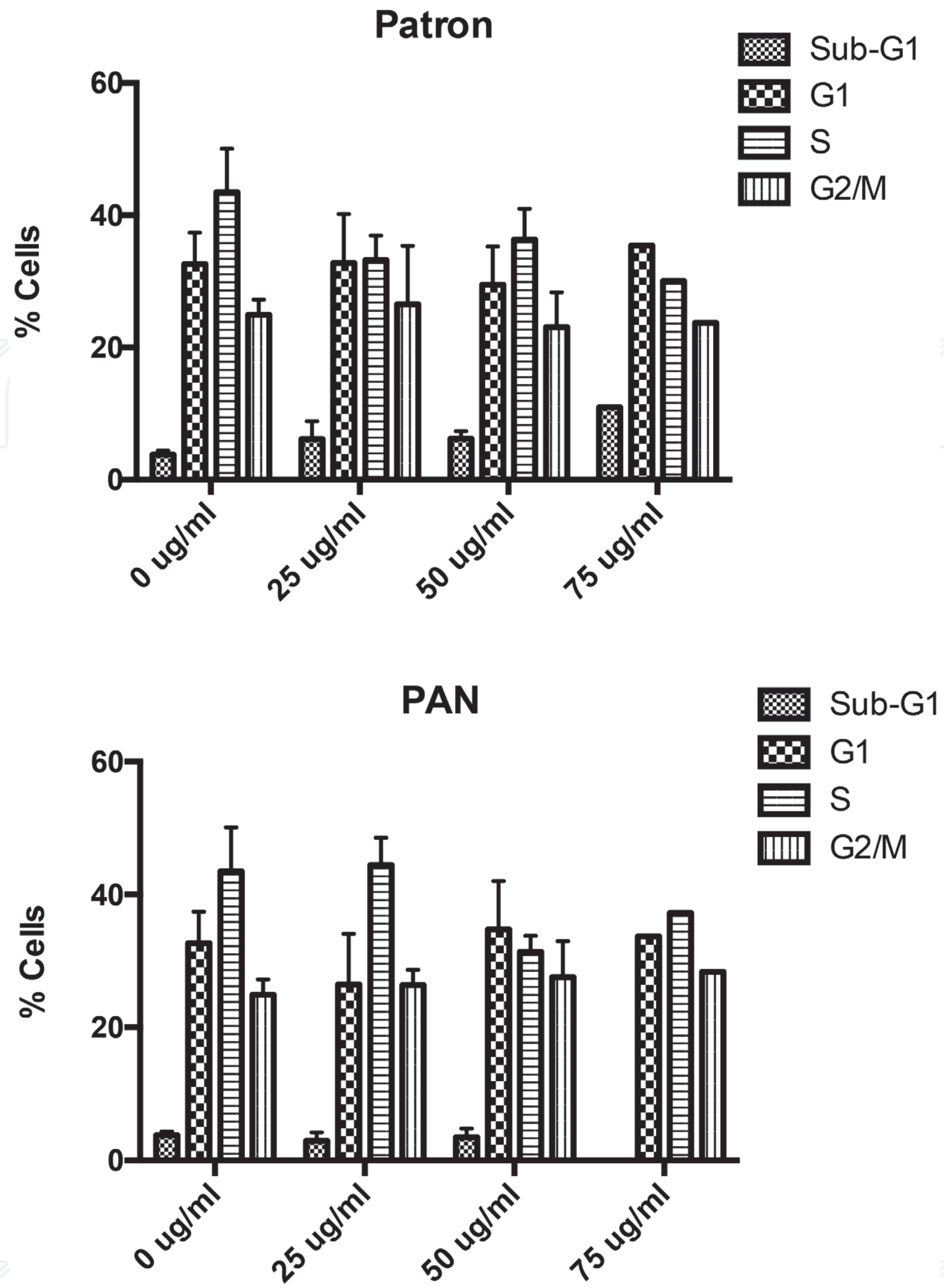

Figure 12.
Cell cycle distribution in HaCaT cells. Cells were treated with 25, 50 and 75 g/mL of GMF (A) and PAN (B) solutions. Values are expressed as mean ± SEM of three independent experiments for concentrations of 25 and 50 g/mL and one experiment for 75 g/mL.

analyses as a measure to monitor the evolution of the air polution and air quality in the valley.

