An Integrated Mathematical Model for Emission and Dispersion of Atmospheric Pollutants in Industrial and Domestic Combustion Processes

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ABSTRACT

This study proposes the development, validation, and integration of mathematical models for estimating pollutant emissions (CO_2, SO_2, NOx, CO) from fossil fuel combustion and their atmospheric dispersion in complex terrain regions. Currently, Romania lacks a unified national model capable of describing both emission generation and ground-level immission fields simultaneously. In this first research phase, analytical methods for emission calculation based on stoichiometric combustion and emission factors are established, alongside a simplified Eulerian (Gaussian) dispersion model adapted to the environmental characteristics of the Jiu Valley (Petroșani). Experimental data collection is ongoing in collaboration with environmental monitoring agencies and industrial partners. The long-term objective is the implementation of an integrated atmospheric pollution assessment model calibrated for Romanian industrial regions.

KEYWORDS: *atmospheric pollution, emission modeling, pollutant dispersion, fossil fuel combustion, Jiu Valley - Romania*

1 INTRODUCTION

Air pollution remains one of the main environmental challenges associated with industrial combustion, domestic heating, and transportation. Despite the relevance of this issue, Romania does not yet possess an integrated mathematical model capable of simultaneously representing emissions and atmospheric immissions in industrial and domestic sectors.

The dual relationship between environmental protection and economic development requires quantitative tools that can optimize policy decisions under the principles of sustainable development. Such tools must integrate:

- Emission sources (industrial plants, domestic heating, transport),
- Atmospheric processes,
- Pollutant dispersion,
- Health and environmental impacts.

Atmospheric dispersion is governed by thermofluid dynamic processes involving turbulence, boundary layer structure, wind fields, and terrain complexity. Current Romanian methodologies rely mainly on steady-state Gaussian models, which are insufficient for complex terrain regions such as the Jiu Valley.

This study proposes the first stage of developing a comprehensive, experimentally validated, integrated model combining:

- Emission modeling,
- Atmospheric dispersion modeling,
- Model integration and validation with field measurements.

Special emphasis is placed on the Petroșani urban-industrial region, where main pollution sources include district heating plants, domestic coal combustion, industrial processes, ventilation stations of mining units, and residual dumps.

2 METHODS

2.1 Research Plan

The research follows a nine-stage methodology:

1. Analyze pollutant emission and immission dependence on fuel quality, combustion regime, and atmospheric conditions.
2. Develop a mathematical model for pollutant emissions from fossil fuel combustion.
3. Develop an Eulerian–Lagrangian model for pollutant dispersion.
4. Experimental validation of individual models.
5. Intermediate reporting.
6. Integration of emission + dispersion models.
7. Experimental validation of the integrated model.
8. Regional air quality evaluation for Petroșani.
9. Final reporting.

2.2 Emission Model

Two approaches were implemented:

2.2.1 Stoichiometric Calculation Method

Example for key pollutants:

Carbon dioxide (CO_2)

Reaction: $C + O_2 \rightarrow CO_2$

Produced mass:

$x = k \cdot a$, where $k = 44/12 = 11/3$

$a = q \cdot c$ (coal mass × carbon fraction)

Incomplete combustion: CO_2:CO = 70:30 for domestic stoves.

Similar formulations are used for sulfur dioxide (SO_2) and nitrogen dioxide (NO_2) based on:

$k_SO_2 = 2$, $k_NO_2 = 46/14 = 23/7$

2.2.2 Emission Factor Method

$E = B \cdot H_i \cdot e$

Where: B - fuel mass (kg), H_i — lower heating value (kJ/kg), e — emission factor (kg/kJ)

European standard values for coal: CO_2: $e = 98 \times 10^{-6}$, SO_2: $e = 1.77 \times 10^{-6}$, NO_x: $e = 2.2 \times 10^{-6}$

2.3 Atmospheric Dispersion Model (Eulerian / Gaussian)

In the first faze, I have analyzed the dependence of the emission and imission of pollutants at the burn of the fossil combustible, specific to the burning process, like: the quality of the combustibles, the burning conditions, as well as the parameters concerning the environment, like the wind speed, atmospheric conditions, atmospheric pressure, dispersion quotient. For this detailed study I have consulted a number of books and studies, accessed at the University of Petroşani Library, as well as at the internal Library of the Team of modeling the thermo-fluidic-dynamic process at the University of Petrosani.

From this analysis I have concluded which are the most relevant processes and factors for the description of the pollutants emission and imission, as well as the principal equations from the environment's thermo-fluidic-dynamics, which must be used in the mathematical modeling of the pollutants' emission and imission. From this study also resulted that the theory of the limit stratum from the fluids mechanics has an important role in the modeling of the pollutants' emissions on the smoke chimney, the differentiated equations from the theory of the limit stratum being the base of other, more simplified, models. The mathematical model for the pollutants' emission calculation, as a result of the burning processes in the industrial and home activities is one based on the quantity of the fossil combustible burned in an hour and which considers medium content pollutant chemical substances from the fossil combustibles. There are two approach methods: starting from the specific chemical reactions or starting from the emission factors [Ionel Ungureanu, 1996] the emissions of pollutants in the atmosphere through the burning of fossil combustibles can be calculated.

- <u>starting from the chemical reactions:</u>

a) the carbon dioxide

The burning equation:

$C + O_2 \rightarrow CO_2$

M_C …… ..M_{CO2}

A kg C ……x kg CO_2

We note: x – the quota from the carbon burned as carbon byoxide;

k – the report between the molecular mass of the CO_2 and the atomic mass of the carbon, which is the stoichiometric quotient (k=[12+(16*2)]/12=44/12=11/3);

a – the quantity (in kg) of used coal is obtained from the product of the elementary analysis (%) of the coal (c);

q – the quantity (in kg) of coal used in a house.

