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Study of the influence of the deposition rate of dust and fine aerosol particles for monitoring and forecasting the state of the surface layer of the atmosphere in industrial regions

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Abstract

For the stable development of society, one of the factors is air quality control, since today reducing the negative impact of pollutants on human health and the ecosystem is especially relevant and in demand. Based on the above, the article examines an important factor: the movement of gravitational deposition of dust and fine aerosol particles on the Earth's surface, which depends on the physical properties of the dispersion phase, temperature, dynamic and kinematic viscosity of the atmospheric air mass, and the horizontal and vertical components of wind speed. Atmospheric stratification affects the deposition of harmful substances in the atmosphere. A mathematical model is presented that takes into account the rate of particle sedimentation, where formulas are provided for calculating it depending on the physical and mechanical properties and characteristics of the medium. For the settling rate of spherical aerosol particles, the Stokes equation is used, which considers all the forces influencing the settling rate. To calculate the dynamic and kinematic viscosity of air, which significantly influences the deposition rate of dust and fine aerosol particles, a regression model is provided that takes into account the temperature and pressure of the atmospheric air mass, and the results of numerical calculations are presented in the form of graphs and histograms.

Keywords: Deposition, Dynamic, Kinematic viscosity of air, Pressure, Regression model, Speed, particle, Temperature.

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1. Introduction

The current accelerated pace of economic development requires the construction of even more powerful industrial facilities. However, their creation has a negative impact not only on the ecological state of the territories where they are built but also on neighboring areas. Especially if the construction of industrial facilities does not comply with sanitary atmospheric standards, this leads to increased air pollution. Particulate matter pollution caused by accelerated industrialization poses a serious threat to human health, increasing morbidity and mortality. Particulate matter is classified by size: coarse (PM10), fine (PM2.5), and ultrafine particles (UFP). External sources of pollution include emissions from transport, construction, biomass combustion, and industry, while internal sources include fuel combustion, smoking, and nanoparticles. Incomplete combustion of fuel, especially indoors, releases high concentrations of harmful particles, which constitute a major health hazard, especially in developing countries. Regardless of the source, fine particles and ultrafine particles (particles with an aerodynamic equivalent diameter of less than 100 nm, UFP) have serious impacts on atmospheric visibility and human health [1].

Scientists from the Netherlands, in [Erisman and Draaijers \[2\]](#), provide an overview of factors influencing the dry deposition of gases and particles in forests during turbulent transport, such as wind speed, tree height, canopy density, precipitation, relative humidity, and global radiation, which affect the state of the surface. They considered the advantages of these factors for determining temporal and spatial changes in the deposition of sodium and sulfur. They found that, due to the limited parameters of moisture exchange with the surface, intermediate changes are poorly modeled. [Mallios, et al. \[3\]](#) studied the influence of non-sphericity and orientation of particles on the gravitational settling of mineral dust for elongated spheroids with numbers $Re < 100$ to numerically calculate the steady-state settling velocity in the momentum equation. They calculated new drag coefficients, taking into account the orientation of the particles.

[Zhao and Wu \[4\]](#) present an analysis of the factors that affect the sedimentation of particles in closed spaces based on the analytical model and three-dimensional drift flow model. The authors found that the increase in the particle sedimentation rate is associated with surface roughness and higher friction velocity near the walls for small particles, while for larger particles (1-5 μm), these factors are not significant. The change in the particle concentration distribution at the same air exchange rate and particle source, which affects the sedimentation flow, revealed that uneven particle distribution often occurs in ventilated spaces. In addition, particle inertia affects the settling velocity, and particles with weak inertia tend to follow certain trajectories in the flow, with inertia slowing down but not preventing this behavior. [Maxey and Corrsin \[5\]](#) and [Garcia-Nieto \[6\]](#) examine the removal mechanisms of aerosol emissions from coal-fired power plants and find that respirable dust is most difficult to capture. Compared to the initial volume of respirable dust, approximately 20% remains after 18 hours of gravity settling. It follows that gravitational settling is the primary mechanism for removing respirable dust compared to condensation and coagulation.

Researchers in [Derevich \[7\]](#) modeled the coagulation of particles and droplets in turbulent flows, taking into account the influence of turbulent diffusion, inertia, and gravity on this process. They developed methods for calculating the coagulation intensity and investigated its dependence on the characteristics of turbulence.

[Baklanov and Sørensen \[8\]](#) propose an improved parameterization of radionuclide removal processes by dry and wet deposition, taking into account the particle size dependence, and present modeling results that can be used in emergency situations to assess atmospheric pollution. For dry deposition, gravity effects are considered through a combination of Stokes' law for small particles, along with a Cunningham correction, and an iterative solution for large particles. Scientists from the Norwegian Institute for Air Research, [Pisso, et al. \[9\]](#), developed a deposition framework for aerosols, including a more detailed parameterization of gravity deposition, which is important for dispersion models near pollution sources. They presented tools for preparing meteorological input data and processing output data; their model offers great potential for modeling and analyzing atmospheric pollutant transport at different scales.

In [Bonnecaze, et al. \[10\]](#), the theory and experimental studies of particle-induced gravity flows are considered, taking into account the influence of particle concentration and fluid depth. The flow models are well-verified experimentally, and the results of the theory correspond to observations. [Camenen \[11\]](#) provides a universal formula for the particle settling velocity, considering their shape and roundness. It is based on two asymptotic forms of the drag coefficient for small and large Reynolds numbers. Three coefficients in the proposed equation are selected for different shapes and roundness using explicit dependencies. The authors [Tirabassi and Moreira \[12\]](#) presented the settling velocity of solid particles on the Earth's surface in an analytical solution of the advection-diffusion equation, where the effect of particle diameters on the concentration distribution at ground level was studied under various conditions of atmospheric stability.

The work of [Giardina and Buffa \[13\]](#) presents a new model for calculating the rate of dry deposition of particles, which takes into account the interaction of inertial and turbulent processes and shows good results when compared with experimental data. [Mariraj Mohan \[14\]](#) considered a general scenario for dry deposition research, focusing on various methods for measuring dry particle deposition flux, comparing various published dry deposition rate numbers, and examining factors controlling the dry deposition rate. A technical review of research into the current state of dry deposition and the limitations of various measurement methods is presented.

[Guha \[15\]](#) discusses the physical processes responsible for particle transport and deposition and their theoretical modeling. Both laminar and turbulent processes are considered, emphasizing the physical understanding of the different transport mechanisms. Modern computational methods for determining particle motion and deposition are discussed, including stochastic Lagrangian particle tracking and the unified Eulerian advection-diffusion approach.

The authors of [Giardina and Buffa \[13\]](#) in their model take into account the resistances that affect the flow of particles in quasilaminar layers, as well as the mutual influence of inertial impact processes and turbulent processes. The developed model estimates the rate of particle sedimentation, taking into account local features such as turbulence and inertia. The

model can be integrated into codes for modeling atmospheric dispersion, allowing for the diversity of deposition surfaces and particle types to be considered.

Having analyzed literary sources on the problem of mathematical modeling of the process of mass and heat transfer in complex systems, we came to the following conclusion: when developing an appropriate mathematical apparatus for monitoring and predicting the concentration of harmful substances in the atmosphere, in addition to weather and climatic factors, it is necessary to take into account changes in the concentration of harmful substances in the atmosphere due to the rate of particle deposition, which depends on the viscosity of the medium. This process is characterized by the laws of aerodynamics and particle mechanics in a liquid or gas, where the main factors are the kinematic and dynamic viscosity of air.