Figure 14 depicts the Simple module measurements of ethanol and propane over the Aburrá Valley. The mission started in the military base near an urban area called Valle de San Nicolas. Flying north at a low altitude, the concentrations of C2H5OH were lower than when the aircraft entered the valley above Girardota. During the entire measurement campaign, and at several altitudes within the valley, there was no significant difference in ethanol concentrations in the vertical profiles, except for some portions in the south of the valley, where the land is not heavily urbanized. Human activities increase the concentration of ethanol, but when vegetation is present, it is mitigated. Similar behavior was detected by the measurements of

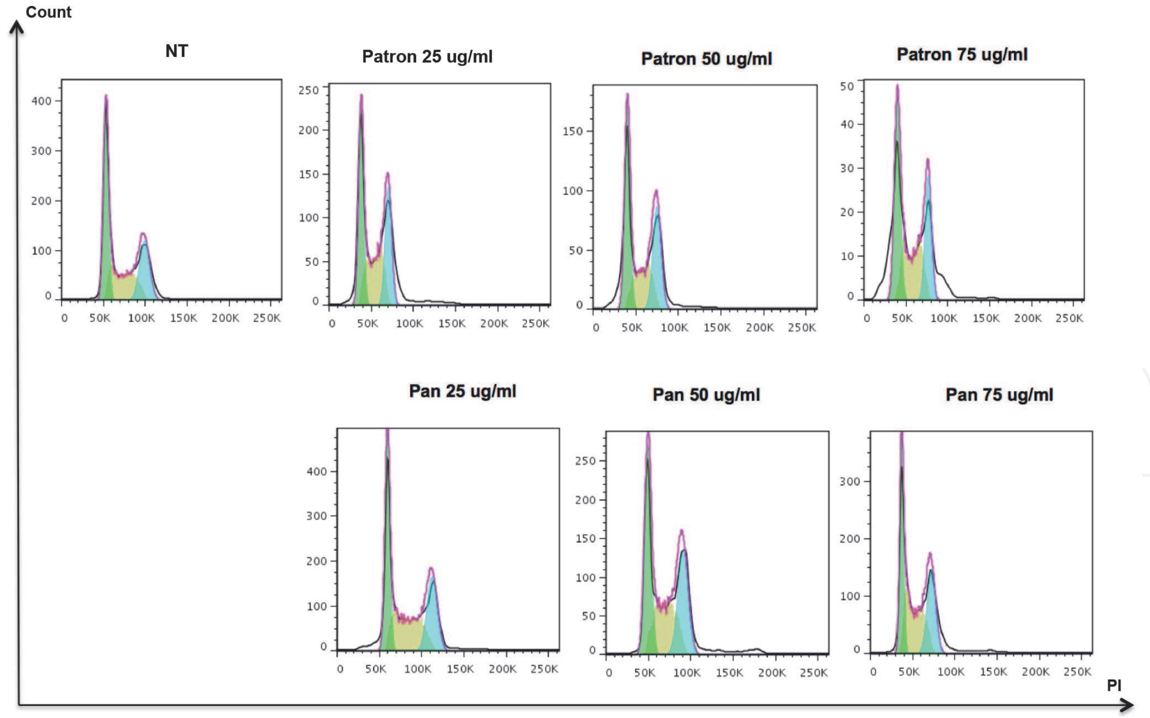

Figure 13.
Representative histograms of cell cycle distributions in HaCaT cells treated with GMF and PAN solutions.