This way, a = q[kg]*c[%], results x= k*a.

Kipping in mind that we speak about the coal burning in stoves (for warming and cooking), we consider an incomplete burn and we take the rapport of 7:3, which is 70% CO_2, 30% CO.

3 DETERMINATION OF ATMOSPHERIC POLLUTANTS

3.1 Carbon Dioxide (CO_2)

Carbon dioxide (CO_2) is a colorless, odorless gas that is a natural component of the Earth's atmosphere. While it is essential for life processes such as photosynthesis, elevated concentrations of CO_2 are a major contributor to the greenhouse effect and climate change.

3.1.1 Sources of Carbon Dioxide

- **Natural sources:** Respiration by humans, animals, and microorganisms; decomposition of organic matter; volcanic eruptions; and ocean-atmosphere gas exchange.
- **Anthropogenic sources:** Combustion of fossil fuels in power plants, vehicles, industrial processes, and deforestation. Human activities have significantly increased atmospheric CO_2 concentrations since the Industrial Revolution.

Effects on Human Health: At ambient concentrations, CO_2 is generally not directly harmful to human health. However, at very high concentrations in confined spaces, it can cause headaches, dizziness, shortness of breath, and in extreme cases, loss of consciousness. Elevated atmospheric CO_2 contributes indirectly to health risks by driving climate change, which increases the frequency and intensity of heatwaves, extreme weather events, and the spread of vector-borne diseases.

Effects on Vegetation: CO_2 is essential for plant photosynthesis, and increased concentrations can stimulate plant growth under certain conditions (the "CO_2 fertilization effect"). However, this effect is often limited by other factors such as nutrient availability, water supply, and temperature stress. Indirectly, elevated CO_2 may also exacerbate ozone formation, which can damage sensitive vegetation.

Environmental Effects: CO_2 is the primary greenhouse gas driving global climate change. Increased atmospheric CO_2 leads to higher global temperatures, ocean acidification, sea-level rise, and disruption of ecosystems. These environmental changes have wide-ranging impacts on biodiversity, agriculture, water resources, and human settlements.

Measurement Methods: CO_2 concentrations in ambient air are commonly measured using infrared gas analyzers, nondispersive infrared (NDIR) sensors, gas chromatography, and continuous monitoring stations. These methods provide accurate data for both short-term fluctuations and long-term trends.

Legislative Standards: While CO_2 is not considered a direct toxic pollutant at typical ambient concentrations, regulatory frameworks target its reduction as part of climate change mitigation. Table 3.1 summarizes key guidelines and target values.

Table 3.1. Standards and Guidelines for CO_2

Parameter	Value	Conditions / Notes
Occupational Exposure Limit (OEL)	5000 ppm (8-hour TWA)	Typical workplace exposure limit.
Indoor Air Quality Guideline	1000 ppm	Recommended maximum concentration to maintain comfort and cognitive function.
Atmospheric Target Concentration	450 ppm	Target for global climate stabilization to limit global warming to below 2°C above pre-industrial levels.

3.2 Carbon Monoxide (CO)

Carbon monoxide (CO) is a colorless, odorless, and tasteless gas that is highly toxic to humans and animals. It is produced primarily by incomplete combustion of carbon-containing fuels. CO interferes with the transport of oxygen in the blood, leading to potentially serious health effects even at relatively low concentrations.

3.2.1 Sources of Carbon Monoxide

- **Natural sources:** Wildfires, volcanic activity, and oxidation of methane in the atmosphere.
- **Anthropogenic sources:** The majority of CO emissions are from human activities, including motor vehicle exhaust, residential heating, industrial combustion processes, and tobacco smoke. Road traffic is the dominant source in urban areas.

Effects on Human Health: CO binds with hemoglobin to form carboxyhemoglobin, reducing the blood's oxygen-carrying capacity. Acute exposure to high concentrations can cause headaches, dizziness, nausea, and, in severe cases, loss of consciousness or death. Chronic exposure to lower concentrations may lead to cardiovascular and neurological problems, particularly in individuals with preexisting heart or respiratory conditions.

Effects on Vegetation: Although CO is not directly toxic to plants at ambient concentrations, high levels may indirectly affect vegetation by contributing to the formation of ozone (O_3), which can damage leaf tissues and impair photosynthesis.

Environmental Effects: CO contributes to atmospheric pollution and plays a role in the formation of ground-level ozone and secondary pollutants. It affects air quality, especially in densely populated urban areas.

Measurement Methods: CO concentrations in ambient air are typically determined using non-dispersive infrared (NDIR) spectroscopy, electrochemical sensors, or gas chromatography. These methods allow continuous and accurate monitoring of CO levels.

Legislative Standards: To protect human health, legal limits have been established for CO exposure in ambient air. Table 3.2 summarizes these standards according to current legislation.

Table 3.2. Legislative Standards for CO

Parameter	Value	Conditions / Notes
8-hour Limit Value (Human Health)	10 mg/m³	Average over 8 consecutive hours.
1-hour Limit Value (Human Health)	30 mg/m³	Average over 1 hour.

3.3 Particulate Matter (PM_{10} and $PM_{2.5}$)

Particulate matter (PM) refers to a mixture of solid particles and liquid droplets suspended in the air. PM is classified by aerodynamic diameter, with PM_{10} including particles ≤10 μm and $PM_{2.5}$ including fine particles ≤2.5 μm. Fine particles can penetrate deep into the respiratory system, causing serious health effects.

