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Environmental Simulation Model Using System Dynamics to Estimate Air Pollution: A Case Study of Mexico City Metropolitan Area

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Abstract: Air pollution in megacities worldwide has been a severe public health and environmental problem; it contributes to climate change and threatens life. Among all services, the transport sector accounts for most of these pollutants. However, despite the strategies implemented to reduce these pollutants, mitigate their effects, and promote prosperity and sustainability, emission reduction targets remain unmet, causing the average global temperatures to keep increasing. In this study, the air pollution in the Mexico City Metropolitan Area (MCMA) is estimated through the design of an environmental simulation model using system dynamics, which constitutes a possibility for authorities to foresee the evolution of air quality in MCMA by assessing the emissions from the transport sector from a holistic perspective, based on the region DESTEP analysis factors. Simulation results estimate a more significant reduction than predicted by the local government's current forecast; this emission reduction would be up to 106% lower for PM_{10}, 176% for $PM_{2.5}$, 34% for NOx, and 17% for VOC. The conclusion demonstrated that one of the main factors with the most significant impact on the control and reduction of emissions is the use and promotion of public transportation, along with the improvement of its road infrastructure.

Keywords: simulation model; system dynamics; sustainability; systemic analysis; air pollution; transport sector; metropolitan area; megacities

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1. Introduction

Air pollution in megacities worldwide has been a severe public health and environmental problem [1–3]. The World Health Organization (WHO) estimates that the combined effect of ambient air pollution and household air pollution causes approximately 7 million premature deaths worldwide every year, mainly as a result of increased mortality from stroke, heart disease, chronic obstructive pulmonary disease, lung cancer, and acute respiratory infections [4].

For instance, according to The United Nations Human Settlements Program (UN-Habitat), Mexican cities have severe environmental pollution problems, with transportation being one of the leading causes, contributing to 20.4% of greenhouse gas (GHG) emissions, 60% of particle matter with a diameter of 10 µm (PM_{10}), and 18% of carbon dioxide (CO_2) emissions. This air pollution costs around 6% of the gross domestic product (GDP) and causes the death of approximately 21,000 people in Mexico annually [5,6].

Given the adverse effects on the environment and public health, it is essential to develop and explore models, methodologies, and techniques to evaluate scenarios and estimate the propagation of the different atmospheric pollutants in the medium and long term. Based on the implementation of measures and actions established by government agencies, these scenarios would help to predict whether they will be sufficiently effective in reducing pollutants from motor vehicles [3,7].

Previous studies have applied various methodologies to estimate and predict pollutant dispersion, including statistical, regression, and dynamic models. However, many of these studies have focused on short-term estimations, without addressing the interaction between socioeconomic and technological factors that influence long-term air quality. Additionally, while some models have incorporated innovative aspects, there is a lack of integration and application of these models into effective public policies that can be adapted for various megacities.

Therefore, this study addresses a significant gap in current research by proposing a dynamic simulation model that anticipates pollution levels under various scenarios and offers a holistic approach to managing air quality. Through this model, we seek to provide more effective tools for decision-makers to implement policies that result in tangible and sustainable improvements in urban health and the environment.

Our approach seeks to fill these methodological and practical gaps by estimating, through designing an environmental simulation model using system dynamics, the emissions of air pollutants from the transport sector that will be emitted in the MCMA by 2030 from a holistic perspective, based on the region's DESTEP analysis factors.

The novelty of the proposed model relies on improving the estimation of criteria air pollutants from the transport sector by incorporating DESTEP factors into the environmental model using dynamic systems that ultimately alter the vehicle kilometers traveled (VKT).

After this introduction, the paper is structured as follows: Section 2 presents a detailed literature review, focusing on the evolution of air quality simulation models and the application of system dynamics within urban contexts. Section 3 describes the methodology, outlining our approach to modeling air pollution in the Mexico City Metropolitan Area using dynamic systems and DESTEP analysis. Section 4 discusses the results, comparing our model's predictions with existing emission inventories and other models. Finally, Section 5 summarizes the findings and their implications for policy and future research.

2. Literature Review

Different environmental simulation models have been developed, implemented, and used to estimate multiple effects of air pollution in metropolitan areas. These models are tools to simulate complex systems and processes in the natural environment and how they behave under various conditions. Such is the case of the environmental model to assess morbidity based on population exposure to $PM_{2.5}$ pollutants [8], or the Newey–West estimators used to estimate transport strategy in the Guadalajara Metropolitan Area [9].

Another example is the OLYMPUS modeling platform, which aims to estimate pollutant emissions from energy-consuming activities [3], or the CHIMERE chemistry-transport model designed for atmospheric composition [10]. Additionally, different analyses have been carried out to evaluate environmental sustainability. For instance, the Moderate Resolution Imaging Spectroradiometer assessed the air quality index in the Kolkata Metropolitan Area, India [11].

More recently, different approaches have been implemented in the Asian continent for analyzing the advancement in air quality. One of these modeling tools is the Weather Research and Forecasting Model, coupled with chemistry (WRF-Chem), which determines the contributions of meteorological conditions and emission reduction on air quality improvement in China [12]. A deep learning model has been developed to acquire hourly mass concentrations of $PM_{2.5}$ chemical components [13], and Central China has developed an updated high-resolution emission inventory based on the Long-range Energy Alternatives Planning System (LEAP) [14].

System dynamics is also one of these environmental simulation models; in this methodology, the aspects involved in the environment are considered as the causal interaction between attributes that describe it [15]. System dynamics facilitates the description of a system, the construction of a dynamic system, and the recreation of its behavior [16]. Moreover, it advantageously simulates non-formal models of complex systems and abstract mathematical models [17].

System dynamics modeling has been utilized to help decision- and policy-makers understand and predict the behavior of a complex system in different fields of study, such as transportation, public utilities, water, housing, food, agriculture, and urban and regional planning [18]. Simulating a complex dynamic system generates relevant information to solve problems in the supply, production, and distribution processes [19] or to develop technological solutions to improve manufacturing processes such as wood and pallets [20].

By developing an integrated model, authorities of megacities could make informed decisions based on different assumptions to improve concentration levels and meet air quality standards. Such is the case of Bogota, a Latin American city and the capital of Colombia, where a simulation model utilizing system dynamics was proposed and applied for evaluating and reducing PM_{10} [7,21]. Another example is the model using system dynamics proposed in Tehran, Iran, to estimate air pollution, including transportation and industrial subsystems [22].

Based on the models utilized in these megacities, the purpose of this study is to estimate, through the design of an environmental simulation model using system dynamics, the air pollution in the Mexico City Metropolitan Area (MCMA). This model will estimate the emissions from the transport sector through 2030 from a holistic perspective, based on the region DESTEP (demographic, economic, social, technological, environmental, and political) analysis factors.