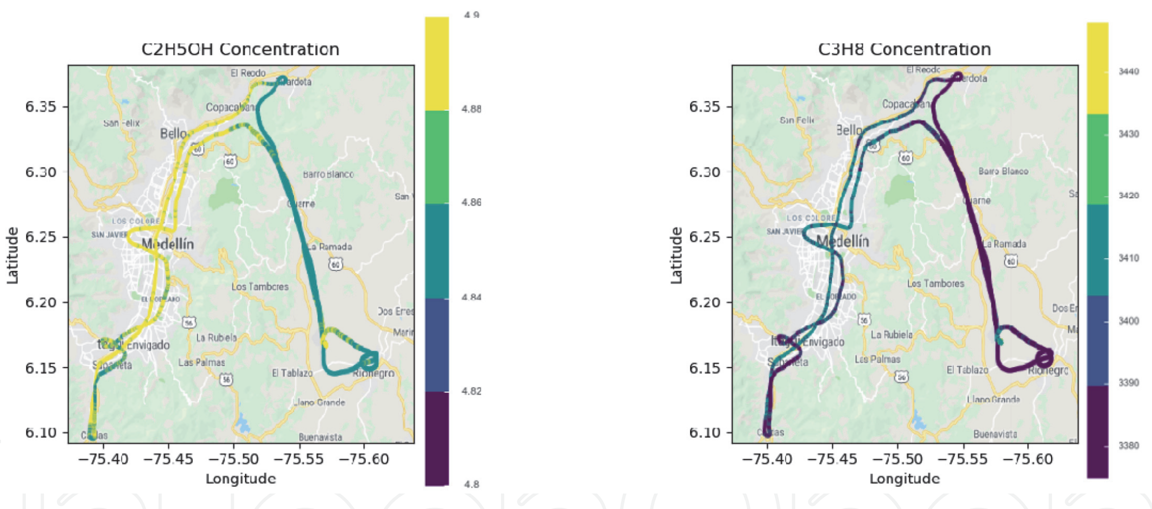

Figure 14.
Simple module measurements of C_2H_5OH and C3H8 over the Aburrá Valley.

propane, which reflect the presence of vegetation in urban areas with lower concentrations. Nevertheless, the highest urban concentration of propane was approximately 3410 ppm.

Simple module measurements of carbon monoxide and hydrogen over the Aburrá Valley are depicted in **Figure 15**. Carbon monoxide is toxic when encountered in concentrations above about 35 ppm. In the atmosphere, it is spatially variable and short-lived, having a role in the formation of ground-level ozone. Its presence indicates that tropospheric ozone is present in this urban area, having consequences for human health and nearby ecosystems. These measurements will enable several reaction schemes to be tested within a chemical transport modeling in the valley.

Simple module measurements of carbon monoxide and hydrogen over the Aburrá Valley are depicted in **Figure 15**. Carbon monoxide is toxic when encountered in concentrations above about 35 ppm. In the atmosphere, it is spatially

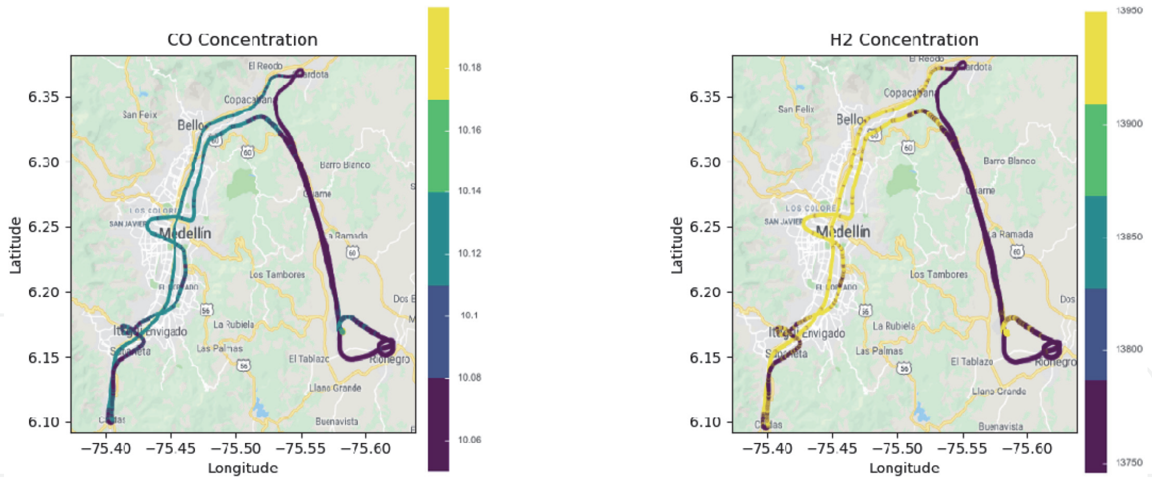

Figure 15.
Simple space measurements of CO and H_2 over the Aburra Valley.