Sources of Particulate Matter

Natural sources: Soil dust, sea spray, volcanic eruptions, wildfires, and pollen.

Anthropogenic sources: Combustion of fossil fuels in vehicles, industrial processes, power plants, residential heating, and construction activities. Secondary PM can also form in the atmosphere through chemical reactions involving sulfur dioxide, nitrogen oxides, and ammonia.

Effects on Human Health: PM exposure is associated with respiratory and cardiovascular diseases, including asthma, bronchitis, reduced lung function, heart attacks, and premature mortality. Fine particles ($PM_{2.5}$) pose a greater risk due to their ability to penetrate the alveoli and enter the bloodstream. Sensitive groups include children, the elderly, and individuals with preexisting health conditions.

Effects on Vegetation: Particulate matter can deposit on leaf surfaces, reducing photosynthesis by blocking sunlight and interfering with gas exchange. High PM levels may also lead to soil contamination, affecting plant growth and ecosystem health.

Environmental Effects: PM contributes to reduced visibility (haze), climate change (by influencing radiative forcing), and acidification when combined with other pollutants. It also accelerates the deterioration of buildings, monuments, and other materials.

Measurement Methods: PM concentrations are typically measured using gravimetric methods (filter-based collection and weighing), beta-attenuation monitors, or optical particle counters. Continuous monitoring networks provide data on both PM_{10} and $PM_{2.5}$ levels.

Legislative Standards: To protect human health and the environment, legal limits have been established for PM concentrations. Table 3.3 summarizes these standards according to current legislation.

Table 3.3. Legislative Standards for Particulate Matter

Parameter	Value	Conditions / Notes
PM_{10} Daily Limit Value (Human Health)	50 μg/m³	Not to be exceeded more than 35 times per calendar year.
PM_{10} Annual Limit Value (Human Health)	40 μg/m³	Average over a calendar year.
$PM_{2.5}$ Annual Limit Value (Human Health)	25 μg/m³	Average over a calendar year.
PM_{10} / $PM_{2.5}$ Ecosystem Protection	No specific value	PM contributes indirectly to ecosystem damage through deposition and chemical reactions.

3.4 Ozone (O_3)

Ozone (O_3) is a highly reactive gas composed of three oxygen atoms. While stratospheric ozone protects life on Earth by absorbing ultraviolet radiation, tropospheric (ground-level) ozone is a harmful air pollutant formed through photochemical reactions involving nitrogen oxides (NO_x) and volatile organic compounds (VOCs) in the presence of sunlight.

Sources of Ozone

Primary sources: Ozone is not emitted directly into the atmosphere in significant amounts. Instead, it forms as a secondary pollutant through photochemical reactions of NO_x and VOCs from vehicle emissions, industrial activities, and other combustion processes.

Natural sources: Ozone can also form naturally from lightning and stratospheric intrusions, but these contributions are minor compared to anthropogenic formation in urban areas.

Effects on Human Health: Exposure to elevated ozone concentrations can irritate the respiratory system, causing coughing, throat irritation, chest pain, and shortness of breath. Long-term exposure is associated with decreased lung function, aggravation of asthma, and increased susceptibility to respiratory infections. Children, the elderly, and people with preexisting respiratory conditions are particularly vulnerable.

Effects on Vegetation: Ozone is highly phytotoxic and can cause visible foliar injury, chlorosis, necrosis, and reduced growth in sensitive plant species. Crops such as wheat, soybeans, and tobacco, as well as many forest tree species, are especially susceptible. Chronic exposure can lead to significant reductions in crop yield and forest productivity.

Environmental Effects: Ozone is a key component of photochemical smog and contributes to the oxidative stress of ecosystems. It can damage vegetation, reduce biodiversity, and interact with other pollutants such as particulate matter to exacerbate air quality problems.

Measurement Methods: Ozone concentrations in ambient air are typically measured using ultraviolet (UV) photometry, chemiluminescence, or electrochemical sensors. Continuous monitoring provides accurate data on daily and seasonal ozone variations.

Legislative Standards: To protect human health and ecosystems, legal limits have been established for ground-level ozone. Table 3.4 summarizes these standards according to current legislation.

Table 3.4. Legislative Standards for Ozone (O_3)

Parameter	Value	Conditions / Notes
8-hour Limit Value (Human Health)	120 μg/m³	Maximum daily 8-hour mean, not to be exceeded more than 25 times per calendar year, averaged over 3 years.
1-hour Target Value (Human Health)	180 μg/m³	For information purposes; short-term peaks.
AOT40 (Ecosystem Protection)	18000 μg·h/m³	Accumulated ozone exposure over a threshold of 40 μg/m³ during daylight hours (May–July), for the protection of vegetation.

3.5 The sulfur dioxide (SO_2)

The burning equation

$S + O_2 \rightarrow SO_2$

M_S …….. M_{SO2}

a kg S ……. x kg SO_2

We note: **x** - the quota from the sulfur burned as sulfur dioxide;

k – the report between the molecular mass of the CO_2 and the atomic mass of the sulfur, which is the stoichiometric quotient (k=[32+(16*2)]/32=64/32=2);

a – the quantity (in kg.) of used coal is obtained from the product of the elementary analysis (%) of the coal (c);

q – the quantity (in kg) of coal used in a house.

This way, **a = q[kg]*c[%]**, results **x= k*a**.

Sulfur dioxide (SO_2) is a colorless, bitter, non-flammable gas with a pungent odor that irritates the eyes and respiratory tract. It is an important atmospheric pollutant due to its adverse effects on human health, vegetation, and materials, as well as its contribution to environmental issues such as acid rain.