To obtain a holistic perspective on air pollutant emissions in MCMA from the transportation sector, the DESTEP analysis will be used [23]. This methodology made it possible to analyze the demand for transportation, the number and type of vehicles, travel patterns, the impact on air quality derived from investment policies in public transportation and clean technologies, absorption of cleaner technologies, and environmental factors, among others.

The systemic approach is explained and can be modeled by its composition, environment, total structure, mechanism, and links resulting from the interaction of the elements of the system [24]. This DESTEP methodology analyzes different factors that help gather information and is a valuable tool for representing a current situation, presenting trends and future predictions in an organized manner [25].

3. Materials and Methods

3.1. Air Pollutants Simulation Models

The MCMA has been developing emissions inventories for the last four decades; these inventories estimate the emissions from the transport sector utilizing traffic counts, with PM_{10}, particle matter with a diameter of 2.5 μm ($PM_{2.5}$), nitrogen oxides (NOx), carbon monoxide (CO), volatile organic compounds (VOC), black carbon (BC), and GHG, expressed as carbon dioxide equivalents (CO_{2eq}), being the highest emissions from this sector. In this sense, air quality models can be air pollution forecasting tools for emission inventories [26].

The 2018 MCMA Emissions Inventory includes the use of MOVES-Mexico 2018 software (Motor Vehicle Emission Simulator) based on the MOVES2014 developed by the U.S. Environmental Protection Agency (EPA) and adapted for MCMA to calculate the pollutant emissions from different sources [26–28]. However, this package has undergone updates, making the MOVES4 version the most recent. This latest version updates the data of the vehicle fleet, fuel type, travel activity, emission rates, and emission factors, in addition to including the possibility of simulating electric cars, among other additional features [29], which led to the version used in Mexico being somewhat outdated.

The Management Program to Improve Air Quality in the Mexico City Metropolitan Area (ProAire ZMVM 2021–2030, Spanish acronym) estimates emissions from mobile sources [30,31]. However, designing an environmental simulation model using system dynamics to estimate pollutant emissions from the transport sector will make it possible to incorporate additional variables or scenarios to the simulation, understand the underlying dynamics of emissions in-depth, explore different policies that would affect air quality, adjust the model to the observed data, adapt the model to unexpected changes, and evaluate its impact.

To carry out the environmental modeling, this research used Stella Professional Online 3.7.1 from isee Exchange, a software specialized in system dynamics, whose modeling capabilities allowed the design of an environmental simulation with ease and enabled the analysis of the dynamics of the variables related to the emissions of atmospheric pollutants. For a better understanding of the model, a causal diagram and a flow diagram, with their respective variables, attributes, and mathematical models, were created [32].

Implementing this environmental simulation model using system dynamics in the methodology used by the MCMA emission inventories, which in turn is used by the ProAire ZMVM 2021–2030, could provide a more accurate picture of the emissions estimation, which would also help to establish more precise strategies, measures, and actions aimed at reducing air pollutants.

As a result, the main contribution of this research is the proposal of the environmental simulation model using system dynamics from a holistic perspective based on DESTEP analysis factors in MCMA, which could be homologated to carry out an estimation of the different atmospheric pollutants coming from the transportation sector, foresee the evolution of air quality, and help decision- and policy-makers understand and predict the behavior of complex systems in different megacities worldwide.

3.2. MCMA Air Pollutants Estimation

The emissions of criteria air pollutants from the transportation sector in the MCMA by 2030 were estimated by the local authorities by calculating the tons of emissions per year. To obtain the estimated tons per year of these compounds, it is necessary to know the different emission factors (EFs) associated with each constituent applied to an activity data; in the case of mobile sources, this activity is the VKT.

For an accurate emissions estimation from mobile sources, it is necessary to use detailed information on their main precursors and factors that promote their chemical reaction, such as geographic area, fuel quality, mobility, and roadway type [33]. The emissions modeling process of MCMA uses these data to estimate EFs directly. An emission factor is the quantity of a pollutant, typically expressed in grams per kilometer or grams per mile, released into the atmosphere, with an activity associated with releasing that pollutant [34]. These already processed data, expressed as EFs, were taken from the 2018 MCMA Emissions Inventory Calculation Report (Memoria de Cálculo del Inventario de Emisiones de la Zona Metropolitana del Valle de México 2018) [35].

In the case of mobile sources, the activity related to releasing criteria air pollutants consists of VKT (or VMT—vehicle miles traveled), which measures a motor vehicle operation within a specific geographic area over a given period [36]. Local authorities calculate VKT based on the kilometers traveled per day, the number of days of circulation per year, and the number of vehicles per model year. The VKT per year varies according to the vehicle type, model year, and hologram established in the Vehicle Verification Program based on their emission control systems.

The ProAire ZMVM 2021–2030 estimates emissions from 94 categories that constitute four different emission sources, including 25 point sources, 56 area sources, 11 mobile sources, and 2 natural sources. Mobile sources (transportation sector) consume 50% of the fossil fuels in the MCMA and are also the primary source of $PM_{2.5}$, CO, and NOx emissions, significantly contributing to PM_{10}. Likewise, mobile sources account for one-fifth of VOC emissions, mainly from gasoline-powered cars [30].

According to the 2018 MCMA Emissions Inventory, the transportation sector comprises just over 6 million cars, classified as the private sector, which consists of 89.4%, the public sector, with 5.5%, and the cargo transportation sector, with 5.1%. Table 1 details the estimated vehicle fleet for the MCMA by type of vehicle and fuel; 97.1% correspond to gasoline-powered cars and 2.1% to diesel vehicles. This study considered only information from gasoline-powered cars from the private vehicle sector (private vehicles/passenger cars, SUVs, and motorcycles), representing 5,330,838 cars and almost 44.4% of fossil fuel consumption in the metropolitan area.

Table 1. Vehicle fleet in the MCMA by type of car and fuel.

Type of Vehicle	Total Fleet	Gasoline	Diesel
Private vehicles/Passenger cars	3,711,770	3,683,360	10,042
SUV	1,108,092	1,102,608	3514
Motorcycles	544,870	544,870	NA
Cabs	213,187	212,355	369
Wagons	61,492	52,742	8679
Microbuses	26,736	7612	262
Buses	26,539	528	25,895
Metro buses	862	NA	862
Cargo (3.8 tons)	201,828	174,395	25,614
Cargo (<3.8 tons)	96,488	47,819	41,090
Tractor-trailers	9337	NA	9337
Total units	6,001,201	5,826,289	125,664
Contribution		97.1%	2.1%

Author's own elaboration of the 2018 MCMA Emissions Inventory.