2. Statement of the Problem

To study, predict, and analyze the process of distribution of aerosol emissions in the atmosphere, a mathematical model of the distribution of harmful substances in the atmosphere has been developed. Taking into account the above factors, the transport and diffusion equation based on the law of conservation of mass and energy momentum is presented in the following form [16-20]:

$$\begin{aligned} \frac{\partial \theta}{\partial t} + u \frac{\partial \theta}{\partial x} + v \frac{\partial \theta}{\partial y} + (w - w_g) \frac{\partial \theta}{\partial z} + (\Phi_r + \Phi_v + \alpha)\theta = \\ = \frac{\partial}{\partial x} \left(\mu \frac{\partial \theta}{\partial x} \right) + \frac{\partial}{\partial y} \left(\mu \frac{\partial \theta}{\partial y} \right) + \frac{\partial}{\partial z} \left(\kappa \frac{\partial \theta}{\partial z} \right) + \delta Q; \end{aligned} \tag{1}$$

with the corresponding initial and boundary conditions:

$$\theta(x, y, z, t) = \theta^0(x, y, z) \text{ при } t=0; \tag{2}$$

$$-\mu \frac{\partial \theta}{\partial x} \Big|_{x=0} = \gamma(\theta - \theta_a); \quad \mu \frac{\partial \theta}{\partial x} \Big|_{x=L_x} = \gamma(\theta - \theta_a); \tag{3}$$

$$-\mu \frac{\partial \theta}{\partial y} \Big|_{y=0} = \gamma(\theta - \theta_a); \quad \mu \frac{\partial \theta}{\partial y} \Big|_{y=L_y} = \gamma(\theta - \theta_a); \tag{4}$$

$$\kappa \frac{\partial \theta^*}{\partial z} \Big|_{z=0} = \beta \cdot \theta^* - F_0(x, y, z); \quad \kappa \frac{\partial \theta}{\partial z} \Big|_{z=H_z} = \gamma(\theta - \theta_a). \tag{5}$$

Here θ – concentration of harmful substances in the atmosphere, t – time, θ^0 – primary concentration of harmful substances in the atmosphere, θ_a – concentration entering across the boundaries of the area under consideration, x, y, z – coordinate system, u, v, w – wind speed in three directions, w_g – particle settling rate; Φ_r – decrease in the concentration of pollutants in the atmosphere due to decomposition and photochemical transformation, Φ_v – reduction in the concentration of pollutants due to leaching, depending on the intensity of precipitation, α – coefficient of particle capture by vegetation, μ, κ – diffusion and turbulence coefficients, Q – source power, δ – Dirac function, γ – mass transfer coefficient across calculation boundaries, β – coefficient of interaction of particles with the underlying surface, F_0 – a stationary source of emission of harmful substances from the underlying surface of the earth.

Calculation of particle deposition rates is important for monitoring and predicting the concentration of harmful particles in the atmosphere, liquid, or other media. From the World Bank report, it is known that 83% of the capital's residents live in areas with high levels of air pollution. The report emphasizes that one of the main air pollutants is fine particulate matter with a diameter of 2.5 microns. PM2.5 and PM10 can persist in the atmosphere for a long time and spread over long distances. They penetrate the respiratory tract have a negative impact on human health, and sometimes can be fatal. Determining settling velocity helps estimate how long particles will remain in the air and how far they can travel.

The concentration of fine particles plays a key role in air quality assessment, environmental monitoring, and the development of health standards. Conducted studies of the process of transfer and diffusion of pollutants in the atmosphere showed that a significant factor in changing the concentration of harmful substances is the rate of gravitational deposition of particles on the surface of the Earth, and it depends on the physical properties of the dispersion phase, temperature dynamics, and kinematic viscosity of the air mass of the atmosphere, horizontal and vertical components of wind speeds, and stratification of the atmosphere, which can be stable, unstable, or indifferent to dry and saturated air, along with other factors.

The fall of a particle under the influence of gravity is called gravitational settling, the speed of which depends on the size, density, and shape of the particles, as well as on environmental parameters. As practice has shown, large and heavy PM10 particles settle faster, while small PM2.5 and ultrafine particles can remain in the air for a long time. Soot particles

settle more slowly than sand particles. Spherical particles settle faster. Irregularly shaped particles (such as pollen) have higher air resistance, which slows down their settling. The denser the particle, the faster it settles.

As is known, the Stokes equation represents the settling velocity for spherical particles in the form

$$W_{sph} = \frac{d^2(\rho_T - \rho_C)g}{18\mu_c}, \tag{6}$$

where in relation (6) W_{sph} - the rate of deposition of solid spherical particles in the atmosphere, m/s ; d - particle diameter, m ; ρ_T - solid particle density, kg/m^3 ; ρ_C - medium density (atmospheric air mass), kg/m^3 ; g - free fall acceleration, m/s^2 ; μ_c - dynamic viscosity of atmospheric air mass, $Pa.s$.

It should be noted that the Stokes equation can only be used for a laminarly moving particle, for which $Re < 1.6$. The sedimentation rate (6) is lower for particles with irregular shapes, so we multiply dependence (6) by the correction factor φ , which is called the shape coefficient, and the sedimentation rate will be:

$$W_g = W_{sph}\varphi, \tag{7}$$

here W_g - settling speed of solid particles of arbitrary shape, m/s ; φ - form factor.

In (7), the particle shape coefficients take the following values: for particles having a cubic shape $\varphi = 0,806$; $\varphi = 0,58$ for particles having an oblong shape; $\varphi = 0,69$ for particles having a round shape; $\varphi = 0,43$ for plate-shaped particles; $\varphi = 0,66$ for particles with an angular shape.

The settling rate is directly proportional to the size and specific gravity of the particles and inversely proportional to the specific gravity and dynamic viscosity of the atmosphere.

From Equations 6, 7 it is clear that the rate of particle deposition depends on μ_c - dynamic and kinematic viscosity of the atmospheric air mass.

To calculate the dynamic and kinematic viscosity of the atmospheric air mass, a regression model was obtained, which takes into account changes in temperature and atmospheric air pressure:

$$\begin{cases} \mu_c = (324 * 10^{-9} * P - 1.5 * 10^{-9} * T * P + 16.81 + 0.048 * T) * 10^{-6}, \\ \mu_x = (324 * 10^{-9} * P - 1.5 * 10^{-9} * T * P + 16.81 + 0.048 * T) * 10^{-6} * 287 * (T + 273) / P, \end{cases} \tag{8}$$

here T - air temperature, P - atmospheric air pressure.

3. Solution Algorithm

To simplify the solution of problems (1)-(5), we consider it in a rectangular area, assuming that the source of pollution is located on the surface of the earth. To numerically solve the problems presented by Turimov, et al. [21]; Eshpulatov and Ubaydullaev [22] and Ubaydullaev and Eshpulatov [23], we divide the region of change of the desired value into a grid with steps corresponding to the given boundary conditions:

$$\Omega_{xyzt} = \left\{ \left(x_i = i\Delta x, y_j = j\Delta y, z_k = k\Delta z, \tau_n = n \Delta t \right), i = \overline{0, N}; j = \overline{0, M}, k = \overline{0, L}, n = \overline{0, N_t}, \Delta t = \frac{1}{N_t} \right\}.$$

In the process of solving problem (1)-(5), an implicit scheme is used to ensure stability. Equation 1 is approximated in the direction of the Ox axis as follows:

$$\begin{aligned} & \frac{1}{2} \frac{\theta_{i,j,k}^{n+1/3} - \theta_{i,j,k}^n}{\Delta t / 3} + \frac{1}{2} \frac{\theta_{i+1,j,k}^{n+1/3} - \theta_{i+1,j,k}^n}{\Delta t / 3} + \left(\frac{u - |u|}{4} \right) \frac{\theta_{i+1,j,k}^{n+1/3} - \theta_{i,j,k}^{n+1/3}}{\Delta x} + \\ & + \left(\frac{u - |u|}{4} \right) \frac{\theta_{i+1,j,k}^n - \theta_{i,j,k}^n}{\Delta x} + \left(\frac{u + |u|}{4} \right) \frac{\theta_{i,j,k}^{n+1/3} - \theta_{i-1,j,k}^{n+1/3}}{\Delta x} + \\ & + \left(\frac{u + |u|}{4} \right) \frac{\theta_{i,j,k}^n - \theta_{i-1,j,k}^n}{\Delta x} + \left(\frac{v - |v|}{2} \right) \frac{\theta_{i,j+1,k}^n - \theta_{i,j,k}^n}{\Delta y} + \\ & + \left(\frac{v + |v|}{2} \right) \frac{\theta_{i,j,k}^n - \theta_{i,j-1,k}^n}{\Delta y} + \left(\frac{(w - w_g^{n+1/3}) - |w - w_g^{n+1/3}|}{2} \right) \frac{\theta_{i,j,k+1}^n - \theta_{i,j,k}^n}{\Delta z} + \end{aligned}$$

$$\begin{aligned}
 & + \left(\frac{(w - w_g^{n+1/3}) + |w - w_g^{n+1/3}|}{2} \right) \frac{\theta_{i,j,k}^n - \theta_{i,j,k-1}^n}{\Delta z} + (\Phi_r + \Phi_v + \alpha) \theta_{i,j,k}^{n+1/3} = \\
 & = \frac{\mu}{\Delta x^2} (\theta_{i+1,j,k}^{n+1/3} - 2\theta_{i,j,k}^{n+1/3} + \theta_{i-1,j,k}^{n+1/3}) + \frac{\mu}{\Delta y^2} (\theta_{i,j+1,k}^n - 2\theta_{i,j,k}^n + \theta_{i,j-1,k}^n) + \\
 & + \frac{1}{\Delta z^2} (\kappa_{k+0,5} \theta_{i,j,k+1}^n - (\kappa_{k+0,5} + \kappa_{k-0,5}) \theta_{i,j,k}^n + \kappa_{k-0,5} \theta_{i,j,k-1}^n) + \frac{1}{3} \delta_{i,j,k} Q.
 \end{aligned}$$

