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Predicting the Level of Ecological Safety for Man-made Objects

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Abstract: The authors explored the utilization of simulation models as a means to ensure environmental safety, using the industrial hub of Kemerovo as an illustrative example. The article analyzes the factors that have contributed to the deterioration of the environment in the region for decades. It has been established that in terms of the overall percentage distribution of emissions from stationary sources, energy enterprises (73.0%), chemical and petrochemical industries (4.7%), and black metallurgy enterprises (7.8%) are leading in the city of Kemerovo. Simulation modelling has shown that the cause of high concentrations of harmful substances in the atmosphere of Kemerovo is due to the negative factors of industrial and household activities and their impact on environmental safety. High correlation and sensitivity coefficients indicate a lack of new available technologies in the region's industry and transport that could prevent air pollution. The forecasting model has indicated a potential two, three or even greater increase in emissions. For example, in the long-term perspective, by 2063, manufacturing emissions could potentially increase by 35 times, leading to irreversible ecological consequences. Extreme pollution and depletion of natural resources could make living in this region impossible.

Keywords: atmospheric pollution, ecological risk, ecological disaster, environmental safety zone, hazardous industries

1. Introduction

This article assesses and forecasts the level of ecological safety in Kuzbass, a region where the anthropogenic landscape covers half of the territory. Kemerovo, Prokopyevsk, Kiselevsk, Belovo, Leninsk-Kuznetsky, and many other cities have been declared ecological disaster zones. In general, normal functioning of the biosphere there is no longer possible. In the Prokopyevsk-Kiselevsk region, atmospheric pollution reaches 300 tons of dust and soot per hectare per year. The threat of an ecological crisis in the area, which many authors have discussed, has already arrived (Schastlivtsev & Bragin 2007). Due to the intensification of metallurgical, chemical, coal mining, and energy industries, Kemerovo and its surrounding region have emerged as one of the primary industrial areas in Siberia and Russia. Unfortunately, this has led to Kemerovo becoming the most polluted region in terms of air pollution. With even greater intensification of the metallurgical, chemical, coal mining, and energy industries, one of the leading industrial regions of Siberia and Russia (Kemerovo and Kemerovo region) has become the most environmentally disadvantaged area in terms of atmospheric pollution. Due to the prevailing wind direction, the city of Kemerovo is directly affected by emissions from nearby mines; the operation of numerous environmentally hazardous enterprises contributes to the increase in environmental pollution; year after year, the volume of benzopyrene (which is a combustion product of various types of fuel) continues to grow, and it has become a real disaster for the city. The rapid growth of coal mining in the Kuzbass region, predominantly through open-pit mining, is leading to a rapid development of an environmental and social disaster in the area.

In 1943, Kemerovo, a city in the Novosibirsk region, was designated as the administrative centre of the Kemerovo region. This decision was primarily influenced by the Kuznetsk coal basin becoming a major supplier of coal and iron ore during World War II, leading to the relocation of numerous industrial enterprises to the area. However, the concentration of these industrial facilities in the region had a negative impact on production and economic activities, resulting in a significant anthropogenic burden on the environment. For example, the industrial complex of Novokuznetsk includes two metallurgical plants, aluminium and ferroalloy factories, agglomeration and coal enrichment plants, several mines and open pits, three major thermal power plants, and over 60 small boiler houses. Currently, the region is home to roughly 2.6 million people, exacerbating the challenges of ensuring environmental safety due to the presence of numerous mining and metallurgical enterprises that provide employment opportunities but also pose environmental risks (Levakova & Arustamov 2019, Galanina & Ovsiannikova 2012).

The Kuzbass region is characterized by vast lunar landscapes, which experts attribute to the lack of thoughtful and rational legislation, disregard for environmental safety principles, and wasteful practices. The region's overreliance on resource-dependent industries poses risks of resource depletion and environmental degradation (Ryabov et al. 2018, Zaushintsena & Koghevnikov 2017, Pashkevich & Shuvalov 2006). Scientists evaluating the region's natural assets have found that the existing enterprises have a limited coal supply: the remaining resource in mines is projected to last for 47 years, while the open-pit mines are expected to be operational for 30 years. However, enterprise owners often strive to exceed production volumes if they acquire modern equipment. It would have been logical to invest the income generated from coal sales into shaping a non-resource-based future for the region, but unfortunately, this has not occurred. The rapid and often uncontrolled intensification of natural resource extraction, urbanization, and significant emissions have contributed to a critical and dangerous situation (Golokhvast et al. 2017, Smirnova & Larionov 2020, Smirnova & Larionova 2020).