This research focused on estimating the emissions of PM_{10} and $PM_{2.5}$ particles, as well as NOx and VOC compounds (O_3 precursors) from the transportation sector in the MCMA by 2030 for two main reasons. Firstly, because these pollutants generate the most significant damage to the population's health and environment, and secondly, because the same compounds are mainly emitted by cars in the private gasoline sector, with 39.3%, 22.1%, 47%, and 62.2%, respectively, of the total emissions generated by source and category, as shown in Table 2.

Table 2. Emission of pollutants from the private sector in the MCMA in 2018 [tons/year].

Private Sector	PM_{10}	$PM_{2.5}$	NOx	COV
Private vehicles/Passenger cars	3940.51	1118.63	37,716.02	36,755.04
SUV	1093.73	280.28	15,128.12	10,546.68
Motorcycles	371.17	172.33	5512.08	9753.97
Partial	5405.41	1571.24	58,356.22	57,055.69
Total Mobile Sources	13,763	7098	124,115	91,771
% of emissions from Private vehicles	39.3%	22.1%	47%	62.2

Author's own elaboration based on the 2018 MCMA Emissions Inventory.

In the first instance, an initial simulation was performed to evaluate the model's reliability; that is, the simulation model's results are, to some extent, comparable to the estimation of atmospheric pollutants conducted by the local authorities. For this purpose, PM_{10}, $PM_{2.5}$, NOx, and VOC emissions from the private sector of mobile sources were calculated using Equation (1), which states that the emissions generated by mobile sources for each pollutant are equal to the product of the VKT by type of vehicle and its respective EF, divided by the conversion factor, with the result expressed in grams per kilometer [35]:

$$E_{ijk} = (VKT_{ij}) \times (EF_{ijk})/(1{,}000{,}000), \quad (1)$$

where

E_{ijk} = emissions for vehicle type i, model year j, pollutant k [tons/year];
VKT_{ij} = vehicle kilometers traveled by vehicle type i, model year j [km/year];
EF_{ijk} = emission factor for vehicle type i, model year j, pollutant k [g/km];

1,000,000 = conversion factor, from grams to tons.

For this first simulation, data from the 2018 MCMA Emissions Inventory Calculation Report were used, specifically the VKT by vehicle type and model year, as well as the EFs for vehicle type, model year, and pollutant. The results of this simulation were, in turn, compared with the results obtained by MOVES-Mexico 2018 software, whose estimates were published in the 2018 MCMA Emissions Inventory.

3.3. System Dynamics Simulation Design

Once the correlation between the initial environmental simulation model and the results obtained by MOVES-Mexico 2018 software was verified, indicating that the simulation generated plausible results and was sufficiently reliable to be used in the system dynamics simulation, an environmental simulation model was designed, considering the factors of the DESTEP analysis to have a holistic simulation, to include the different aspects involved in the generation of air pollutant emissions from the transportation sector in the MCMA by 2030.

The DESTEP analysis is a valuable tool for obtaining a holistic perspective of the factors that influence the increase or decrease of mobile sources in MCMA (vehicle fleet), specifically passenger cars, SUVs, and motorcycles. This vehicle fleet behavior directly impacts the VKT and, consequently, the emission and accumulation of PM_{10} and $PM_{2.5}$ particles, NOx, and COV, which are the criteria air pollutants to be estimated in this study by 2030.

Table 3 shows the main study variables of the environmental simulation model. The increase or decrease in the values of the variables representing atmospheric pollutants (PM_{10}, $PM_{2.5}$, NOx, VOC) was taken as a reference to establish air quality and, therefore, public health. Simulating the dynamics of these variables made it possible to estimate the emission of atmospheric pollutants with greater precision, in addition to establishing the variables that have the most significant impact on the control of pollutant emissions.

Table 3. Study variables.

Variables	Description
PM_{10}	Particle matter with a diameter of 10 µm
$PM_{2.5}$	Particle matter with a diameter of 2.5 µm
VOC	Volatile organic compounds
NOx	Nitrogen oxides
EFs	Emission factors
VKT	Vehicle kilometers traveled
Mobile Sources	Passenger cars, SUVs, and motorcycles in MCMA
DESTEP	Demographic, economic, social, technological, environmental, and political factors

Author's own elaboration, based on the systemic analysis applied to the environmental simulation.

Table 4 shows the DESTEP factors and their proposed attributes for DESTEP analysis. These attributes are considered to have the greatest impact on their corresponding DESTEP factor. This analysis is used to understand, in a broader context, how the generation of pollutant emissions in the MCMA has been influenced. Combining this tool with system dynamics allowed the development of a complete and balanced approach to both external factors and their internal interactions.

Different simulations to estimate air pollutant emissions were conducted with Stella Professional Online 3.7.1 software to start designing the environmental simulation model using system dynamics. This software is a web-based modeling valuable tool for creating dynamic simulation models, policy analysis, and strategy development.

Stella Professional Online 3.7.1 uses probability distribution to quantify uncertainty by assigning probabilities to different possible outcomes and propagating uncertainties through models and estimations. Stella's statistical built-ins enabled the introduction of randomness into the model [37].

Table 4. DESTEP analysis.

DESTEP Factors	Attributes
Demographic	Population density
Economic	Productivity–recession
Social	Mobility preference: private car/public transport
Technological	Vehicle technology–fuel quality
Environmental	Air quality management
Political	Federal regulation–EV charging infrastructure

Author's own elaboration based on DESTEP factors.

The data that fed the system dynamics environmental simulation model were taken from the 2018 MCMA Emissions Inventory, as well as from the ProAire ZMVM 2021–2030. Information on the vehicle fleet, vehicle fleet by type of vehicle and fuel, and pollutant emissions by type of vehicle representative for MCMA was adapted, as well as the different rates of population, economic, social, technological, ecological, and political growth that influence the generation of emissions.

Based on the simulation, the results obtained were analyzed to estimate more precisely the emissions of air pollutants from the transportation sector by 2030 to identify the strategic actions implemented by the ProAire ZMVM 2021–2030 that could be strengthened and updated for this same year.

4. Results

To start with the modeling, a causal loop diagram (CLD) was made, which was used to highlight the structure of the entire model, showing the variables that are most important in causing the system behavior. The structure used in the simulation is based on a developed understanding of the model, while facilitating the explanation of the resulting diagram.

Figure 1 shows the causal diagram, which represents the environmental simulation model through system dynamics, using the DESTEP systemic analysis to estimate air pollutant emissions from the transportation sector in the MCMA. This diagram illustrates the positive and negative effects of the variables on the generation and accumulation of criteria air pollutants.