We open the brackets and, grouping similar terms of the equation, we get:

$$\begin{aligned}
 & - \left(\frac{\mu}{\Delta x^2} + \frac{u + |u|}{4\Delta x} \right) \theta_{i-1,j,k}^{n+1/3} + \left(\frac{2\mu}{\Delta x^2} + \frac{|u|}{2\Delta x} + \frac{3}{2\Delta t} + \Phi_r + \Phi_v + \alpha \right) \theta_{i,j,k}^{n+1/3} - \\
 & + \left(\frac{\mu}{\Delta x^2} - \frac{u - |u|}{4\Delta x} - \frac{3}{2\Delta t} \right) \theta_{i+1,j,k}^{n+1/3} = \left(\frac{u + |u|}{4\Delta x} \right) \theta_{i-1,j,k}^n + \left(\frac{3}{2\Delta t} - \frac{u - |u|}{4\Delta x} \right) \theta_{i+1,j,k}^n + \\
 & + \left(\frac{3}{2\Delta t} - \frac{2\mu}{\Delta y^2} - \frac{\kappa_{k+0,5} + \kappa_{k-0,5}}{\Delta z^2} - \frac{|u|}{2\Delta x} - \frac{|v|}{\Delta y} - \frac{|w - w_g^{n+1/3}|}{\Delta z} \right) \theta_{i,j,k}^n + \\
 & + \left(\frac{\mu}{\Delta y^2} + \frac{v + |v|}{2\Delta y} \right) \theta_{i,j-1,k}^n + \left(\frac{\mu}{\Delta y^2} - \frac{v - |v|}{2\Delta y} \right) \theta_{i,j+1,k}^n + \\
 & + \left(\frac{\kappa_{k-0,5}}{\Delta z^2} + \frac{(w - w_g^{n+1/3}) + |w - w_g^{n+1/3}|}{2\Delta z} \right) \theta_{i,j,k-1}^n + \\
 & + \left(\frac{\kappa_{k+0,5}}{\Delta z^2} - \frac{(w - w_g^{n+1/3}) - |w - w_g^{n+1/3}|}{2\Delta z} \right) \theta_{i,j,k+1}^n + \frac{1}{3} \delta_{i,j,k} Q.
 \end{aligned}$$

Let us simplify such terms and obtain the following system of linear algebraic equations:

$$a_{i,j,k} \theta_{i-1,j,k}^{n+1/3} - b_{i,j,k} \theta_{i,j,k}^{n+1/3} + c_{i,j,k} \theta_{i+1,j,k}^{n+1/3} = -d_{i,j,k}. \tag{9}$$

The coefficients and free term of system (9) are determined as follows:

$$\begin{aligned}
 a_{i,j,k} &= \frac{\mu}{\Delta x^2} + \frac{u + |u|}{4\Delta x}; \quad b_{i,j,k} = \frac{2\mu}{\Delta x^2} + \frac{|u|}{2\Delta x} + \frac{3}{2\Delta t} + \Phi_r + \Phi_v + \alpha; \\
 c_{i,j,k} &= \frac{\mu}{\Delta x^2} - \frac{u - |u|}{4\Delta x} - \frac{3}{2\Delta t}; \\
 d_{i,j,k} &= \left(\frac{3}{2\Delta t} - \frac{2\mu}{\Delta y^2} - \frac{\kappa_{k+0,5} + \kappa_{k-0,5}}{\Delta z^2} - \frac{|u|}{2\Delta x} - \frac{|v|}{\Delta y} - \frac{|w - w_g^{n+1/3}|}{\Delta z} \right) \theta_{i,j,k}^n + \\
 & + \left(\frac{u + |u|}{4\Delta x} \right) \theta_{i-1,j,k}^n + \left(\frac{3}{2\Delta t} - \frac{u - |u|}{4\Delta x} \right) \theta_{i+1,j,k}^n + \left(\frac{\mu}{\Delta y^2} + \frac{v + |v|}{2\Delta y} \right) \theta_{i,j-1,k}^n +
 \end{aligned}$$

$$\begin{aligned}
 & + \left(\frac{\mu}{\Delta y^2} - \frac{v - |v|}{2\Delta y} \right) \theta_{i,j+1,k}^n + \left(\frac{\kappa_{k-0,5}}{\Delta z^2} + \frac{(w - w_g^{n+1/3}) + |w - w_g^{n+1/3}|}{2\Delta z} \right) \theta_{i,j,k-1}^n + \\
 & + \left(\frac{\kappa_{k+0,5}}{\Delta z^2} - \frac{(w - w_g^{n+1/3}) - |w - w_g^{n+1/3}|}{2\Delta z} \right) \theta_{i,j,k+1}^n + \frac{1}{3} \delta_{i,j,k} Q.
 \end{aligned}$$

We also approximate boundary condition (3) for $x=0$ with second-order accuracy as follows:

$$-\mu \frac{-3\theta_{0,j,k}^{n+1/3} + 4\theta_{1,j,k}^{n+1/3} - \theta_{2,j,k}^{n+1/3}}{2\Delta x} = \gamma\theta_{0,j,k}^{n+1/3} - \gamma\theta_a,$$

or

$$3\mu\theta_{0,j,k}^{n+1/3} - 4\mu\theta_{1,j,k}^{n+1/3} + \mu\theta_{2,j,k}^{n+1/3} = 2\Delta x\gamma\theta_{0,j,k}^{n+1/3} - 2\Delta x\gamma\theta_a. \tag{10}$$

From the resulting tridiagonal system of linear algebraic equations $x=1$ we have

$$a_{1,j,k}\theta_{0,j,k}^{n+1/3} - b_{1,j,k}\theta_{1,j,k}^{n+1/3} + c_{1,j,k}\theta_{2,j,k}^{n+1/3} = -d_{1,j,k};$$

and find $\theta_{2,j,k}^{n+1/3}$ it as follows:

$$\theta_{2,j,k}^{n+1/3} = -\frac{a_{1,j,k}}{c_{1,j,k}}\theta_{0,j,k}^{n+1/3} + \frac{b_{1,j,k}}{c_{1,j,k}}\theta_{1,j,k}^{n+1/3} - \frac{d_{1,j,k}}{c_{1,j,k}}. \tag{11}$$

Let's substitute (11) in place $\theta_{2,j,k}^{n+1/3}$ in (10) and get

$$\begin{aligned}
 & 3\mu\theta_{0,j,k}^{n+1/3} - 4\mu\theta_{1,j,k}^{n+1/3} - \mu \frac{a_{1,j,k}}{c_{1,j,k}}\theta_{0,j,k}^{n+1/3} + \mu \frac{b_{1,j,k}}{c_{1,j,k}}\theta_{1,j,k}^{n+1/3} - \\
 & -\mu \frac{d_{1,j,k}}{c_{1,j,k}} = 2\Delta x\gamma\theta_{0,j,k}^{n+1/3} - 2\Delta x\gamma\theta_a.
 \end{aligned}$$

Simplifying, we find $\theta_{0,j,k}^{n+1/3}$ it as follows:

$$\theta_{0,j,k}^{n+1/3} = \frac{4\mu c_{1,j,k} - b_{1,j,k}\mu}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\gamma} \theta_{1,j,k}^{n+1/3} + \frac{\mu d_{1,j,k} + 2\Delta x\gamma c_{1,j,k}\theta_a}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\gamma}.$$

Using the sweep method, we find $\alpha_{0,j,k}$ and $\beta_{0,j,k}$:

$$\alpha_{0,j,k} = \frac{4\mu c_{1,j,k} - b_{1,j,k}\mu}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\gamma}; \quad \beta_{0,j,k} = \frac{\mu d_{1,j,k} + 2\Delta x\gamma c_{1,j,k}\theta_a}{3\mu c_{1,j,k} - a_{1,j,k}\mu + 2\Delta x\gamma}.$$