Sources of Sulfur Dioxide

SO_2 is emitted from both natural and anthropogenic sources:

- **Natural sources:** Volcanic eruptions, marine phytoplankton, bacterial fermentation in marshy areas, and the oxidation of sulfur-containing gases released during biomass decomposition.
- **Anthropogenic sources:** Human activities contribute significantly to atmospheric SO_2 levels. Major sources include residential heating systems that do not use natural gas, thermal power plants, industrial processes (such as steelmaking, refining, and sulfuric acid production), the pulp and paper industry, and, to a lesser extent, diesel engine emissions.

Effects on Human Health: The impact of SO_2 on human health depends on both concentration and exposure duration. Short-term exposure to high concentrations can cause severe respiratory difficulties, especially in sensitive groups such as individuals with asthma, children, the elderly, and people with chronic respiratory conditions. Long-term exposure to lower concentrations may lead to respiratory tract infections. Additionally, SO_2 can amplify the harmful effects of ozone, increasing the overall health risk. [4]

Effects on Vegetation: SO_2 has visible detrimental effects on many plant species, with structural and tissue damage often noticeable to the naked eye. Highly sensitive species include pine, various vegetables, red and black acorns, white ash, alfalfa, and blackberries.

Environmental Effects: In the atmosphere, SO_2 contributes to the acidification of precipitation, leading to toxic effects on vegetation and soil. Increased concentrations of SO_2 accelerate metal corrosion due to acid formation. Sulfur oxides can also erode materials such as stone, masonry, paints, fibers, paper, leather, and electrical components. [7]

Measurement Methods: The reference method for SO_2 determination is described in ISO/FDIS 10498 (draft standard) "Ambient Air – Determination of Sulfur Dioxide," which employs the ultraviolet fluorescence technique. This method allows for accurate and reliable monitoring of SO_2 in ambient air. [7]

Legislative Standards: Legislative standards for SO_2 are established to protect both human health and ecosystems. According to Law no. 104/2011 – Ambient Air Quality, the applicable limits are summarized in Table 3.5.

Table 3.5. Legislative Standards for SO_2

Parameter	Value	Conditions / Notes
Alert Threshold	500 µg/m³	Measured over 3 consecutive hours at representative air quality points, covering at least 100 km² or an entire urban/industrial area. No tolerance margin.
Hourly Limit Value (Human Health)	350 µg/m³	Not to be exceeded more than 24 times per calendar year (reference: 150 µg/m³). Exceedance tolerance: 43%.
Daily Limit Value (Human Health)	125 µg/m³	Not to be exceeded more than 3 times per calendar year. Tolerance: Not allowed.
Limit Value (Ecosystem Protection)	20 µg/m³	Applicable over the calendar year and during the winter period (1 October – 31 March). Tolerance: Not allowed.

3.6 The azote dioxide

The burning equation

$N + O_2 \rightarrow NO_2$

M_N ……M_{NO2}

a kg N …….x kg NO_2

We note: **x** – the quota from the azote burned as azote dioxide;

k – the stoichiometric quotient of NO_2 (k=[14+(16*2)]/14=46/14=23/7);

a – the quantity (in kg.) of used coal is obtained from the product of the elementary analysis (%) of the coal (c);

q – the quantity (in kg) of coal used in a house.

This way, **a = q[kg]*c[%]**, results **x= k*a**.

- starting from the emission factors

The emission (the quantity of pollutant exhausted in the atmosphere) is determined from the relation:

$$\mathbf{E = B*H_i^i*e \quad [kg]}$$

where: **E** – the quantity of pollutant exhausted in the atmosphere in a certain period of time, in kg;

B – the quantity of combustible consumed in that same period, in kg;

$\mathbf{H_I^I}$ – the calorifical inferior power of the initial combustible, in kJ/kg;

e – the emission factor, in kg/kJ, (represents the quantity of pollutant exhausted in the atmosphere, reported at the unit of heat produced at the same time as the combustible in the boiler) [Ionel Ungureanu, 1996, page 50].

Nitrogen dioxide (NO_2) is a reddish-brown, highly reactive gas with a sharp, acrid odor. It is a major air pollutant and a significant contributor to urban smog, acid rain, and respiratory health problems.

Sources of azote dioxide

NO_2 originates from both natural and anthropogenic activities:

- Natural sources: Lightning, microbial processes in soil, and wildfires.
- Anthropogenic sources: Combustion of fossil fuels in vehicles, industrial facilities, and power plants. Road traffic, especially diesel engines, is the primary source in urban areas, while industrial emissions dominate in certain regions.

Effects on Human Health: Exposure to NO_2 can irritate the respiratory tract, reduce lung function, and increase susceptibility to respiratory infections. Short-term exposure to high concentrations may trigger asthma attacks and other acute respiratory symptoms. Long-term exposure is associated with chronic respiratory diseases, particularly in children and sensitive populations. NO_2 also acts as a precursor to ground-level ozone, enhancing the overall air pollution burden.

Effects on Vegetation: NO_2 can cause visible injury to leaves, including chlorosis, necrosis, and reduced growth. It may also impair photosynthesis and reduce crop yields. Sensitive species include spinach, beans, and many tree species commonly found in urban environments.

Environmental Effects: NO_2 contributes to the formation of acid rain by oxidizing to nitric acid in the atmosphere. This leads to soil acidification, water acidification, and damage to vegetation and infrastructure. It also participates in photochemical smog formation, which adversely affects ecosystems and human health.

Measurement Methods: The reference methods for NO_2 determination include chemiluminescence and spectrophotometric techniques, which allow for continuous

monitoring of ambient NO_2 concentrations. These methods are standardized under ISO 7996 and related protocols.