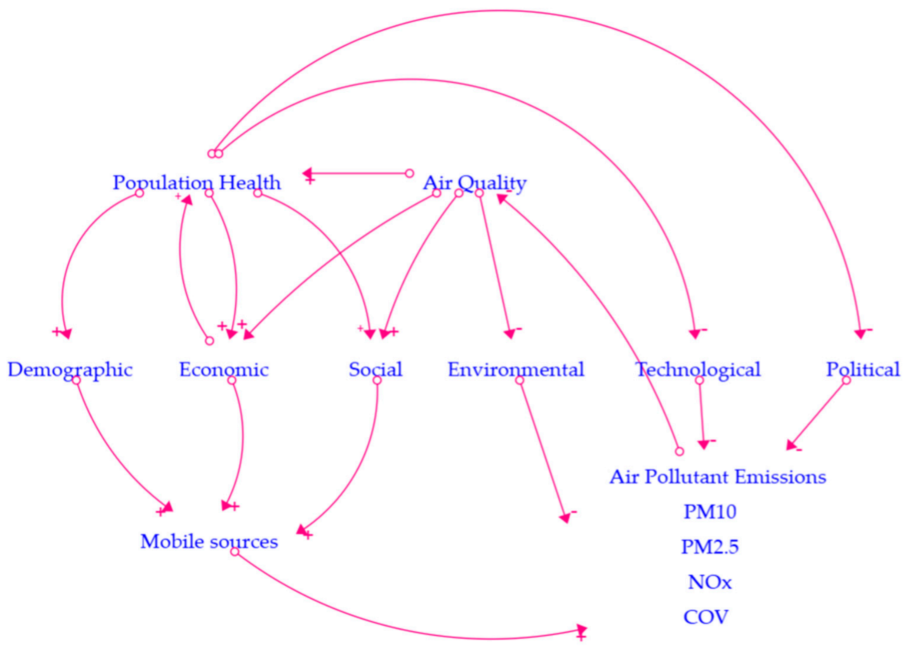

Figure 1. Causal loop diagram of the environmental simulation model for estimating air pollutant emissions from mobile sources. Author's own elaboration in Stella Professional Online 3.7.1.

Once the CLD diagram was completed, an initial simulation was performed to evaluate the model's reliability. For this purpose, PM_{10}, $PM_{2.5}$, NOx, and VOC emissions from the private sector of the mobile sources were estimated using only the EFs and VKT, data taken from the 2018 Emission Inventory Calculation Report [35]. To calculate the VKT, the emission inventory calculation report uses Equation (2), which equals the product of the kilometers traveled per day per type of vehicle, the number of vehicles of that type, and the number of days per year in which the vehicles of that type circulate. The result will be shown in kilometers traveled per year.

$$VKT_{ij} = (KD_i) \times (NV_{ij}) \times (DY_i), \quad (2)$$

where

VKT_{ij} = vehicle kilometers traveled by vehicle type i, model year j [km/year];

KD_i = kilometers traveled per day by vehicle type i [km/day];

NV_{ij} = number of vehicles of type i, model year j [number of vehicles];

DY_i = days per year in which vehicles of type i circulate [days/year].

Figure 2 shows the result of this first simulation, for which both the VKT by vehicle type and model year, as well as the weighted EFs [g/km] for gasoline vehicles in the MCMA were taken from the calculation report [35]. The VKT data used are shown in Table 5. On the other hand, Table 6 shows the corresponding EFs used, and Table 7 shows the emission of pollutants by element in tons per year at 89.4%, which is the amount coming from private cars, SUVs, and motorcycles.

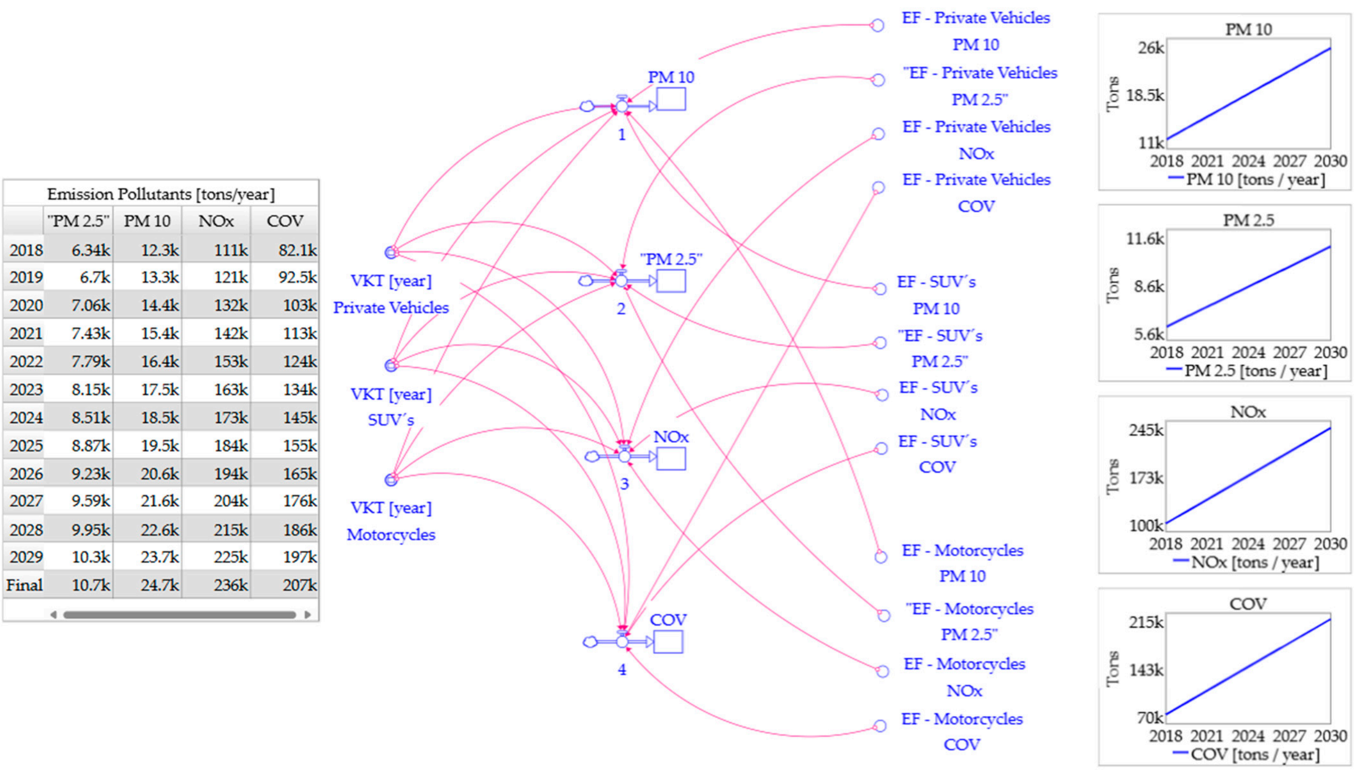

Figure 2. Initial environmental simulation to estimate air pollutant emissions from mobile sources. Author's own elaboration in Stella Professional Online 3.7.1.