Similarly, we approximate the boundary condition (3) for $x = L_x$ with second-order accuracy as follows:

$$\begin{aligned}
 & \mu \frac{\theta_{N-2,j,k}^{n+1/3} - 4\theta_{N-1,j,k}^{n+1/3} + 3\theta_{N,j,k}^{n+1/3}}{2\Delta x} = \gamma\theta_{N,j,k}^{n+1/3} - \gamma\theta_a, \\
 & \mu \frac{\theta_{N-2,j,k}^{n+1/3} - 4\theta_{N-1,j,k}^{n+1/3} + 3\theta_{N,j,k}^{n+1/3}}{2\Delta x} = \gamma\theta_{N,j,k}^{n+1/3} - \gamma\theta_a. \tag{12}
 \end{aligned}$$

Let's apply the sweep method sequentially for $N, N-1$ and $N-2$ and find $\theta_{N-1,j,k}^{n+1/3}$ and $\theta_{N-2,j,k}^{n+1/3}$:

$$\theta_{N-1,j,k}^{n+1/3} = \alpha_{N-1,j,k}\theta_{N,j,k}^{n+1/3} + \beta_{N-1,j,k}, \tag{13}$$

$$\begin{aligned} \theta_{N-2,j,k}^{n+1/3} &= \alpha_{N-2,j,k} \theta_{N-1,j,k}^{n+1/3} + \beta_{N-2,j,k} = \\ &= \alpha_{N-2,j,k} (\alpha_{N-1,j,k} \theta_{N,j,k}^{n+1/3} + \beta_{N-1,j,k}) + \beta_{N-2,j,k} = \\ &= \alpha_{N-2,j,k} \alpha_{N-1,j,k} \theta_{N,j,k}^{n+1/3} + \alpha_{N-2,j,k} \beta_{N-1,j,k} + \beta_{N-2,j,k}, \end{aligned} \tag{14}$$

$\theta_{N-1,j,k}^{n+1/3}$ and $\theta_{N-2,j,k}^{n+1/3}$ in (13) and (14) substituting instead of $\theta_{N-1,j,k}^{n+1/3}$ and $\theta_{N-2,j,k}^{n+1/3}$ in (12), we find $\theta_{N,j,k}^{n+1/3}$:

$$\begin{aligned} &\alpha_{N-2,j,k} \alpha_{N-1,j,k} \mu \theta_{N,j,k}^{n+1/3} + \alpha_{N-2,j,k} \beta_{N-1,j,k} \mu + \beta_{N-2,j,k} \mu - 4\alpha_{N-1,j,k} \mu \theta_{N,j,k}^{n+1/3} - \\ &- 4\beta_{N-1,j,k} \mu + 3\mu \theta_{N,j,k}^{n+1/3} = 2\Delta x \gamma \theta_{N,j,k}^{n+1/3} - 2\Delta x \gamma \theta_a; \\ \theta_{N,j,k}^{n+1/3} &= \frac{2\Delta x \gamma \theta_a - (\beta_{N-2,j,k} + \alpha_{N-2,j,k} \beta_{N-1,j,k} - 4\beta_{N-1,j,k}) \mu}{2\Delta x \gamma + (\alpha_{N-2,j,k} \alpha_{N-1,j,k} - 4\alpha_{N-1,j,k} + 3) \mu}. \end{aligned}$$

The above sequence of actions is applicable for the O_y and O_z directions.

For direction O_y :

$$\bar{a}_{i,j,k} \theta_{i,j-1,k}^{n+2/3} - \bar{b}_{i,j,k} \theta_{i,j,k}^{n+2/3} + \bar{c}_{i,j,k} \theta_{i,j+1,k}^{n+2/3} = -\bar{d}_{i,j,k},$$

where

$$\bar{a}_{i,j,k} = \frac{\mu}{\Delta y^2} + \frac{v+|v|}{4\Delta y}; \quad \bar{b}_{i,j,k} = \frac{2\mu}{\Delta y^2} + \frac{|v|}{2\Delta y} + \frac{3}{2\Delta t} + \Phi_r + \Phi_v + \alpha;$$

$$\bar{c}_{i,j,k} = \frac{\mu}{\Delta y^2} - \frac{v-|v|}{4\Delta y} - \frac{3}{2\Delta t};$$

$$\begin{aligned} \bar{d}_{i,j,k} &= \left(\frac{3}{2\Delta t} - \frac{2\mu}{\Delta x^2} - \frac{\kappa_{k+0,5} + \kappa_{k-0,5}}{\Delta z^2} - \frac{|u|}{\Delta x} - \frac{|v|}{2\Delta y} - \frac{|w_a|}{\Delta z} \right) \theta_{i,j,k}^{n+1/3} + \left(\frac{\mu}{\Delta x^2} + \frac{u+|u|}{2\Delta x} \right) \theta_{i-1,j,k}^{n+1/3} + \\ &+ \left(\frac{\mu}{\Delta x^2} - \frac{u-|u|}{2\Delta x} \right) \theta_{i+1,j,k}^{n+1/3} + \left(\frac{v+|v|}{4\Delta y} \right) \theta_{i,j-1,k}^{n+1/3} + \left(\frac{3}{2\Delta t} - \frac{v-|v|}{4\Delta y} \right) \theta_{i,j+1,k}^{n+1/3} + \\ &+ \left(\frac{\kappa_{k-0,5}}{\Delta z^2} + \frac{(w-w_g^{n+2/3}) + |w-w_g^{n+2/3}|}{2\Delta z} \right) \theta_{i,j,k-1}^{n+1/3} + \end{aligned}$$

$$+ \left(\frac{\kappa_{k+0,5}}{\Delta z^2} - \frac{(w-w_g^{n+2/3}) - |w-w_g^{n+2/3}|}{2\Delta z} \right) \theta_{i,j,k+1}^{n+1/3} + \frac{1}{3} \delta_{i,j,k} Q;$$

$$\theta_{i,M,k}^{n+2/3} = \frac{2\Delta y \gamma \theta_a - \mu \bar{\alpha}_{i,M-2,k} \bar{\beta}_{i,M-1,k} - \mu \bar{\beta}_{i,M-2,k} + 4\mu \bar{\beta}_{i,M-1,k}}{2\Delta y \gamma + \bar{\alpha}_{i,M-2,k} \bar{\alpha}_{i,M-1,k} \mu - 4\mu \bar{\alpha}_{i,M-1,k} + 3\mu}.$$

For direction O_z :

$$\bar{a}_{i,j,k} \theta_{i,j,k-1}^{n+1} - \bar{b}_{i,j,k} \theta_{i,j,k}^{n+1} + \bar{c}_{i,j,k} \theta_{i,j,k+1}^{n+1} = -\bar{d}_{i,j,k},$$

where

$$\bar{a}_{i,j,k} = \frac{\kappa_{k-0,5}}{\Delta z^2} + \frac{(w-w_g^{n+1}) + |w-w_g^{n+1}|}{4\Delta z};$$

$$\bar{b}_{i,j,k} = \frac{\kappa_{k+0,5} + \kappa_{k-0,5}}{\Delta z^2} + \frac{|w-w_g^{n+1}|}{2\Delta z} + \frac{3}{2\Delta t} + \Phi_r + \Phi_v + \alpha;$$

$$\begin{aligned} \bar{c}_{i,j,k} &= \frac{\kappa_{k+0,5}}{\Delta z^2} - \frac{(w - w_g^{n+1}) - |w - w_g^{n+1}|}{4\Delta z} - \frac{3}{2\Delta t}; \\ \bar{d}_{i,j,k} &= \left(\frac{3}{2\Delta t} - \frac{2\mu}{\Delta x^2} - \frac{2\mu}{\Delta y^2} - \frac{|u|}{\Delta x} - \frac{|v|}{\Delta y} - \frac{|w - w_g^{n+1}|}{2\Delta z} \right) \theta_{i,j,k}^{n+2/3} + \\ &+ \left(\frac{\mu}{\Delta x^2} + \frac{u + |u|}{2\Delta x} \right) \theta_{i-1,j,k}^{n+2/3} + \left(\frac{\mu}{\Delta x^2} - \frac{u - |u|}{2\Delta x} \right) \theta_{i+1,j,k}^{n+2/3} + \left(\frac{\mu}{\Delta y^2} + \frac{v + |v|}{2\Delta y} \right) \theta_{i,j-1,k}^{n+2/3} + \\ &+ \left(\frac{\mu}{\Delta y^2} - \frac{v - |v|}{2\Delta y} \right) \theta_{i,j+1,k}^{n+2/3} + \left(\frac{(w - w_g^{n+1}) + |w - w_g^{n+1}|}{4\Delta z} \right) \theta_{i,j-1,k}^{n+2/3} + \\ &+ \left(\frac{3}{2\Delta t} - \frac{(w - w_g^{n+1}) - |w - w_g^{n+1}|}{4\Delta z} \right) \theta_{i,j+1,k}^{n+2/3} + \frac{1}{3} \delta_{i,j,k} Q; \\ \theta_{i,j,L}^{n+1} &= \frac{2\Delta z \xi \theta_E - \kappa \alpha_{i,j,L-2} \bar{\beta}_{i,j,L-1} - \kappa \bar{\beta}_{i,j,L-2} + 4\kappa \bar{\beta}_{i,j,L-1}}{2\Delta z \xi + \alpha_{i,j,L-2} \alpha_{i,j,L-1} \kappa - 4\kappa \alpha_{i,j,L-1} + 3\kappa}. \end{aligned}$$