In the 1990s, Kemerovo ranked third in terms of pollution levels. The city constantly grapples with smog and is considered an "ecological disaster zone." This issue is mainly attributed to its unfavourable location, which results in the accumulation of industrial emissions in the city. Air pollution is the most pressing problem in the region, with cities such as Kemerovo, Novokuznetsk, and Prokopyevsk consistently ranking high on the list of most polluted urban areas in the country. On average, stationary and mobile sources contribute to the emission of almost 2 (1718.8) million tons of pollutants into the atmosphere of Kemerovo and the Kemerovo region (Levakova & Arustamov 2019).

It is important to note that the majority of emissions in the Kemerovo region consist of extremely hazardous and highly dangerous substances, with carbon monoxide (51.6%), sulfuric anhydride (15%), nitrogen oxides (8%), hydrocarbons (3.5%), and suspended solids being the main pollutants. The largest contributors to emissions in Kemerovo are energy enterprises, chemical and petrochemical industries, and ferrous metallurgy enterprises. It is evident that atmospheric pollution from coal mining (Kemerovo region) is directly linked to the production volume, with each thousand tons of coal mined leading to the emission of approximately 2.17 tons of harmful substances into the atmosphere (Nevzorov & Manakov 2017).

However, the current legislation in Russia primarily focuses on regulating stationary sources of pollution, which is inadequate when estimating emissions in urban environments where transportation is a major contributor. There is a significant lack of control over emissions from mobile vehicles. Existing systems for modelling emissions, such as the Unified Program for the Calculation of Atmospheric Pollution (UPRZA "Ecologist" v. 4.70), provide calculations on the dispersion of pollutants in the air. Although UPRZA is relevant and aligned with current methods and standards, it does not fully address the issue of forecasting air pollution in the city, as its calculations are not comprehensive.

To address these challenges and ensure environmental safety in urban atmospheric conditions, the author presents the objective of developing a model capable of predicting criteria related to environmental safety. Such a model would be crucial in effectively managing and mitigating air pollution in the Kemerovo and Kemerovo region.

2. Materials and Methods

2.1. Model analyses

Three important tests were conducted: model calibration, model validation, and sensitivity testing (Xing et al. 2019), to ensure the validity of the model structure

2.1.1. Calibration

Calibration provides values for unknown parameters not considered in the model (Batty 2009). A calibration index was included to set an acceptable value for each sector of the model. Predictions were divided into two parts. The first part of 2022 was used for model calibration, then validated with the second part data for 2023 (Luo et al. 2010). Thus, data for 2022 was initial year data.

For calibration as an additional parameter to optimize values of Particulate Matter Emissions (PM emissions) results for minimizing the difference between actual and simulated values a calibration rate (index) was applied (Pinto et al. 2017):

$$calibration\_index = \frac{actual\_data}{predicted\_data}, \tag{1}$$

where $actual$ is the actual data value, *predicted* is the simulated data value.

2.1.2. Validation

The Simulation Error coefficient (hereafter SER) is widely used to evaluate the performance of an environmental dynamic model for model validation. SER measures the difference between model predictions and observed data and can be used to assess the accuracy of model simulations. Thus, SER can be used to optimize model parameters and reduce prediction errors (Xu et al. 2015). Predicted values can be compared with actual data from 2022 to determine the accuracy of the simulation. If the simulation error rate is low and the errors are less than 10%, then it can be concluded that the sector has passed the validation test and can be considered an effective model sector (Liu et al. 2020). Data from 2023 was used to validate data of further predictions. The mean of the percentage difference was used to evaluate a simulation error rate (Xing et al. 2019). The mean of the absolute difference (hereafter MAD) represents the next equation:

$$absolut\_error = |actual - predicted| \tag{2}$$

The Mean Absolute Percentage Error (MAPE) is represented by equation 3 (%):

$$relative\_error = \frac{absolut\_error}{actual} \times 100\% \tag{3}$$

2.1.3. Sensitivity analyses

Sensitivity analysis was used to validate data from 2023. Sensitivity analysis is conducted to determine how changes in the initial parameters affect the model. Sensitivity analysis shows the model response to small changes. The method is mainly used to identify the key input data of the model and the associated variability in model predictions.