Table 5. Kilometers traveled per day by vehicle type [millions].

Vehicle Type	km/Day
Private vehicles/Passenger cars	5842.42
SUV	1290.59
Motorcycles	1365.45

Author's own elaboration based on the 2018 MCMA Emissions Inventory Calculation Report.

Table 6. Weighted emission factors for gasoline-powered vehicles in MCMA [g/km].

Type of Vehicle	PM_{10}	$PM_{2.5}$	NOx	COV
Private vehicles/Passenger cars	0.139	0.049	1.220	1.253
SUVs	0.141	0.044	2.095	1.544
Motorcycles	0.028	0.013	0.415	0.806

Author's own elaboration, based on the 2018 MCMA Emissions Inventory Calculation Report.

Table 7. Emission of pollutants in MCMA in 2018 [tons/year].

Type of Source	PM_{10}	$PM_{2.5}$	NOx	COV
Mobile source	13,763	7098	124,115	91,771
% Corresponding to the private sector	89.4	89.4	89.4	89.4
Private sector [tons/year]	12,304	6346	110,959	82,043

Author's own elaboration, based on the 2018 MCMA Emissions Inventory Calculation Report.

The results of this first simulation estimate that by 2030, the tons of PM_{10} emitted per year will be 24,700, those of $PM_{2.5}$ will be 10,700, the tons of NOx emitted will be 236,000, and the tons of VOC will be 207,000. These represent increases of 39.3%, 25.1%, 51.3%, and 91.6% of these pollutants criteria, respectively, taking as reference a trend scenario; that is, the scenario that estimates the emissions that would be generated if no action were taken to reduce atmospheric pollutants.

These data initially reveal higher contamination than expected, as shown in Table 8, with the data on O_3 precursors showing the greatest differences in their calculation. Based on the data provided by the Secretariat of the Environment (SEDEMA, Spanish acronym), this simulation shows the urgent need to update the methodology used so far to estimate emissions. This would also imply that the effectiveness of the actions and measures implemented by the ProAire ZMVM 2021–2030 would be compromised and might not be sufficient to control and reduce emissions by 2030.

Table 8. Estimation of atmospheric pollutants, trend scenario [tons/year].

Criteria Air Pollutants	PM_{10}	$PM_{2.5}$	NOx	COV
Trend scenario	17,727	8,555	155,978	108,015

Author's own elaboration, based on the ProAire ZMVM 2021–2030.

After this first simulation of the environmental model, in which only the VKT and EF data were used to calculate air pollutant emissions, a more adverse scenario was observed than the one predicted by SEDEMA. It should be recalled that these data were calculated using MOVES-Mexico 2018 software, and that information related to the vehicle fleet, geographic area, fuel quality, mobility patterns, and type of roads in the MCMA was used for the modeling.

Figure 3 shows the proposed system dynamics environmental simulation model using DESTEP systemic analysis to estimate air pollutant emissions from the transportation sector in the MCMA through 2030. This model mainly comprises three aspects: the first part contains the demographic, economic, and social factors directly related to the increase in mobile sources in the MCMA.

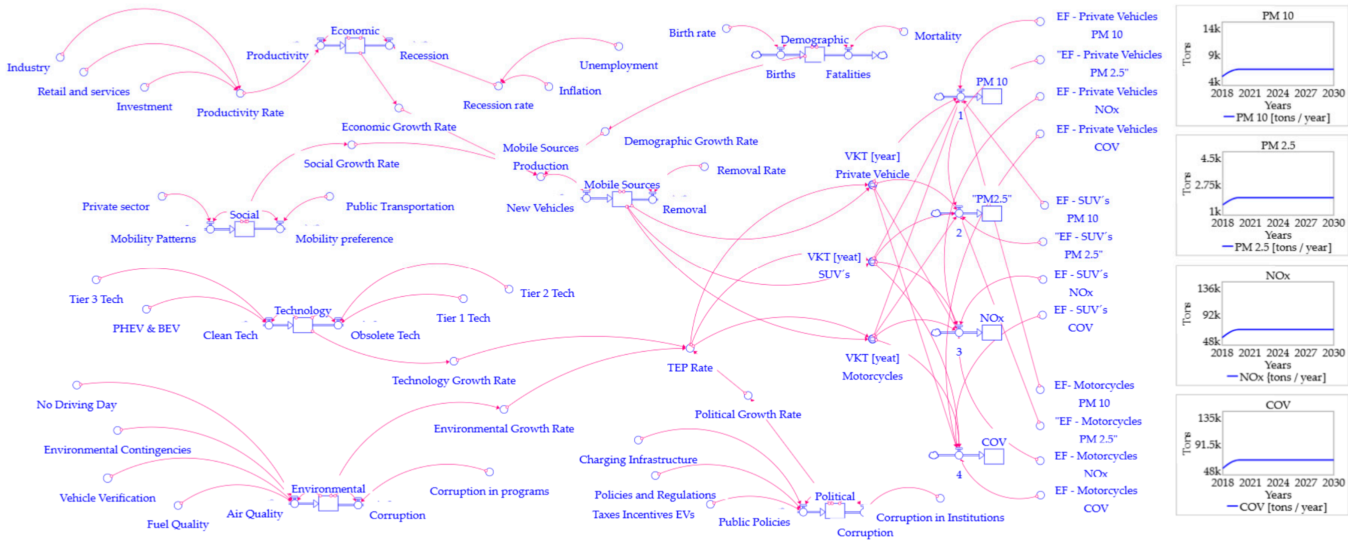

Figure 3. Proposed environmental simulation model using DESTEP systemic factors to estimate air pollutant emissions from the transportation sector in MCMA by 2030. Author's own elaboration in Stella Professional Online 3.7.1.

The second part of this model comprises technological, ecological, and political factors, which do not directly influence the increase in mobile sources, but affect the number of VKT in the metropolitan area. These first two parts are connected and ultimately modify the VKT, which is finally used to estimate criteria air pollutants in the third part of the model. This third part of the simulation corresponds to the first simulation shown in Figure 2; configuring the simulation in this way would allow for forecasting the VKT while keeping the EFs constant. In other words, the factors implemented in the DESTEP analysis alter the dynamics of the system variables, helping to understand the broader context emissions in MCMA.

The simulation took into account birth and death rates for the demographic factor; productivity growth and recession rates for the economic factor; mobility patterns for the social factor; vehicle technology for the technological factor; the effectiveness of the programs, such as No Driving Day (Hoy no Circula), Environmental Contingencies (Contingencias Ambientales), Obligatory Vehicle Verification Program (Verificentros), as well as fuel quality and the perception of corruption for the ecological factor; and, finally, the effectiveness of the infrastructure of battery charging stations, policies, regulations, incentives for the acquisition of clean cars, and the perception of corruption for the political factor.

