Mathematical modeling of the spread of pollutants in the atmosphere from the storage of liquid waste of pig complexes during reagent treatment

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Abstract. The effect of treatment of liquid organic waste from pig farms with various calcium-containing reagents, followed by neutralization to pH 7.0-8.5, on reducing the emissions of pollutants such as ammonia, hydrogen sulfide, methyl mercaptan, nitrogen and carbon oxides at various stages of treatment was studied. The article deals with mathematical modeling of changes in the concentration fields of pollutants over time. Dynamic processes of gaseous pollutants propagation in the surface air layer above liquid organic waste accumulators are simulated. The developed model will allow calculating the distribution of pollutants over the storage of liquid organic waste in a given period of time and calculate the concentrations of gaseous pollutants in steady-state and non-stationary modes during reagent treatment. The time of reducing the concentrations of pollutants to the required values is determined based on the results of a computational experiment in the VITECON software package. The corrected sizes of sanitary protection zones of the pig complex before and after reagent treatment are presented.

The problem of spreading pollution in the air near pig complexes is very relevant all over the world. Thus, in research [1], a comparative assessment of the influence of gases generated in pig complexes (ammonia (NH₃), carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O)) on the occurrence of ecological problems is given. NH₃ and N₂O are released at all stages of handling liquid waste from pig complexes, while CO₂ is released both from animal respiration and waste accumulation, and CH₄ is released both from enteric fermentation in animals and during waste storage. [2] presents the results of studies of the effect of mineral additives on the release of gaseous pollutants during composting. It is known that acidification of animal waste is used to reduce emissions of ammonia and methane [3,4], but such methods involve the use of aggressive reagents for the biosphere or a long shelf life. The research [5] describes methods for adequate measurements of gaseous pollutants from pig complexes; the selection method was tested using artificial sources of emissions set up at the facilities.

The aim of the research was to model the spread of pollutants in the atmosphere from the storage of liquid waste from pig complexes that are subjected to reagent treatment to obtain organic fertilizer, and to adjust the size of the sanitary protection zone. To achieve this goal, it is necessary to solve a problem describing the propagation of gaseous pollutants in the surface layer of air at a known speed of its movement at various stages of processing.

The results of studies of the efficiency of fractionation of liquid organic waste of pig complexes using various calcium-containing (calcium carbide slurry, defecation lime suspension, lime milk suspension)
and acidifying (superphosphate suspensions, ammophos, nitrophosca solutions, oxalic acid) reagents for the production of organic-mineral fertilizers are presented in [6-8].

The research was conducted on the basis of the South Russian State Polytechnic University (NPI) named after M. I. Platov. The objects of the study were the surface layer of air above the accumulators of liquid waste from a pig-breeding farm in the Rostov region with a population of 14,000 pigs.

To identify the dynamics of the content of gases that pollute the atmosphere near liquid waste storage facilities, polluted air was sampled and concentrations were measured using the GANK-4RB gas analyzer at various stages of treatment: I-liquid waste without treatment; II-after the introduction of calcium-containing reagents; III-after the introduction of acidifying reagents figure 1.

![Graph](image1.png)

**Figure 1.** Concentrations of pollutants at various stages of liquid waste treatment in a) CH$_3$SH and H$_2$S, b) CO, NO, NO$_2$, NH$_3$.

A significant decrease in the content of pollutants in the air above the surface of pig complexes liquid organic waste accumulators was observed with the sequential introduction of calcium-containing and acidifying reagents. So, the concentration of methyl mercaptan decreased from 41 to 0.52 maximum acceptable concentrations (MAC) and hydrogen sulfide decreased from 4 to 0.05 MAC. The content of ammonia, nitrogen oxides, and carbon in the air near storage sites decreased by 90-99% after treatment.

Based on the data obtained, the calculation of dispersion of gas emissions near liquid organic waste storage facilities was carried out using the unified program for calculating atmospheric pollution UPRZA "ECOLOGIST"-4.60, which makes calculations in accordance with the "methods for calculating the dispersion of harmful (polluting) substances in the atmospheric air" (approved by order of the Ministry of natural resources of Russia 273 of 06.06.2017). The program made it possible to calculate the maximum one-time (averaged over a 20-30-minute interval) concentrations of pollutants in the air before and after treatment of liquid organic waste (in MAC fractions) under adverse weather conditions. The results of calculating the dispersion of methyl mercaptan and hydrogen sulfide are shown in figure 2,3.
The size of the sanitary protection zone (SPZ) for a complex with working treatment facilities should be 1000 m [9].

Clarification of the size of the sanitary protection zone was carried out with an adjustment for the wind rose for the area where the pig complex is located. As a result, we got the values, m: North-2600; North-East-2600; East-4000; South-East-1000; South-600; South-West-2400; West-4600; North-West-2200. The maximum permissible concentration of methyl mercaptan after reagent treatment was reached at a distance of 230 m from the pig complex, H$_2$S+NO-at a distance of 100 m, the recommended size of the sanitary protection zone can be reduced to 300 m. The specified SPZ dimensions are equal to m: North-169; North-East-169; East-260; South-East-65; South-39; southwest-156; West-299; Northwest-143 figure 4.
However, the program does not allow us to estimate changes in concentration fields over time, especially over large areas. Therefore, the authors solved the problem of modeling the dynamic processes of propagation of gaseous pollutants in the boundary layer of the atmosphere over accumulators of liquid organic waste. At this stage, the concentrations of polluting gases in the three-kilometer zone were estimated.