The steps of the sensitivity analyses:

1. Defining the input variables. Identifying the variables that influence the model's predictions for PM emissions. For this step, correlation and Root Mean Square Error (RMSER) analysis methods are used (Pianosi et al. 2016) to determine the strength of relationships between variables. The study used these methods to detect the most significant variables that influence PM emissions.
2. Determining the range of variation. Determining the range of values for each input variable that will be used in the sensitivity analysis. The values were changed by 10%, 15%, 20%, 25%, and 30% (Wei et al. 2012).
3. Implementation and validation. After the model's simulation, the output's sensitivity must be evaluated. A sensitivity coefficient was evaluated (Sourisseau et al. 2008). Equation 4 represents the equation for the sensitivity coefficient.

$$sensitivity\_coefficient = \frac{\Delta y(x)}{\Delta x}, \tag{4}$$

where $\Delta y(x)$ change of dependent variable, Δx change of independent variable. The general sensitivity degree index, i.e. the sensitivity of a dependent variable is given in equation 5:

$$sensitivity\_degree\_index = \frac{1}{n}\sum sensitivity\_coef. \tag{5}$$

where n is the number of indexes.

The sensitivity analysis was performed through the "one-at-a-time" approach, where the value of a single parameter was modified at a time while maintaining the values of the other parameters constant (Wei et al. 2012).

3. Results

3.1. Model predictions: Total PM emissions

3.1.1. Calibration results

Results of the simulation of PM emissions in the model include six values: (1) emission from the household sector, (2) transport sector, industrial sector, which includes (3) manufacturing, (4) power plants and (5) mining sub-sectors. The model was calibrated against actual data collected from air quality monitoring stations in Kemerovo city to ensure the accuracy of the model predictions.

It should be noted that there is a large discrepancy in the statistical data on emissions of pollutants into the atmosphere from stationary sources of pollution in Kemerovo and the Kemerovo region. For example, the state report for 2017 tells about 1 487.7 ths tons (Rosprirodnadzor 2017). The article by Levakova and Arustamov indicated 1 348.7 ths tons (Levakova & Arustamov 2019).

According to the South Siberian Interregional Department of Rosprirodnadzor (2017), 4 912 ths tons of pollutants were released into the atmosphere, of which 1 603 ths tons fell in the Kemerovo region (Rosprirodnadzor 2017). In 2020, emissions amounted to 1 612 ths tons (Rosprirodnadzor 2021). The maximum allowable emissions (solid particles) set for power plants is exceeded by 5 814.75 ths tons per year (Kemerovo Administration 2022).

The article uses up-to-date data received in 2022 at the request of Rosprirodnadzor in Kemerovo. The final calibration results are illustrated in Table 1, where actual data for 2022, predicted values and the index of calibration are presented.

Table 1. Comparison of actual and predicted data for 2022 with the calibration index

Sector	Predicted	Actual	Calibration index
Household	232.26	243.87	1.049
Transport	256.40	256.66	1.001
Manufacture	283.59	256.40	0.904
Power Plants	748.49	672.74	0.899
Mining	2342.96	2056.44	0.878

The closer the calibration index is to 1, the more reliable the results of the model are considered. The values closest to 1 are those of the household and transport, while other sectors also show low differences between actual and predicted values. Forecasting emissions for these two pollution sources (household and transport) shows that the calculation results have the smallest relative error.

3.1.2. Validation results

The validation of results using SER is first conducted using 2022 data to compare the actual and predicted data without calibration. The SER results for the 2022 data without calibration, presented in Table 2, demonstrate the high efficiency of the household and transport sectors, with a MAPE test result of less than 5%.

Table 2. Comparison of predicted and actual data (tons/year) for 2022 without calibration

Sector	Predicted	Actual	MAD	MAPE, %	Sector efficiency
Household	232.26	243.87	11.61	4.76	yes
Transport	256.40	256.66	0.26	0.10	yes
Manufacture	283.59	256.40	27.19	10.60	no
Power Plants	748.49	672.74	75.75	11.25	no
Mining	2342.96	2056.44	286.52	13.93	no

The efficiency of other sectors is significantly lower, particularly for the power plants and mining subsectors, indicating the absence of additional parameters that should have been included in the model.