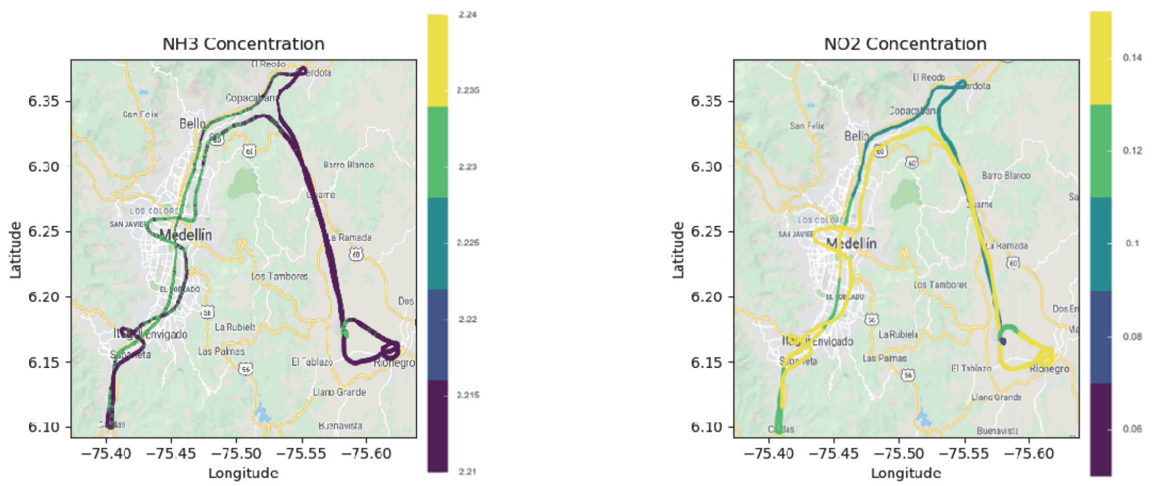

Figure 16.
Simple space measurements of NH3 and NO2 over the Aburra Valley.

variable and short-lived, having a role in the formation of ground-level ozone. Its presence indicates that tropospheric ozone is present in this urban area, having consequences for human health and nearby ecosystems. These measurements will enable several reaction schemes to be tested within modeling in the valley.

Simple module measurements of ammonia and nitrogen dioxide over the Aburrá Valley are depicted in **Figure 16**. The presence of elevated concentrations of nitrogenated species in the highest-altitude layers is deeply concerning. Ammonia is an irritant compound whose potency increases with its concentration. The permissible exposure limit is 25 ppm, and it becomes lethal above 500 ppm.

Author details

Andres Yarce Botero[1,2,3,4*], Olga Lucia Quintero Montoya[1,4], Santiago Lopez-Restrepo[1,2,4], Nicolás Pinel[2], Jhon Edinson Hinestroza[1], Elias David Niño-Ruiz[5], Jimmy Anderson Flórez[6], Angela María Rendón[7], Monica Lucia Alvarez-Laínez[8], Andres Felipe Zapata-Gonzalez[8], Jose Fernando Duque Trujillo[9], Elena Montilla[10], Andres Pareja[11], Jean Paul Delgado[12], Jose Ignacio Marulanda Bernal[13], Jaime Andres Betancur[6], Alejandro Vélez[6], Arjo Segers[14], Arnold Heemink[3], Juan Ernesto Soto[6], Bibiana Esperanza Boada Sanabria[1] and Sara Lorduy[1,6]

1 Mathematical Modelling Research Group, Universidad EAFIT, Medellin, Colombia

2 Department of Biological Sciences, Evolution and Conservation, Research Group on Biodiversity, Universidad EAFIT, Medellin, Colombia

3 Department of Applied Mathematics, TU Delft, Delft, The Netherlands

4 SimpleSpace, Universidad EAFIT, Medellin, Colombia

5 Applied Math and Computer Science Lab, Universidad del Norte, Colombia

6 Fuerza Aerea Colombiana, Colombia

7 Grupo de Ingenieria y Gestion Ambiental, Escuela Ambiental, Facultad de Ingeniería, Universidadde Antioquia, Medellín, Colombia

8 Design Engineering Research Group–GRID, Universidad EAFIT, Colombia

9 Departamento de Ciencias de la Tierra, Universidad EAFIT, Colombia

10 Applied Optics Research group, Universidad EAFIT, Colombia

11 Unidad de Toxicidad in vitro, Universidad CES, Colombia

12 Research Group of Genetics, Regeneration and Cancer, Institute of Biology, Universidad de Antioquia, Colombia

13 Applied Electromagnetism Reseacrh Group, Universidad EAFIT, Colombia

14 TNO Department of Climate, Air and Sustainability, Utrecht, The Netherlands

*Address all correspondence to: a.yarcebotero@tudelft.nl

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