Since each factor uses different types of units, the values were normalized using Equation (3), which indicates that the growth rate per factor equals the final value of that factor minus its corresponding initial value, divided by the initial value of the same factor. This normalization is used to obtain the rate of increase or reduction that the mobile sources or VKT undergo, given the modification of each factor included in the system.

$$\text{Growth rate}_d = (\text{Factor}_{df} - \text{Factor}_{di})/(\text{Factor}_{di}), \quad (3)$$

where

Growth rate_d = rate of increase or reduction of factor d [%];

Factor_{di} = initial value of factor d;

Factor_{df} = final value of factor d;

Finally, the factors of the DESTEP analysis are integrated into the simulation using Equation (4), which shows that the VKT by type of vehicle is equal to the product of the number of vehicles in the metropolitan area, the corresponding percentage of vehicle type, the kilometers traveled per day, the days of circulation per year, and the rate of increase or reduction in the technological, ecological, and political factors, all added to the initial value of the VKT.

$$VKT_t = ((NV_t) * (PV_t) * (KD_t) * (Dy_t) * (1 - TEP\_rate)) + VKT_{ti} \quad (4)$$

where

VKT_t = vehicle kilometers traveled by vehicle type t [km/year];
NV_t = number of vehicles of type t [number of vehicles];
PV_t = corresponding percentage for vehicle type t [%];
KD_i = kilometers traveled per day by vehicle type t [km/day];
DY_i = days per year in which vehicles of type t circulate [days/year];
TEP_rate = growth rate of technological, ecological, and political factors [%];
VKT_{ti} = initial vehicle kilometers traveled by vehicle type t [km/year]

5. Discussion

The proposed model, shown in Figure 3, aims to improve the calculation carried out by the local entities shown in Figure 2 by incorporating into the simulation the DESTEP factors that ultimately modify the complex dynamic of the environmental system, and whose behavior alters the VKT. Figure 4 shows the simulation of the proposed environmental simulation model.

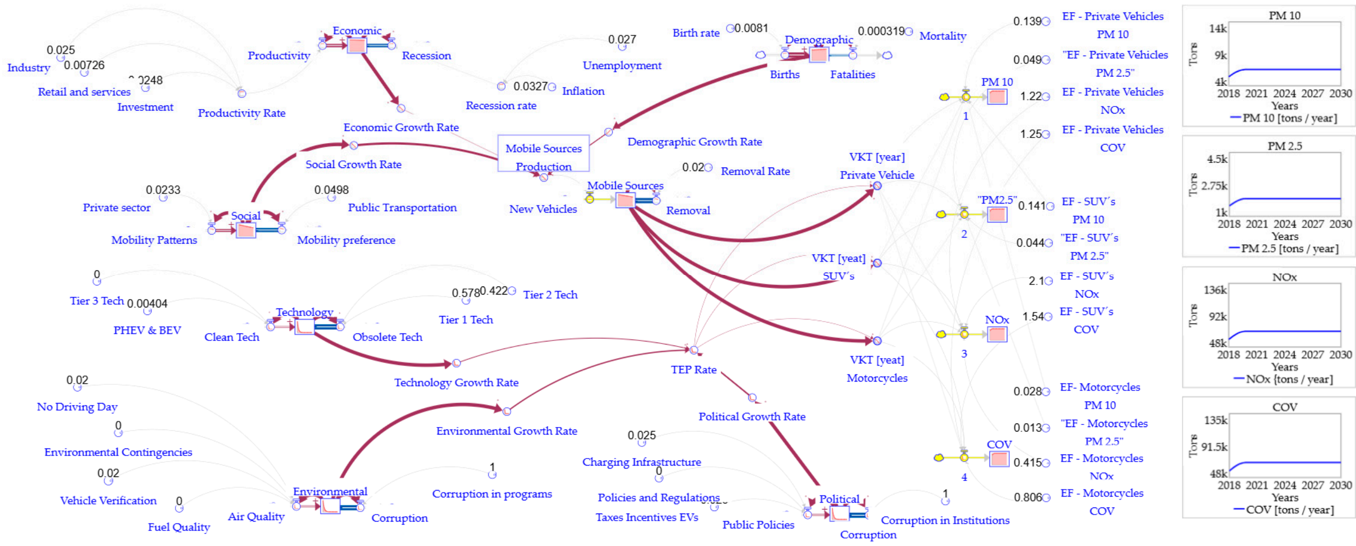

Figure 4. Proposed environmental simulation model using DESTEP systemic analysis and the results. Author's own elaboration in Stella Professional Online 3.7.1.

Unlike the first simulation, which used only the VKT and EFs, the second simulation model used updated data taken from the ProAire ZMVM 2021–2030 and the 2018 MCMA Emissions Inventory, as well as from the National Institute of Statistics and Geography (INEGI, Spanish acronym) and the Bank of Mexico (Mexico's central bank) to estimate more accurately the emissions of criteria air pollutants by 2030, and thus obtain an updated and realistic picture of the effectiveness of the measures and actions implemented by SEDEMA to reduce emissions.

Table 9 shows the results of the second simulation model using the DESTEP systemic analysis to estimate air pollutant emissions from the transportation sector in the MCMA by 2030. As can be seen, the obtained results improve significantly, even becoming better than the levels predicted by ProAire, once the measures and actions to try to counteract the emission of pollutants criteria by 2030 are implemented.

Table 9. Results of the proposed environmental simulation model [tons/year].

Air Pollutants Estimation	PM_{10}	$PM_{2.5}$	NOx	COV
2018	5.41k	1.57k	58.4k	57.1k
2019	6.29k	1.88k	67.2k	65.9k
2020	6.56k	1.97k	69.8k	68.4k
2021	6.56k	1.97k	69.8k	68.4k
2022	6.56k	1.97k	69.8k	68.4k
2023	6.56k	1.97k	69.8k	68.4k
2024	6.56k	1.97k	69.8k	68.4k
2025	6.56k	1.97k	69.8k	68.4k
2026	6.56k	1.97k	69.8k	68.4k
2027	6.56k	1.97k	69.8k	68.4k
2028	6.56k	1.97k	69.8k	68.4k
2029	6.56k	1.97k	69.8k	68.4k
2030	6.56k	1.97k	69.8k	68.4k

Author's own elaboration in Stella Professional Online 3.7.1.

Comparing these results against the values estimated by ProAire, shown in Table 10, it is shown that the results given by the simulation are 106% lower for PM_{10}, 176% for $PM_{2.5}$, 34% for NOx, and 17% for VOCs.

Table 10. Estimation of atmospheric pollutants, ProAire Estimations [tons/year].