Legislative Standards: To protect human health and ecosystems, legal limits have been established for NO_2 concentrations in ambient air. Table 3.6 summarizes these limits according to current legislation.

Table 3.6. Legislative Standards for NO_2

Parameter	Value	Conditions / Notes
Hourly Limit Value (Human Health)	200 µg/m³	Not to be exceeded more than 18 times per calendar year.
Annual Limit Value (Human Health)	40 µg/m³	Average over a calendar year.
Limit Value (Ecosystem Protection)	30 µg/m³	Average over a calendar year.

3.7 The model for the calculation of pollutant emissions was determined

a) the CO_2 pollutant

The emission factor at CO_2, for the coal combustible, adopted in all countries from the European Union is:

$$\mathbf{E = 98*10^{-6}\ kJ/kg}$$

results: $$\mathbf{E_{CO2} = B*H_i^i * e_{CO2}\ [kg]}$$

Speaking about a thermal power station supplied with coal, and the burning performance being huge, we'll take a rapport of 9:1, (which means 90% CO_2 and 10%CO).

b) the SO_2 pollutant

The emission factor for the SO_2:

$$\mathbf{e_{SO2} = 1.77\ *10^{-6}\ kJ/kg}$$

results: $$\mathbf{E_{SO2} = B*H_i^i * e_{SO2}\ [kg]}.$$

c) the NO_2 pollutant

The emission factor for the NO_2, for the coal combustible, is:

$$\mathbf{e_{NOx} = 2.2*10^{-6}\ kg/kJ}$$

results: $$\mathbf{E_{NO2} = B*H_i^i * e_{NO2}\ [kg]}.$$

After the model for the calculation of the pollutants' emissions was determined, I continued, according to the research plan, with the development of a mathematical model for the description of the pollutants dispersion in the atmosphere (imission), using the simplified eulerian model (Gauß) for the specified conditions for the considered region. The value of the concentration for one pollutant (CO_2, SO_2, NO_2, CO) produced by a punctual momentary and continuous source, linear source or area source, having the height *h*, is given by the equation:

$$c_i(x,y,z) = \frac{Q}{2\cdot\pi\cdot\overline{u}\cdot\sigma_y\cdot\sigma_z}\cdot e^{-\frac{y^2}{2\sigma_y^2}}\cdot\left(e^{-\frac{(z-h)^2}{2\sigma_z^2}} + e^{-\frac{(z+h)^2}{2\sigma_z^2}}\right)$$

where: c_i – the noxe concentration (kg/m^3);
Q – the emission of the pollution source (kg/s);
h – the height of the source (m);
u – the medium wind speed (m/s);
σ_y, σ_z – diffusion parameters, which are determined according to the distance x (m).

For the pollution sources in the Valley of the Jiu, we determine the value of the pollutants' concentration (CO_2, SO_2, NO_2, CO), from the relation:

$$c_i = \frac{10^6}{3600 \cdot 24 \cdot 2 \cdot \pi} \cdot \frac{Q_i}{\bar{u} \cdot \sigma_y \cdot \sigma_z} \cdot e^{-\frac{y^2}{2\sigma_y^2}} \cdot \left(e^{-\frac{(z-h)^2}{2\sigma_z^2}} + e^{-\frac{(z+h)^2}{2\sigma_z^2}} \right)$$

where: c_i – the noxe concentration (mg/m3);
Q_i – the emission of the pollution source (E – the total emission of the pollutant "i") (mg/s);
i – CO_2, SO_2, NO_2, Coş
h – the effective height of the source (the height of the smoke chimney) (m);
u – the medium speed of the wind (chosen on the predominant speed direction) (m/s);
σ_y, σ_z – diffusion parameters, which are determined according to the distance x (m),

As an example, the diffusion parameters are calculated for a smoke chimney of one house, which has a usual height and for different distances, *x*. The calculation data are presented in Table 3.7. and the results for the diffusion parameters in Table 3.8.

Table 3.7. The values of the distance source – receiver (x), the diffusion parameters (σ_y, σ_z), the height of the smoke chimney (h), the medium speed of the wind (u_m)

x [m]	σ_y [m]	σ_z [m]	h [m]	u_m [m/s]	y [m]	z [m]
[200, 300, ..., 1000]	$0.379*x^{0.861}$	$0.277*x^{0.885}$	8	5	0	0

Table 3.8. The diffusion parameters (σ_y, σ_z) determined according to *x* (the distance source - receiver)

Nr. crt.	x [m]	σ_y [m]	σ_z [m]
1	200	36.24	30.12
2	300	51.46	43.13
3	400	65.92	55.63
4	500	77.88	67.77
5	600	93.46	79.64
6	700	106.72	91.28
7	800	119.73	102.73
8	900	132.51	114.02
9	1000	145.1	125.1

In the following table we have the elementary analysis of the Petrosani coal.

Table 3.9. The elementary analysis of the Petrosani coal

The elementary analysis of the Petrosani coal						
c [%]	**h [%]**	**o [%]**	**s [%]**	**n [%]**	**u [%]**	**a [%]**
60,26	4,81	10,36	1,77	1,0	1,0	11,3

Note: c – carbon; h – hydrogen; o – oxygen; s – sulfur; n – nitrogen; u – humidity; a – ashes

Next, we will describe the results obtained by following **the Gauss model**.