After calibrating the parameters, SER is performed using the 2023 data. The results, presented in Table 3, demonstrate a high-efficiency level across all sectors.

Table 3. Comparison of predicted and actual data for 2023 without calibration

Sector	Predicted	Actual	MAD	MAPE, %	Sector efficiency
Household	244.98	270.25	25.27	9.35	yes
Transport	275.13	284.42	9.29	3.27	yes
Manufacture	1 338.44	1 483.2	144.76	9.76	yes
Power Plants	669.65	745.50	75.85	10.17	no
Mining	2 254.91	2 278.86	23.95	1.05	yes

The efficiency of the power plants sector is slightly lower than the others, with a MAPE value of more than 10%, exceeding the threshold by 0.17%. However, it can be said that the results have approximately the same relative error, indicating that an additional unaccounted for external factor and an additional calibration index are applied to further forecasts.

The correlation coefficient shows the highest direct proportional relationship between total emissions and enterprise emissions, as shown in Table 4.

Table 4. Correlation coefficients of emissions by types of agents

Agent	Transport	Manufacture	Household
Correlation coefficients	-0.292	1.0	0.313

That means that enterprises are the main source of pollution in the city of Kemerovo.

3.1.3. Sensitivity analyses

A series of sensitivity analyses were conducted in the study to investigate how input parameter changes affect the system's responses. The model consists of 12 initial parameters, 3 initial variables, 2 table (lookup) functions, and 37 constants (parameters) that change the values of 109 variables, driving changes in 9 stocks overall. The sectors with the greatest impact on final PM emissions from all sectors were first identified with a correlation test to select the most significant parameters for the test.

There is the emissions output for 2022-2063 and correlation results. All sectors show a high correlation coefficient between simulated final emissions and emissions from their respective sectors: the industrial sector (R = 1.0), the transport sector (R = 1.0), and the household sector (R = 0.88). The regression test identified the most significant inputs from the transport and industrial sectors. It can be concluded that the presence of solid particles in the gas composition of the air can double. First of all, this growth occurs in connection with the activity of the coal mining industry and the industry associated with energy production. There is also a significant increase in emissions from transport, which can also be associated with industry growth.

The contribution to the result of the model is all the more significant as the value of the sensitivity coefficient is greater. The variable with the highest response to changes in input values was "energy_consumption_dynamic", with a sensitivity degree index of 80.453. That means that even small changes in the independent variable (Fig. 1a), which is a stock driver, significantly influence the value of all PM emissions, which is a dependent variable (Fig. 1b).

a.

b.

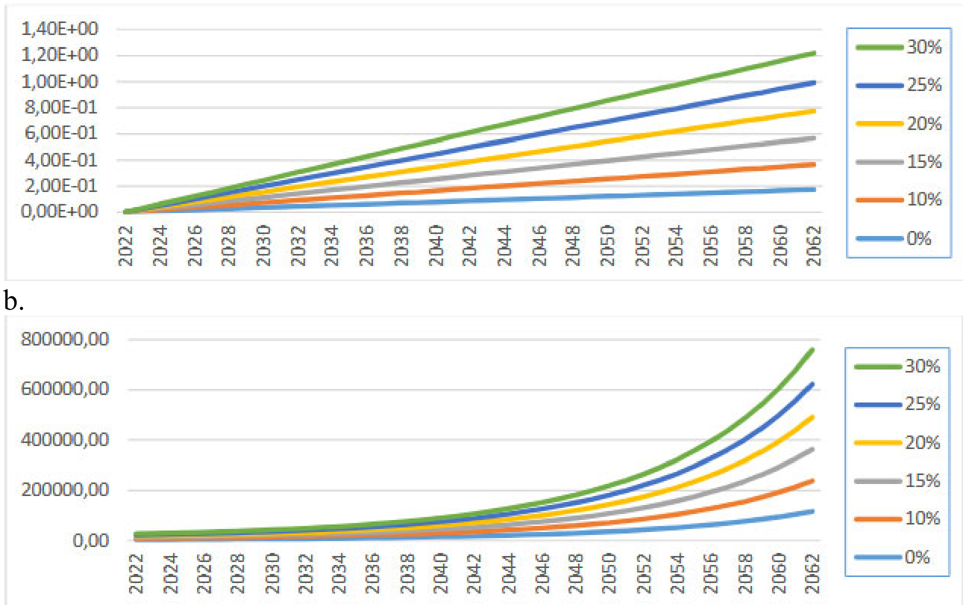

Fig. 1. (a, b). Sensitivity test: change of independent variable "energy consumption_ dynamic" (a) and the dependent variable "PM emissions" (b)

Fig. 2 shows that the sensitivity coefficient starts showing significant changes (70.895) even with the smallest change of 10% and continues to grow proportionately.