Criteria Air Pollutants	PM_{10}	$PM_{2.5}$	NOx	COV
Estimations from ProAire ZMVM 2021–2030	13,530	5,442	93,223	80,196

Author's own elaboration, based on the ProAire ZMVM 2021–2030.

These results could be biased due to the input data of the simulation and the country's current situation. Although the simulation results indeed estimate a lower emission of pollutants criteria than that predicted by the ProAire, these data can be observed to result from a decreasing economy. Based on the GDP in 2018, which was 5.09 trillion pesos [31], it is estimated, based on the current data, that in 2030, the GDP will be 4.93 trillion, which generates a reduction in mobile sources and, therefore, a reduction in pollutant emissions.

However, as should be the goal of every government, public policy decision-making is mainly focused on providing security, generating adequate conditions for access to public health and education, and promoting economic growth at municipal, state, and federal levels; therefore, if the economy in the central zone of the country was to increase, lowering unemployment and inflation levels, while increasing the number of trips, a very different scenario than the one shown in the current simulation could be presented.

It would be enough for the unemployment rate to drop from 2.7% to 2% for inflation to drop from 3.27% to 2.27%, and for the number of trips in private vehicles, given the changes in the inflation and unemployment rates, to increase from 21.09% to 27.12%, for emissions of criteria air pollutants to undergo a very significant increase. With these variations in these variables, emissions would go from being within the ProAire estimates to being well above the estimates for NOx and VOCs, putting PM2.5 and PM10 levels at risk as well. Figure 5 shows the simulation, given the changes in unemployment, inflation, and private mobility pattern rates. Table 11 shows the estimated tons by 2030 in the event of this scenario.

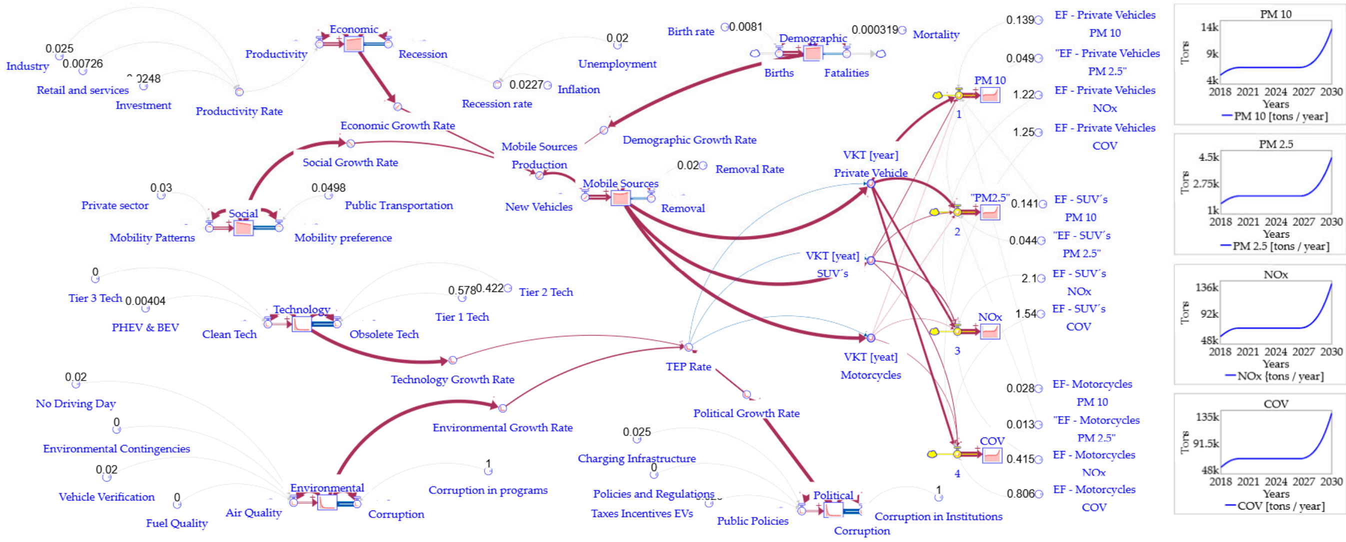

Figure 5. Proposed environmental simulation model given variations in unemployment, inflation, and commuting rates [tons/year].

Table 11. Results of the proposed environmental simulation model given variations in unemployment, inflation, and commuting rates [tons/year].

Air Pollutants Estimation	PM_{10}	$PM_{2.5}$	NOx	COV
2018	5.41k	1.57k	58.4k	57.1k
2019	6.29k	1.88k	67.2k	65.9k
2020	6.62k	1.99k	70.3k	69k
2021	6.62k	1.99k	70.3k	69k
2022	6.62k	1.99k	70.3k	69k
2023	6.62k	1.99k	70.3k	69k
2024	6.62k	1.99k	70.3k	69k
2025	6.62k	1.99k	70.3k	69k
2026	6.62k	1.99k	70.3k	69k
2027	6.7k	2.02k	71k	69.6k
2028	7.49k	2.3k	78.9k	77.5k
2029	9.37k	2.96k	98k	96.8k
2030	12.7k	4.11k	132k	131k

Author's own elaboration in Stella Professional Online 3.7.1.

Among the measures related to limiting pollution from exhaust gas emissions are the design of public policies, updating the corresponding regulations, improving the efficiency of government programs such as the No Driving Day, Environmental Contingencies, Obligatory Vehicle Verification Program, or by updating the technology of the vehicle fleet. However, the simulation suggests that one of the strategies with the most significant impact on the control and reduction of emissions would be focused on the use and promotion of public transportation [38,39].

The abovementioned measures would benefit citizens most significantly by reducing emissions, improving air quality, and protecting the population's health. Figure 6 shows the system's dynamics by increasing public transport use. If public transport use were to increase from 45.05% to 50% (1.71 million trips approximately), even with changes in unemployment rates, inflation, and the number of trips, the emissions of pollutants criteria would remain well below those estimated by ProAire.