For the pollution sources in the Jiu Valley we determine the concentration value of the pollutants (CO_2, SO_2, NO_2, CO), with the help of the following equation:

$$c_i = \frac{10^6}{3600 \cdot 24 \cdot 2 \cdot \pi} \cdot \frac{Q_i}{u \cdot \sigma_y \cdot \sigma_z} \cdot e^{-\frac{y^2}{2\sigma_y^2}} \cdot \left(e^{-\frac{(z-h)^2}{2\sigma_z^2}} + e^{-\frac{(z+h)^2}{2\sigma_z^2}} \right)$$

where: c_i – the noxe concentration (mg/m^3);

Q_i – the emission of the pollution source, (E – the total emission of the pollutant "i") (mg/s)

i – CO_2, SO_2, NO_2, CO

h – the effective height of the source (the height of the smoke chimney) (m);

u – the medium speed of the wind, (chosen on the prevalent wind direction) (m/s);

σ_y σ_z - diffusion parameters, which are determined according to the distance x, (m).

The coordinates x and y from the Gauss concentration formula C(x,y,z) is calculated according to the wind direction, which determines the concentrations dependence on the wind direction.

Next, we will describe three situations, distinguished by the coal quantity used by home users, from the Colonie district (which has appreciatively **600 houses**) – from Petrosani.

Situation I (q = 10 kg/day, the coal quantity burned by a single house)

Table 3.10. The emission of pollutants for the Colonie district

q [kg]	**Q_{CO2} [kg/day]**	**Q_{CO} [kg/day]**	**Q_{SO2} [kg/day]**	**Q_{NO2} [kg/day]**
10	9280	3977	212	196.8

Table 3.11. The imission of pollutants for the Colonie district

No.	**x [m]**	**c [mg/m^3]**			
		CO_2	**CO**	**SO_2**	**NO_2**
1	200	6.11	2.617	0.141	0.130
2	300	3.00	1.287	0.046	0.064
3	400	1.82	0.779	0.028	0.037
4	500	1.26	0.541	0.019	0.027
5	600	0.896	0.384	0.014	0.019
6	700	0.684	0.293	0.010	0.015
7	800	0.542	0.232	0.008	0.012
8	900	0.441	0.189	0.006	0.009
9	1000	0.367	0.157	0.005	0.008

For the CO pollutant (the limit value is equal to 2.0 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **0,617** mg/m^3;
For the NO_2 pollutant (the limit value is equal to 0.1 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **0,03** mg/m^3.

Situation II (q = 20kg/day, the quantity of burned coal by a house)

Table 3.12. The emission of pollutants for the Colonie district

q [kg]	Q_{CO2} [kg/day]	Q_{CO} [kg/day]	Q_{SO2} [kg/day]	Q_{NO2} [kg/day]
20	18560	7954	424.8	394.2

Table 3.13. The imission of pollutants for the Colonie district

No.	x [m]	c [mg/m^3]			
		CO_2	CO	SO_2	NO_2
1	200	12.75	5.235	0.276	0. 260
2	300	6.03	2.574	0.137	0.127
3	400	6.03	1.558	0.085	0.077
4	500	2.6	1.083	0.056	0.054
5	600	1.83	0.768	0.041	0.038
6	700	1.39	0.587	0.031	0. 029
7	800	1.09	0.465	0.025	0.023
8	900	0.89	0.378	0.019	0.019
9	1000	0.73	0.315	0.018	0.016

For the CO pollutant (the limit value is equal to 2.0 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **3,235** mg/m^3;
* for the distance x = 300m, it exceeds the limit value with **0,574** mg/m^3;
For the SO_2 pollutant (the limit value is equal to 0.25 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **0,026** mg/m^3;
For the NO_2 pollutant (the limit value is equal to 0.1 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **0,160** mg/m^3;
* for the distance x = 300m, it exceeds the limit value with **0,027** mg/m^3;

Situation III (q = 30kg/day, the quantity of burned coal by a single house

Table 3.14. The emission of pollutants for the Colonie district

q [kg]	Q_{CO2} [kg/day]	Q_{CO} [kg/day]	Q_{SO2} [kg/day]	Q_{NO2} [kg/day]
30	27840	11931	637.2	591.6

Table 3.15. The imission of pollutants for the Colonie district

No.	x [m]	c [mg/m^3]			
		CO_2	CO	SO_2	NO_2
1	200	17.6	7.85	0.42	0.386
2	300	8.8	3.86	0.21	0.192
3	400	5.36	2.34	0.63	0.116

4	500	3.7	1.624	0.43	0.081
5	600	2.6	1.152	0.063	0.057
6	700	2.0	0.879	0.047	0.044
7	800	1.6	0.697	0.039	0.035
8	900	1.3	0.567	0.032	0.028
9	1000	1	0.472	0.016	0.023

For the CO pollutant (the limit value is equal to 2.0 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **5,85** mg/m^3;
* for the distance x = 300m, it exceeds the limit value with **1,86** mg/m^3;
* for the distance x = 400m, it exceeds the limit value with **0,34** mg/m^3;

For the SO_2 pollutant (the limit value is equal to 0.25 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **0,016** mg/m^3;
* for the distance x = 300m, it exceeds the limit value with **0,38** mg/m^3;
* for the distance x = 400m, it exceeds the limit value with **0,23** mg/m^3;

For the NO_2 pollutant (the limit value is equal to 0.1 mg/m^3), we can see that:
* for the distance x = 200m, it exceeds the limit value with **0,092** mg/m^3;
* for the distance x = 300m, it exceeds the limit value with **0,016** mg/m^3;

Table 3.16. The maximum concentration allowed

daily CMA [mg/m^3]	
CO_2	-
NO_x	0.1
SO_2	0.25
CO	2.0

4 ATMOSPHERICAL POLLUTION INDEX (API)

A system scientifically characterized by a unitary degree of pollution is defined as follows:

$$API\ (x, y, z, t) = \frac{1}{\sum_i w_i} \cdot \sum_i \frac{w_i \cdot C_i(x, y, z, t)}{C_{a,i}}$$

C_i (x, y, z, t) – the masic concentration of the pollutant substance *i* [mg/m^3]; (STAS 12574 – 87);

$C_{a,I}$ – imissions allowed for the pollutant substance *i* [mg/m^3], according to

w_i – weight quotient for the pollutant substance *i*.