Based on the proposed regression models (8), calculations were carried out to determine changes in the dynamic and kinematic viscosity of the atmospheric air mass depending on temperature and pressure, which are shown in Figures 1-7.

In Figure. 1-3, the dynamics of changes in the kinematic viscosity of air depending on pressure at different air temperatures are shown. From Figure 1, it can be seen that with increasing pressure, the viscosity of air increases at low temperatures according to a linear law.

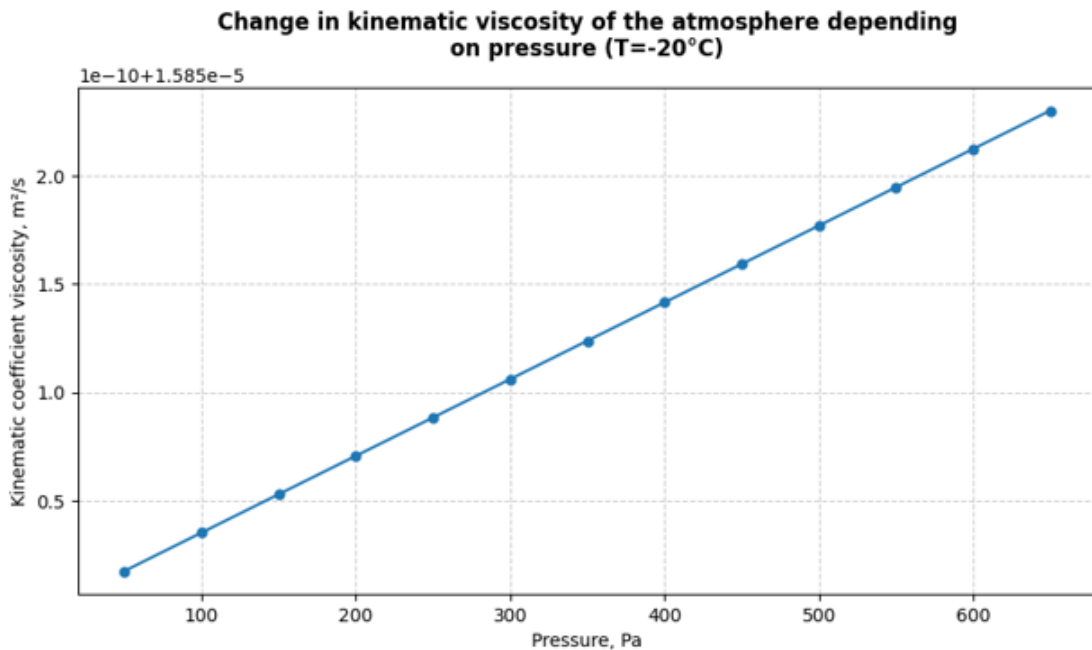


Figure 1. Change in the kinematic viscosity of the atmosphere depending on pressure at T = -20 °C.

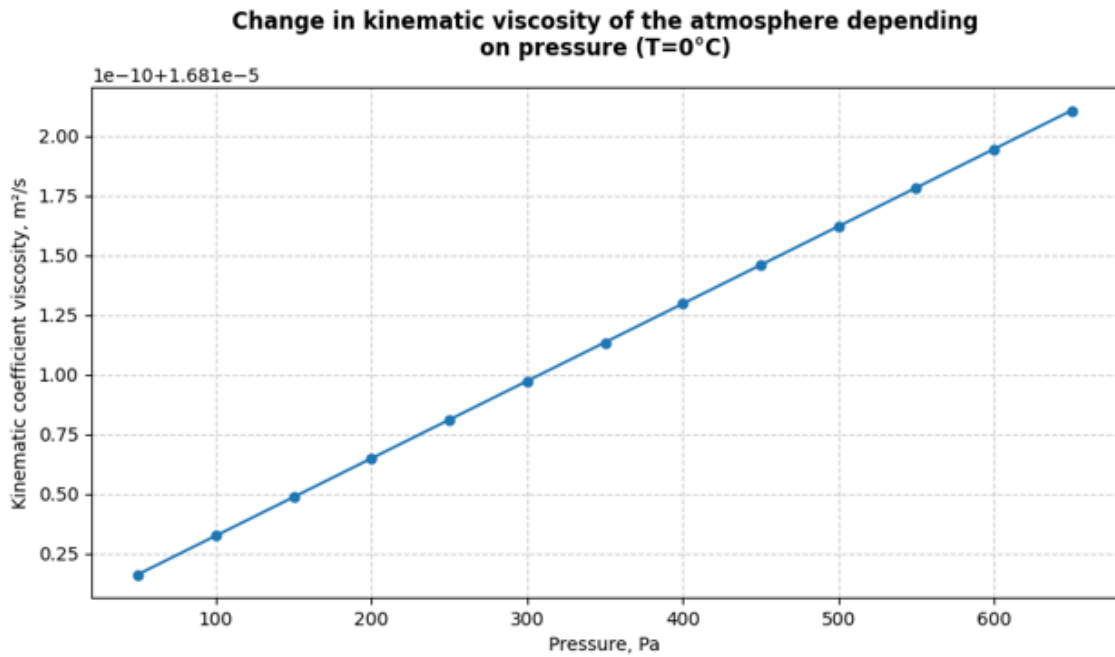


Figure 2.
Change in the kinematic viscosity of the atmosphere depending on pressure at T=0°C.

And at T = 0°C, the viscosity of air increases less intensely than at negative temperatures [Figure 2](#), which indicates a moderate increase in air density. [Figure 3](#) indicates that the viscosity of air changes little with increasing temperature and increasing pressure.

As can be seen from the straight lines in [Figures 1-3](#), the kinematic viscosity of the atmosphere increases linearly depending on the increase in pressure and temperature in the atmosphere. Temperature is the main factor determining the kinematic viscosity of air, as it directly affects the dynamic viscosity and density. Understanding this relationship allows us to accurately predict the state of air masses and develop effective technical and environmental solutions.

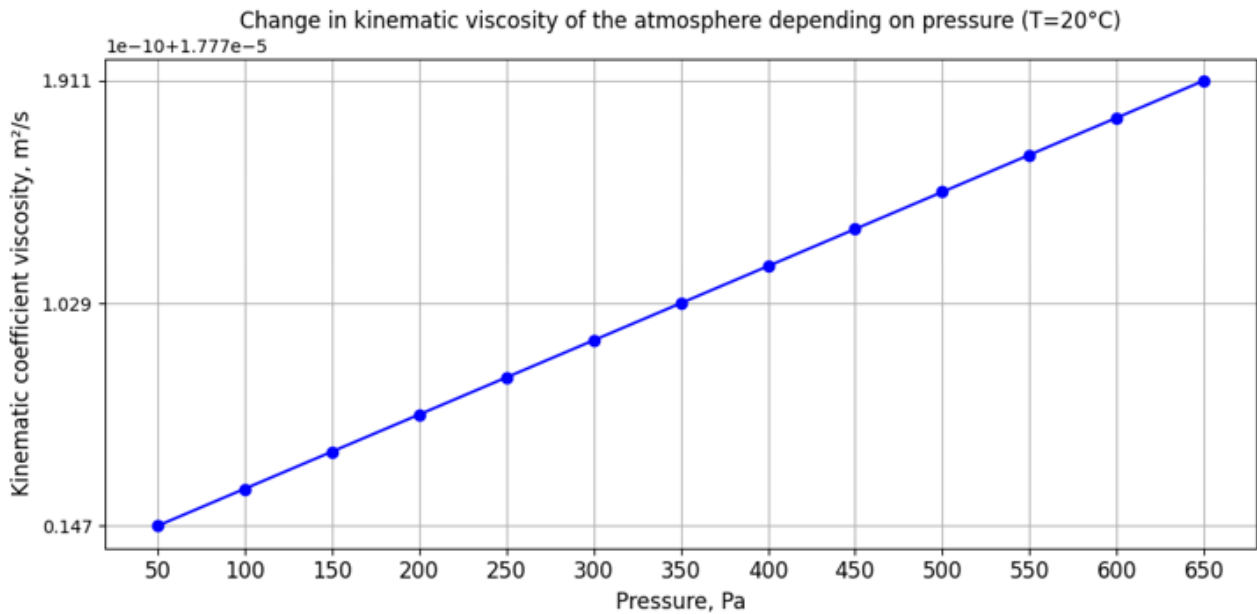


Figure 3.
Change in the kinematic viscosity of the atmosphere depending on pressure at T = 20 °C.