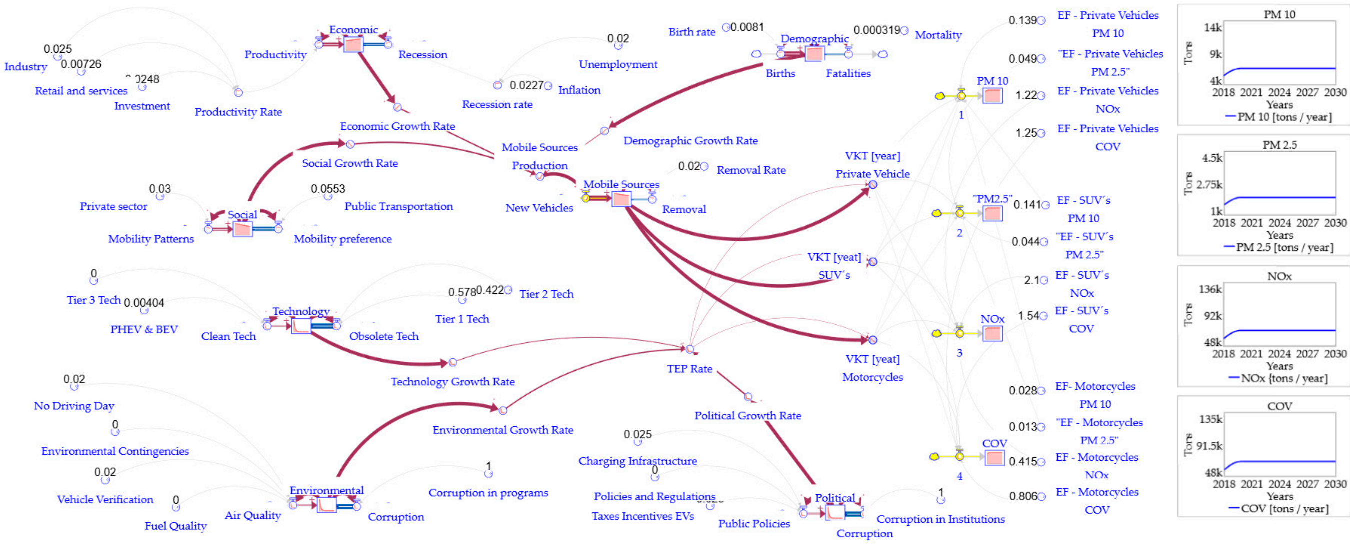

Figure 6. Proposed environmental simulation model using DESTEP systemic analysis to estimate air pollutant emissions from the transportation sector in MCMA by 2030. Measures and actions implemented to foster the use of public transport. Author's own elaboration in Stella Professional Online 3.7.1.

Table 12 shows the results of the estimates of pollutant criteria by 2030, given the implementation of measures and actions focused on the use and improvement of public transportation and road infrastructure. As stated in the ProAire ZMVM 2021–2030, implementing measures concentrated on updating the regulatory framework to reduce VOCs, fine particles, and combustion gases, as well as updating vehicle emissions regulations, is of utmost importance. However, this simulation shows the different strategies that could be implemented, aimed at promoting the use of public transport, such as improving the conditions of both roads and units, updating the public transport fleet, improving the perspective in terms of safety and efficiency, as well as providing better working conditions for drivers.

Table 12. Results of the proposed environmental simulation model given an increment in the use of public transportation to estimate air pollutant emissions from the transportation sector [tons/year].

Air Pollutants Estimation	PM_{10}	$PM_{2.5}$	NOx	COV
2018	5.41k	1.57k	58.4k	57.1k
2019	6.29k	1.88k	67.2k	65.9k
2020	6.56k	1.97k	69.8k	68.4k
2021	6.56k	1.97k	69.8k	68.4k
2022	6.56k	1.97k	69.8k	68.4k
2023	6.56k	1.97k	69.8k	68.4k
2024	6.56k	1.97k	69.8k	68.4k
2025	6.56k	1.97k	69.8k	68.4k
2026	6.56k	1.97k	69.8k	68.4k
2027	6.56k	1.97k	69.8k	68.4k
2028	6.56k	1.97k	69.8k	68.4k
2029	6.56k	1.97k	69.8k	68.4k
2030	6.56k	1.97k	69.8k	68.4k

Author's own elaboration in Stella Professional Online 3.7.1.

Through the simulations of the dynamics of the environmental model in the MCMA, it can be observed that the estimates from ProAire ZMVM 2021–2030 are very optimistic compared to the results of the first simulation in Stella (Figure 2). The simulation estimates that by 2030, the annual emissions will be 24,700 tons of PM_{10}, 10,700 tons of $PM_{2.5}$, 236,000 tons of NOx, and 207,000 tons of VOCs, representing an increase of 82.6%, 96.6%, 153.2%, and 158.1% of these pollutants criteria, respectively.

However, by performing the environmental simulation model from a holistic perspective, through the implementation of the DESTEP analysis, more accurate estimates of pollutant criteria emissions are obtained. These results, shown in Table 12, demonstrate that, unlike the forecast of ProAire ZMVM 2021–2030, the tons emitted by 2030 would be even lower than expected.

Despite the positive results of this simulation, it is essential to consider how variable the results can be, since these data are mainly due to the current situation in the country. However, if the economy in the central part of the country were to grow, if unemployment and inflation levels were to drop, and if the number of trips in private vehicles were to increase, among other things, a very different picture could emerge from the one shown in this subsequent simulation.

6. Conclusions

This study aimed to design an environmental simulation model using system dynamics to estimate air pollution from the transportation sector in the most important Megacity in Mexico by 2030 from a holistic perspective, based on the region's DESTEP analysis factors, to foresee the evolution of air quality. The proposed model is shown in Figure 3, with the study variables shown in Table 3 and the DESTEP analysis attributes depicted in Table 4.

This model is made up of three main components: demographic, economic, and social factors, which are directly related to the increase in mobile sources; technological, ecological, and political factors, which do not directly influence the rise in mobile sources but do affect the number of VKT in the megacity. Finally, these first two parts are connected and used to estimate criteria air pollutants (tons/year) in the third part of the model (Figure 2).

One of the main advantages of this simulation structure design is how the DESTEP analysis factors are integrated for both the estimation of the increase in mobile sources (in this case, private cars) and the calculation of VKT per year by vehicle type. In addition, this model allows the inclusion of different variables, which provide more accurate results by simulating the system's dynamics from a holistic perspective.

While the environmental simulation model using system dynamics proposed in this study is tailored to the MCMA, the structure itself, the variables, as well as the DESTEP analysis factors utilized in this study's environmental model might be applied to different megacities worldwide to estimate air pollutant emissions from other sources by calibrating its initial values or reevaluating its sub-variables.

Derived from these data, with a higher level of reliability, priorities and public policy proposals could be established, focusing on the primary factors and variables that have the most significant impact on the generation of pollutants criteria and, therefore, on air quality and the population's health. Measures and actions to be implemented should be mainly focused on promoting the use of public passenger transportation through the improvement and expansion of roads and high-capacity units, updating the public transportation fleet, renewing its technology, and improving its perception in terms of safety and efficiency, as well as providing better working conditions for drivers, without neglecting the improvement in the infrastructure and the increase in non-motorized transportation trips in the metropolitan area.

This study was limited by the information utilized for the attribute values inputted into the proposed simulation. The availability of historical data would have improved the resolution of the simulation's initial values. Future work, calibrating the simulation model, should include more accurate information regarding Tier 3 technology, PHEV, and BEV adoption rates, governmental program effectiveness, and fuel quality standards.

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