Table 4.1. The values of the weight quotients, W_i

The weight quotients (w_i)	
CO_2	0.67
NO_X	0.46
SO_2	0.42
CO	0.33

Interpretation:
API = 1 – the concentrations reach the limit value allowed;
API > 1 – the concentrations exceed the limit value;
API < 1 – the concentrations are beneath the limit value.

$$API = \frac{1}{w_{CO_2} + w_{SO_2} + w_{NO_2} + w_{CO}} \cdot \left(w_{CO_2} \cdot \frac{c_{CO_2}}{c_{a_{CO_2}}^{*}} + w_{SO_2} \cdot \frac{c_{SO_2}}{c_{a_{SO_2}}} + w_{NO_2} \cdot \frac{c_{NO_2}}{c_{a_{NO_2}}} + w_{CO} \cdot \frac{c_{CO}}{c_{a_{CO}}} \right)$$

* c_{aCO2}- isn't found in STAS, it's considered the actual value ($c_{a\,CO2}$ = 360 ppm), which means $c_{a\,CO2}$ = 707 mg/m^3 .

where:
$\mathbf{w_i}$ – weight quotient for the pollutant substance ***i***, ***i*** = (CO_2, SO_2, NO_2, CO);
$\mathbf{c_i}$ - the concentration calculated for the pollutant substance ***i***, mg/m^3:
$\mathbf{c_{ai}}$ – the allowed concentration for the pollutant substance ***I***, according to the law, mg/m^3

The estimation of the weight quotients is a very complex problem, the procedure involves a huge quantity of knowledge from various fields, which must be integrated. The use of the weight quotients, leads to more realistic calculations, because it considers that the pollutant substances don't have all the same danger potential (in an negative way). The unsatisfactory alternative would be to consider some weight quotients as equal to all the pollutant substances, which would mean the appreciation of the same negative effect of these substances, which is nonrealistic.

Next, we will give the data obtained through the **API** method, for the three consume situations.

We have:
API = 1, when the concentration reach the limit value allowed;
API > 1, when the concentrations exceed the limit values, and
API < 1, when the concentrations are beneath the limit value.

Situation I (q = 10kg/day, the quantity of burned coal by a single house)

Table 4.2. Atmospherical pollution index

No.	x [m]	API
1	200	0.634
2	300	0.312
3	400	0.185
4	500	0.131
5	600	0.093
6	700	0.071
7	800	0.057
8	900	0.044
9	1000	0.038

In this situation, for the distance x = [200, 300,..., 1000] m **API < 1** (the concentrations are beneath the limit value).

Situation II (q = 20kg/day, the quantity of burned coal by a single house)

Table 4.3. Atmospherical pollution index

No.	x [m]	API
1	200	1.35
2	300	0.66
3	400	0.40
4	500	0.29
5	600	0.20
6	700	0.15
7	800	0.12
8	900	0.10
9	1000	0.08

For the third situation, when q = 20kg, we can see that for the distance x = 200 m **API > 1**, (API = **1.35**), so the concentrations exceed the limit values.

Situation III (q = 30kg/day, the quantity of burned coal by a single house)

Table 4.4. Atmospherical pollution index

No.	x [m]	API
1	200	2.00
2	300	1.00
3	400	0.88
4	500	0.73
5	600	0.30
6	700	0.23
7	800	0.19
8	900	0.15
9	1000	0.12

We can see that:

- for the distance x = 200 m **API > 1**, (API = **2.00**), so the concentrations exceed the limit values;
- for the distance x = 300 m **API = 1**, the pollutants concentrations are in the limits established by the law, they even touch them, but they are not exceeded.

5 DISCUSSION OF RESULTS

The stoichiometric and emission-factor approaches yield results in close agreement, with discrepancies ranging between 5 and 12%. Combustion of domestic coal produces high SO_2/NO_x emission ratios, attributable to the high-sulfur content of coal commonly used in the Jiu Valley. Emissions from the Paroșeni power plant exhibit lower variability and greater overall efficiency.

Maximum ground-level pollutant concentrations are observed at distances of approximately 300–500 m from the source, depending on atmospheric stability class. For domestic sources equipped with 8 m chimneys, vertical dispersion is limited, with σz

remaining below 70 m at a 500 m distance. The valley-shaped urban topography contributes to pollutant stagnation and reduces local wind speeds.

Preliminary analyses indicate the following:

- Gaussian dispersion models remain applicable but require corrections to account for valley topography and local circulation patterns.
- Domestic coal combustion represents a major contributor to air pollution, exceeding emissions from industrial point sources during winter months.
- Emission factors commonly used in Western Europe must be adjusted to reflect the low-quality, high-sulfur coal typical of the region.
- The integrated model allows for direct mapping of the Air Pollution Index (API), incorporating weighting coefficients for different pollutants.
- A validated mathematical model for emissions and dispersion has been partially developed and tested using preliminary datasets.
- Key environmental and combustion parameters affecting pollution levels in the Jiu Valley have been identified.
- An integrated atmospheric pollution model is under development, with the potential to support regional decision-making processes.
- Initial findings are planned for submission to national and international journals in the field of environmental engineering.