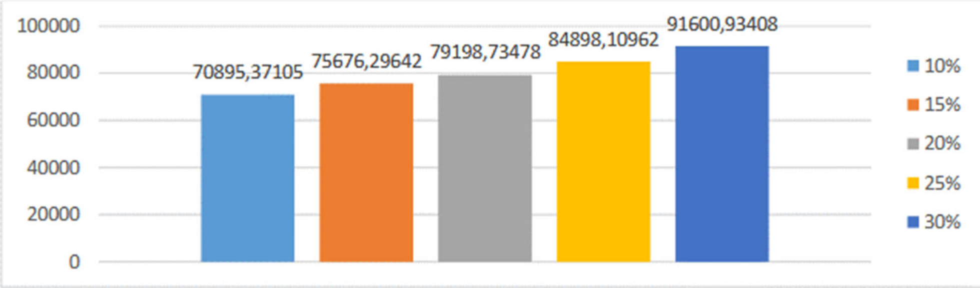

Fig. 2. The sensitivity coefficient change

During the calibration phase of the model, which aimed to incorporate unaccounted parameters and improve the accuracy of predictions, the predicted values for two sectors (transport and household) were found to be close to the real values. A difference between the actual and simulated values was noticed for other sectors, which is not unexpected given the high level of abstraction involved in dynamic simulation modelling compared to discrete-event or agent-based modelling approaches.

The mining and power plants sub-sectors have the lowest sector efficiency, according to the results of the sector validation before applied calibration. These findings suggest that the parameters used to model these sectors may be insufficient, and additional data collection may be necessary to obtain more accurate results. A common practice for validating and calibrating simulation model predictions is to use data covering at least five years (Van Vliet et al. 2016). However, in this study, only two years of data were used for validation, which may have a negative impact on the accuracy and reliability of the validation results.

The predicted values until 2063 show a doubling, tripling, and more harmful emissions into the atmosphere (Table 5).

Table 5. Emissions of pollutants into the atmosphere in 2022 and forecast for 2063 by pollution sources

Sources	2022 ths tonn	2063 ths tonn
Household	243.87	686.00
Transport	256.66	1 230.00
Manufacture	256.40	9 054.03
Power Plants	672.74	1 292.00
Mining	2 056.44	6 330.00

4. Conclusions

Testing of the constructed model showed the dynamics of pollutant emissions from different sources in the city of Kemerovo and the Kemerovo region. Correlation results indicate that industries, especially coal mining and power generation, are the main sources of particulate matter emissions. The modelling results show the projected growth of industrial emissions, emphasizing the need to regulate and prevent environmental hazards. The forecasting model indicated a potential two, three, or even greater increase in emissions. For instance, by 2063, production-related emissions could rise up to 35 times in the long term, leading to irreversible environmental consequences. This extreme pollution and depletion of natural resources could make habitation in this region impossible. In Kemerovo, benzopyrene, a combustion byproduct of various fuel types, remains predominant despite the absence of active mines. That indicates that zones where fuel combustion is used are the city's primary pollution sources. These sources include industrial enterprises (including numerous chemical plants), transportation, and the private sector. Despite the availability of new technologies, the intensive development of environmental and social catastrophes in the region has not been prevented. The Kemerovo region is characterized as a collection of "hot spots" with significant chemical pollution that threatens the environment and the population's health. The depletion of natural assets cannot be a stabilizing factor or a strategic direction for ensuring environmental safety and protecting the atmosphere from pollution caused by household, transportation, and industrial waste. The region has successfully achieved an appropriate level of production and consumption of mineral and biological resources to ensure the sustainable utilization of the natural environment. Consequently, it is crucial for the activities of industrial facilities and the population in all parts of the region to be structured in a manner that effectively mitigates atmospheric air pollution and aligns the high concentration of raw material and processing industries with the principles of green management and environmental safety.

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