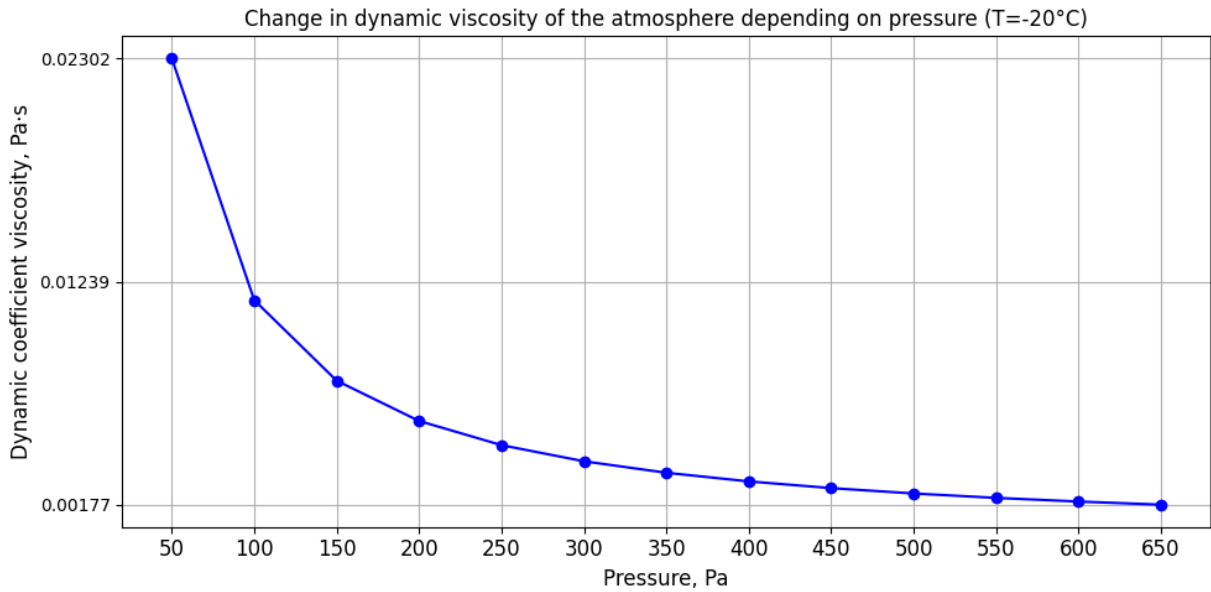


Figure 4.
Change in dynamic viscosity of the atmosphere depending on pressure at T=-20°C.

The dynamic viscosity of the atmosphere (Figures 4-6) decreases depending on the increase in pressure in the atmosphere. This is especially noticeable when the pressure changes in the ranges. Low temperature increases the viscosity of air, but as pressure increases, the viscosity decreases rapidly. This is explained by an increase in air density, which reduces the relative influence of dynamic viscosity. Computational experiments were carried out on the dynamics of changes in the kinematic viscosity of the atmosphere at various pressures with increasing temperature, from which it was determined that an increase in temperature contributes to an increase in kinematic viscosity.

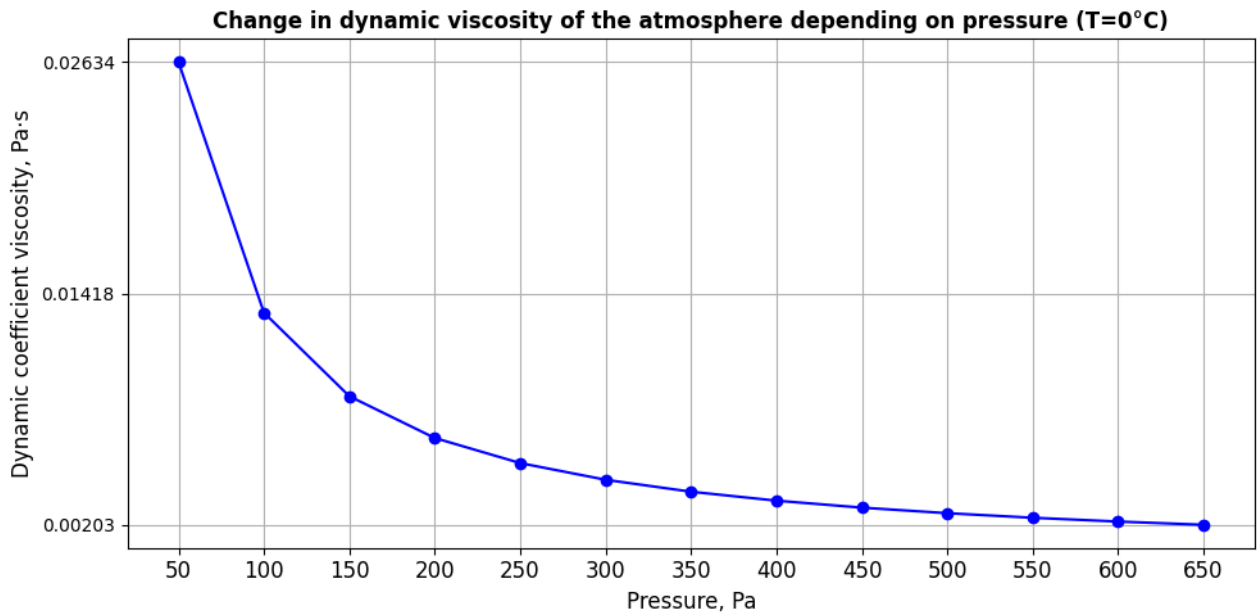


Figure 5.
Change in dynamic viscosity of the atmosphere depending on pressure at T=0°C.

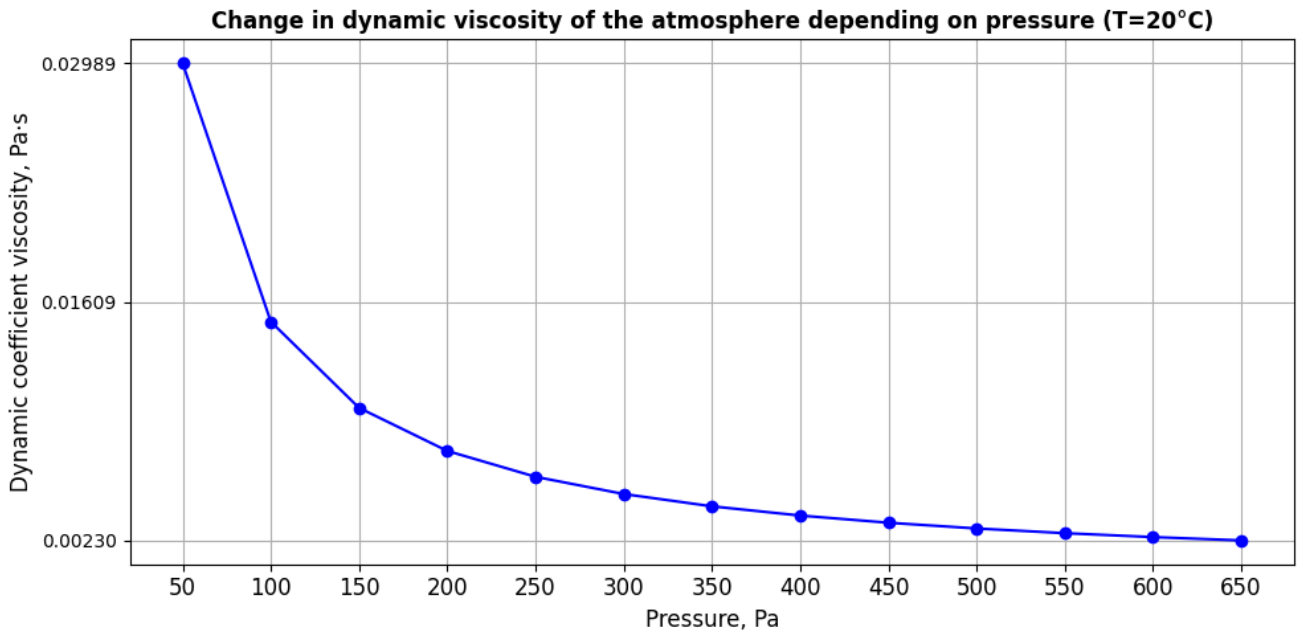


Figure 6. Change in dynamic viscosity of the atmosphere depending on pressure at T=20°C.