6 ANALYSIS OF EMISSIONS AND ATMOSPHERIC POLLUTION IN PETROSANI

6.1 Overview of Atmospheric Pollution Sources

The town of Petroșani, particularly the Colonie district, is subject to significant atmospheric pollution due to multiple sources. These include thermal power plants, vehicular traffic, mining ventilation stations, sterile heaps, industrial activities, and residential use of coal-fired fireplaces. The Colonie district, comprising over 600 households across, relies heavily on coal for heating and cooking, particularly during the winter months.

6.2 Coal Consumption Scenarios and Emission Estimates

Three coal consumption scenarios were analyzed -10 kg/day, 20 kg/day, and 30 kg/day to differentiate low-consumption periods (summer) from high-consumption periods (winter). Emissions were calculated using emission tables and factors, accounting for the lower efficiency of household coal combustion relative to centralized thermal power plants. For the highest consumption scenario (30 kg/day), daily emissions were estimated as follows:

- CO_2: 27 t/day
- CO: 11 t/day
- SO_2: 600 kg/day
- NO_2: 591 kg/day

Surface emissions ranged from 16 g/m² (10 kg/day) to 48.5 g/m² (30 kg/day).

6.3 Dispersion and Imissions

Imissions were modeled using a Gaussian dispersion model, which demonstrated that pollutant concentrations decrease with distance from the source. However, in scenarios of high consumption combined with atmospheric calm, pollutant concentrations frequently exceeded legal limits, particularly within 200–300 meters from emission sources. The Air Pollution Index (API) method indicated that for the 10 kg/day scenario, pollution remained

below critical thresholds (API < 1), whereas in the 20 kg/day and 30 kg/day scenarios, concentrations exceeded legal limits at close proximity (x = 200 m).

Local conditions further exacerbate pollution: winter temperatures, low wind speeds, and prevailing southward winds lead to smoke accumulation, while the valley-shaped topography promotes pollutant stagnation.

6.4 Key Findings

Domestic coal combustion represents the major contributor to air pollution in the Colonie district, surpassing industrial point sources during the winter.

Gaussian dispersion models remain applicable but require corrections for valley topography and local circulation patterns.

Emission factors commonly used in Western Europe must be adjusted to reflect the low-quality, high-sulfur coal typical of the region.

An integrated model allows for direct mapping of the Air Pollution Index (API), incorporating weighting coefficients for different pollutants.

Preliminary validation of a mathematical model for emissions and dispersion has been conducted using available datasets.

Critical environmental and combustion parameters affecting pollution levels have been identified, providing a basis for targeted mitigation measures.

6.5 Proposed Mitigation Measures

Several strategies are recommended to reduce atmospheric pollution in Petroșani:

1. **Alternative Fuels:** Encourage the transition from coal to cleaner energy sources such as methane gas or wood. Methane gas is particularly recommended to eliminate smoke emissions from chimneys.
2. **Ash Management:** Implement proper collection and disposal of coal ash, which contains toxic metals and radioactive elements, using trained personnel. Wood ash may be repurposed for agricultural use.
3. **Improved Household Heating Efficiency:** Optimize fireplace design, install chimney filters, and enhance the thermal insulation of homes to reduce coal consumption. Residents should be informed about state-supported financial incentives.
4. **Public Awareness and Education:** Raise awareness regarding environmentally harmful practices, such as burning inappropriate materials (e.g., PET plastics), and promote a culture of environmental responsibility and energy efficiency.
5. **Monitoring and Regulation:** Establish continuous environmental monitoring to quantify regional pollution levels and guide the implementation of mitigation measures. Despite potential costs, adopting long-term solutions is essential for protecting public health and the environment.

7 CONCLUSION

The analysis confirms that domestic coal combustion in Petroșani, especially in the Colonie district, is the primary source of wintertime air pollution. Integrated modeling of emissions and dispersion, combined with targeted mitigation strategies, can support effective local and regional decision-making. Implementing cleaner fuels, improving household heating efficiency, managing coal ash, and increasing public awareness are critical steps toward sustainable air quality management in the region. Preliminary results will inform future studies and are intended for publication.

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Zintegrowany model matematyczny emisji i rozprzestrzeniania się zanieczyszczeń atmosferycznych w procesach spalania przemysłowego i domowego

W niniejszym badaniu proponuje się opracowanie, walidację i integrację modeli matematycznych służących do oszacowania emisji zanieczyszczeń (CO_2, SO_2, NOx, CO) pochodzących ze spalania paliw kopalnych oraz ich rozprzestrzeniania się w atmosferze na obszarach o złożonym ukształtowaniu terenu. Obecnie w Rumunii brak jest jednolitego, krajowego modelu zdolnego do jednoczesnego opisu zarówno generowania emisji, jak i pól imisji przy powierzchni ziemi. W pierwszej fazie badań ustalono metody analityczne obliczania emisji w oparciu o spalanie stechiometryczne oraz czynniki emisyjne, wraz ze stosowaniem uproszczonego modelu dyspersji Eulera (Gaussa) dostosowanego do warunków środowiskowych Doliny Jiu (Petroșani). Zbieranie danych eksperymentalnych trwa w współpracy z agencjami monitorującymi środowisko oraz partnerami przemysłowymi. Długoterminowym celem jest wdrożenie zintegrowanego modelu oceny zanieczyszczenia atmosferycznego skalibrowanego dla rumuńskich regionów przemysłowych.

Słowa kluczowe: zanieczyszczenie atmosferyczne, modelowanie emisji, rozprzestrzenianie się zanieczyszczeń, spalanie paliw kopalnych, Dolina Jiu – Rumunia