The boundary value problem expressing the dependence of the distribution of pollutants in the air above the surface of storage devices on the speed of air movement is set in the region $\Omega$ [10], shown in figure 5.

\[
\begin{align*}
\frac{\partial c}{\partial t} + \nabla \cdot (\bar{v}c) &= \Delta c + \sigma c + Q_c, \quad x \in \Omega; \\
\alpha_1 \frac{\partial c}{\partial n} + \alpha_2 c + \alpha_3 \varphi(x, y) &= 0 \quad \text{if} \quad z = z_0, \\
\frac{\partial c}{\partial n} &= 0 \quad \text{for} \quad \Sigma n u v_n \geq 0; c = c_{\Sigma} \quad \text{for} \quad \Sigma n u v_n < 0; \\
c &= 0 \quad \text{if} \quad z = l_3, \\
c(x, 0) &= c_\Phi(x), \quad x \in \Omega \cup \partial \Omega.
\end{align*}
\]

Here is $\Omega$ calculated area.
\[ \Omega = \{ x \mid x = (x_1, x_2, x_3), \quad 0 < x_\alpha < l_\alpha, \quad \alpha = 1, 2; \quad z_0(x_1, x_2) < x_3 < l_3 \} \]

which \( x = (x_1, x_2, x_3) \leftrightarrow (x, y, z), \quad z_0(x, y) \) – a function of the height of the underlying surface; \( \Sigma \) - a side surface of the computational area.

\( \mathbf{C} \) - the impurity concentration; \( \mathbf{v} = (v_1, v_2, v_3) \leftrightarrow (u, v, w) \) the speed of air; \( \sigma \) - the speed of chemical transformation of admixtures; \( v_n \) – normal component of the speed vector of the wind; \( C_\Sigma \) – background value of impurity concentration on \( \Sigma \); \( c_\phi(x) \) - is the background concentration of impurity components; \( \partial \Omega \) – border area \( \Omega \).

The functions \( \alpha_1, \alpha_2, \alpha_3 \), are determined by the conditions of interaction of the impurity with the underlying surface. There may be the following cases:

- full reflection of the pollutant in the area \( \Omega_1 \): \( \partial c / \partial n = 0, \quad (x, y) \in \Omega_1 \), (in this case \( \alpha_1=1, \alpha_2=0, \alpha_3=0 \));
- areal emission with intensity \( \phi_1(x, y) \) in \( \Omega_2 \): \( \partial c / \partial n = \phi_1(x, y), \quad (x, y) \in \Omega_2 \), (\( \alpha_1=1, \alpha_2=0, \alpha_3=-1 \));
- full sedimentation in \( \Omega_3 \): \( c(x, y) = 0, \quad (x, y) \in \Omega_3 \), (\( \alpha_1=0, \alpha_2=1, \alpha_3=0 \));
- partly reflection in contact with the surface in \( \Omega_4 \): \( \partial c / \partial n + \lambda c = 0, \quad (x, y) \in \Omega_4 \), (\( \alpha_1=1, \alpha_2=\lambda, \alpha_3=0 \));
- in \( \Omega_3 \) pollutants are neutralized and the intensity should not be higher than the set value: \( c(x, y) = \phi_2(x, y), \quad (x, y) \in \Omega_4 \), (\( \alpha_1=0, \alpha_2=1, \alpha_3=-1 \));

The choice of this mathematical model is due to: the variety of cases of interaction of an impurity with the surface, depending on weather conditions. The boundary value problem (1-5) is solved by the difference method.

The method of numerical solution and properties of a possible difference scheme are presented in research [10]. The VITECON software package made it possible to implement algorithms under the most unfavorable weather conditions - no wind at low humidity (no wet deposition: \( \sigma=0 \); the underlying surface is completely reflected by the pollutant \( \partial C/\partial n=0 \)). In this situation, even without the treatment of liquid organic waste, the concentrations of methyl mercaptan and H₂S will remain significantly higher than the maximum acceptable even in a three-kilometer zone.

Figure 6 shows graphs of the dependence of the content of gaseous pollutants: H₂S and methyl mercaptan (at \( y=3 \) km) before processing pig complex waste (line C₁), 15 minutes after the introduction of the alkaline reagent (line C₂), 15 (line C₃) and 45 (line C₄) minutes after the introduction of the acidifying reagent.
Figure 6. The contents of gaseous pollutants over liquid waste storages in 2-6 hours after treatment where: a) H\(_2\)S; b) CH\(_3\)SH.

The decrease of H\(_2\)S and methyl mercaptan concentrations to acceptable levels at a distance of three kilometers from the source of discharge under the worst meteorological conditions was achieved over a period of 18 hours figure 7.

Figure 7. Content of gaseous pollutants after 18 hours of treatment: a) H\(_2\)S; b) CH\(_3\)SN.

The steady state (constant concentrations of pollutants) under constant conditions occurs 18 hours after its treatment. The criterion for establishing a stationary state was the condition:

\[
\frac{c_{i+1} - c_i}{h_i} < \varepsilon
\]

which \(c_{i+1}, c_i\) - concentration in subsequent and previous time steps, \(h_i\)-time step selected \(\varepsilon=10^{-5}\).

Figure 8 shows changes in the content of gaseous pollutants in the immediate vicinity of the pig complex’s liquid waste storage facilities, after 18 hours of settling. So the concentration of H\(_2\)S was – 0.25 MPC, and methyl mercaptan-2.0 MPC. At a distance of up to three kilometers, the concentrations were 0.05 MPC and 0.9 MPC, respectively.
The structure of the mathematical model made it possible to determine the period of probable reduction of the content of gaseous substances in the atmosphere above the surface of the storage tanks at a distance of three kilometers. This period was 18h for the worst weather conditions, which is much faster than the time required for any other known options for preparing liquid organic waste from pig complexes. Thus, the reagent treatment of liquid organic waste from pig complexes in order to obtain organic fertilizers also helps to reduce emissions of pollutants and improve ecological safety.

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