Based on the graph presented in Figure 7, it was revealed that dynamic viscosity depends on temperature, i.e., it decreases with increasing pressure and temperature. Meanwhile, kinematic viscosity increases linearly with pressure and temperature.

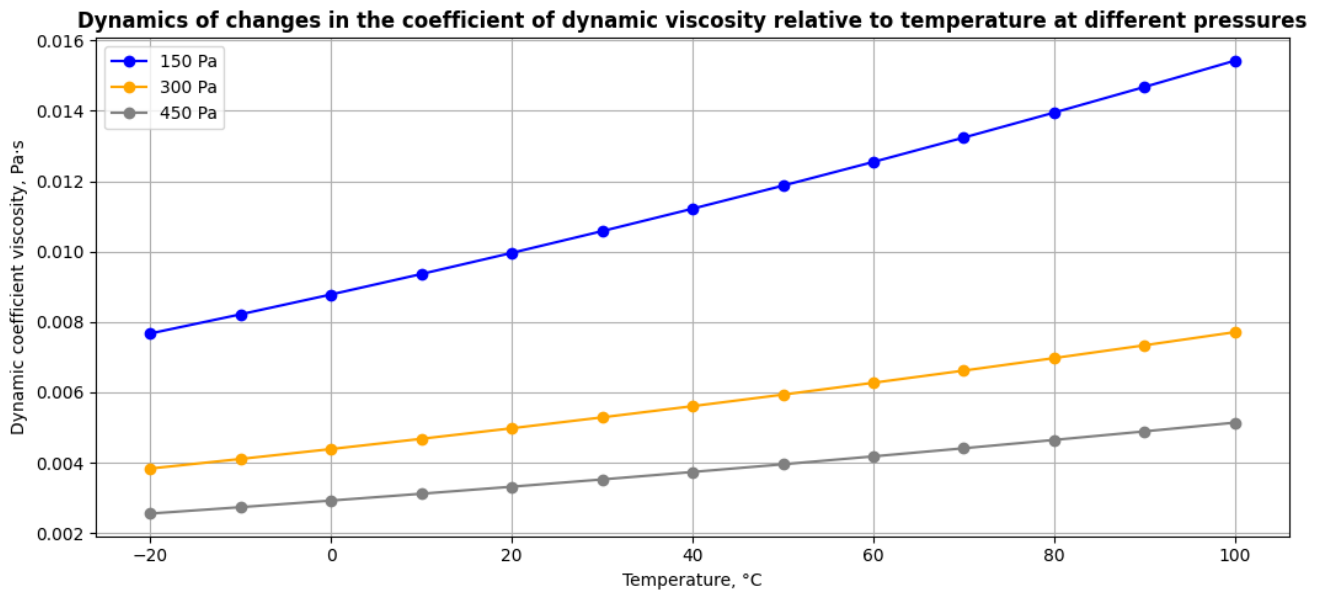


Figure 7. Change in dynamic viscosity of the atmosphere depending on temperature at different pressure.

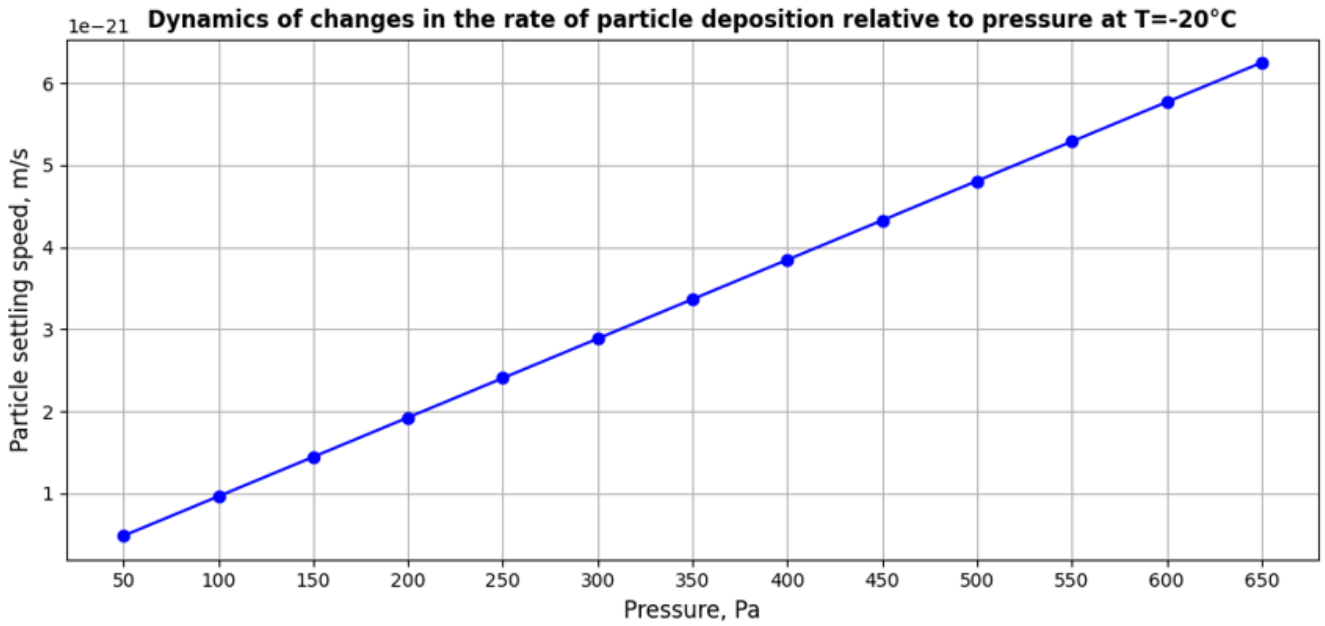


Figure 8.
Change in particle sedimentation rate relative to pressure.

In Figure 8-10 show the results of changes in the rate of deposition of harmful particles relative to air pressure at different temperatures. The results of a comparison of these graphs show that the deceleration of the deposition of harmful particles is influenced by an increase in air temperature, at which its density decreases. From the above results, it was revealed that at higher temperatures, the viscosity of air increases, which also helps to reduce the rate of deposition of harmful particles.

Graph Figure 11 demonstrates the dynamics of changes in the rate of deposition of harmful particles depending on temperature at a fixed pressure. Analysis of the figure shows that at low temperatures, there is a sharp decrease in the deposition rate, and with an increase in air temperature, the deposition rate of particles decreases. From the above results, this is justified by a decrease in air density and an increase in its viscosity with increasing temperature. This confirms the strong influence of the temperature factor.

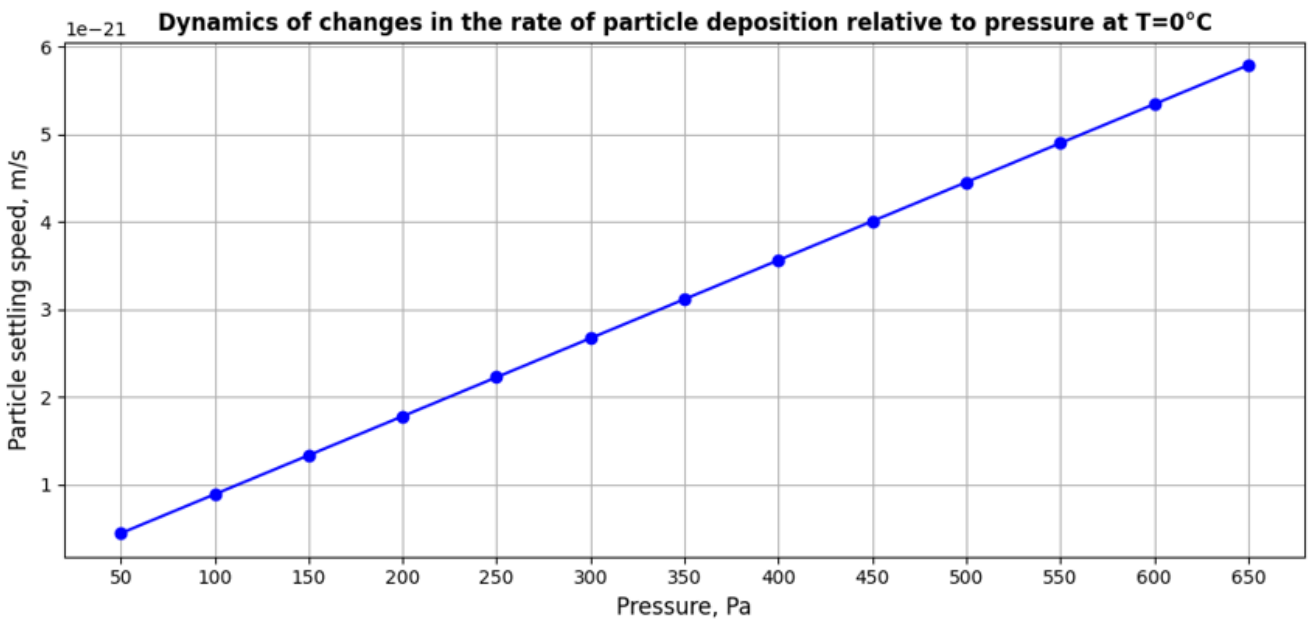


Figure 9.
Change in particle sedimentation rate relative to pressure.

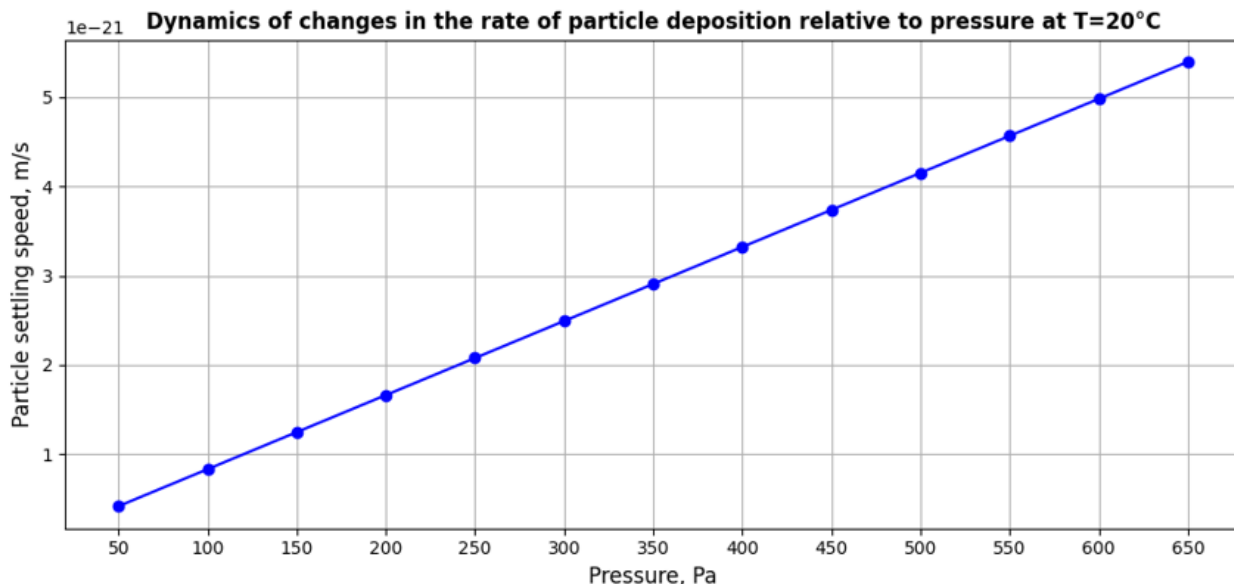


Figure 10.
Change in particle sedimentation rate relative to pressure.

Based on computational experiments, results were obtained from which it follows that the rate of deposition of particles in the atmosphere is a complex function of pressure, temperature, and the physical parameters of the particles themselves. If pressure accelerates deposition, temperature slows it down, as it increases the viscosity of air and reduces its density. Additional factors include particle size and density.

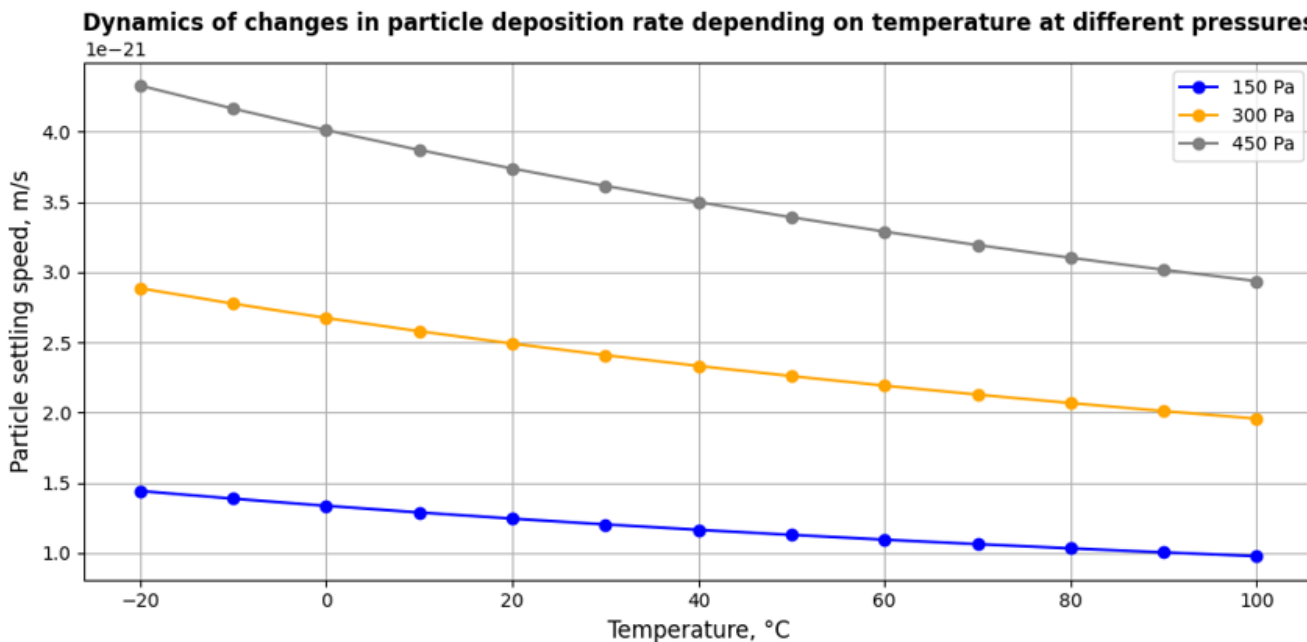


Figure 11.
Change in the rate of particle deposition relative to temperature at different atmospheric pressures

4. Conclusion

This work confirms that in the processes of transport and diffusion of pollutants, many factors are important and significantly influence the deposition of pollutants in the atmosphere to the surface of the Earth. From the numerical calculations performed, it is clear that the kinematic viscosity of the atmosphere increases according to a linear law, and the dynamic viscosity of the atmosphere decreases according to an exponential law, depending on the increase in pressure in the atmosphere. The regression models used are effective in determining the influence of temperature and pressure on dynamic and kinematic viscosity. The results of which make it possible to estimate the duration of the persistence of harmful particles in the atmosphere and the distance of their spread through the air. It plays an important role in environmental monitoring and air quality management systems. The conducted study emphasizes that the considered factors influencing the deposition of pollutants in the atmosphere are very important. In particular, they make it possible to effectively control the rate of deposition of harmful substances, taking into account climatic conditions. The developed models can be used to predict the behavior of

dust and fine aerosol particles and assess their impact on the environment, which can be useful for monitoring and predicting the state of the surface layer of the atmosphere in industrial regions and in developing air protection measures.

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