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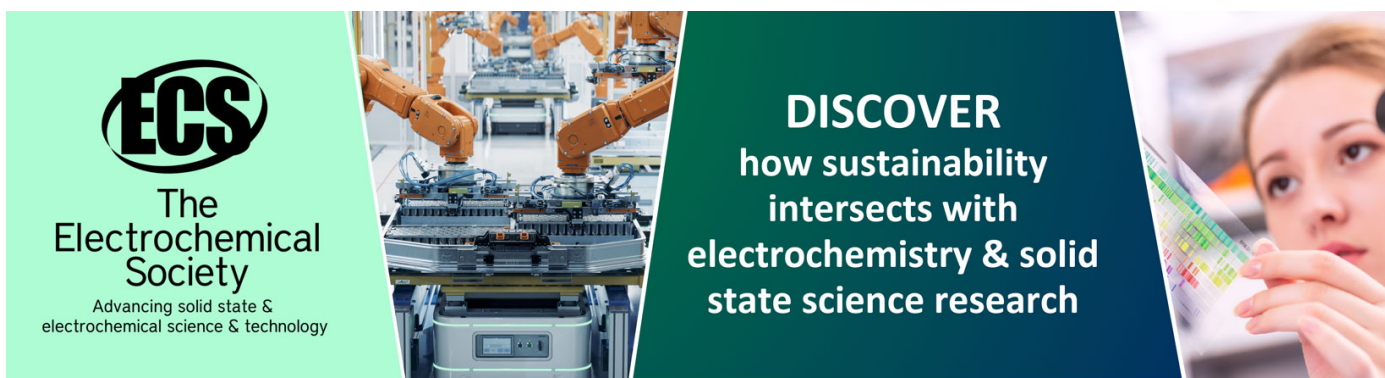
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Phenol monitoring in the air of the city residential part

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Abstract. In order to monitor the chemical composition of atmospheric air in cities located in the zone of petrochemical enterprises influence, automatic atmospheric air monitoring stations (AAAMS) are being established. The concentration of phenol and methanol in the air of the residential part of the city is recorded at AAAMSs. In the industrial zone air, the methanol content is measured at the source of pollution. Processing the numerical series of the measured concentrations values using the cross-correlation function allows you to get the time lag of the contaminated gas cloud moving from the source of emission to the city. Models have been developed for changes in concentration of phenol in the air of the residential area using the factor regression method, taking into account the concentration of the analyzed compounds, the time lag from the source of pollution to the living area and weather conditions: - air temperature and humidity, wind direction and speed.

1.Introduction

Phenol is one of the large-tonnage products of basic organic synthesis. Global phenol production capacities exceed 8.5 million tons per year [1]. In 2018, more than 201 thousand tons of phenol was produced in Russia [1]. The most significant uses of phenol are the production of bisphenol A and phenol-formaldehyde resins - more than 70% of global consumption [1]. About 10% of phenol is used in the production of caprolactam [1]. Phenols enter the environment in various ways: as a result of processing solid fuels, in the production of paper, paints and varnishes, the production of phenol-formaldehyde resins, adhesives, and various plastics. Powerful anthropogenic sources of phenol in atmospheric air are oil producing, coke, metallurgical plants, production of asphalt concrete, engineering. The amount of phenols emitted into the atmosphere by coke production is determined by the technology of processing coal and its secondary products, the quality of coal, and especially the means used for de-phenolization of wastewater [1]. Significant atmospheric phenol pollution also occurs during forest fires.

In general, the effect of phenol and its homologs on the environment in general and the human body in particular is manifested not only as a result of its release into the environment from the stage of its receipt and processing [1], but also as a result of biogenic processes, for example, the life of hydrobionts [1]. The concentration of phenol in atmospheric air with stable operation of the enterprise depends on the prevailing weather conditions. Observations show that even with constant volumes and compositions of industrial and transport emissions as a result of the influence of meteorological conditions, air pollution levels can vary by several times [1].

Phenols are one of the most common environmental pollution and are considered highly hazardous



to the environment. This compound causes a violation of ecological systems, the recovery period of which, after the complete elimination of the source of harmful effects, is at least 30 years [2,3].

The toxic effect of phenols is manifested at the cellular level (impaired respiration, pigmentogenesis, protein biosynthesis; membrane barrier functions) and at the body level (suppression of growth and reproduction in algae, impaired equilibrium, respiration, loss of motor activity in fish, etc.). The discharge of phenolic waters into water bodies and streams sharply worsens their general sanitary condition, influencing living organisms not only by their toxicity, but also by a significant change in the regime of nutrients and dissolved gases (oxygen, carbon dioxide) [1].

Therefore, monitoring the air of residential areas of urban areas adjacent to petrochemical plants for the production and processing of phenol and its derivatives seems to be a necessary task.

2. Materials and research methods

The objects of the study were the values of phenol concentration measured in the period of 2010–2012 at an automated atmospheric air control station (AAAMS) located in the residential part of the city, and methanol concentrations recorded at the enterprise's emission source. The content of pollutants in the air of the residential area is recorded by control sensors configured to measure every 3 minutes. A chromatograph installed at the enterprise's emission source records the methanol content every 10 minutes. Arrays of hourly values of meteorological parameters were obtained, such as wind direction and speed, air pressure and humidity. To process the statistical results, a correlation and regression analysis of numerical series was used. [5–8]

To determine the influence of the source on the methanol content in the atmosphere of the residential zone, a cross-correlation function was used to determine the time it takes for the methanol polluting the air to reach the atmosphere from the source of the methanol. With its help, the relationship between the time series of the phenol concentration in the residential area and methanol at the source of industrial emissions is displayed, which allows taking into account the delay between the emission and the increase in phenol content in the residential area of the city. Due to the influence of meteorological parameters, the value of the concentration of a substance in the residential area is currently determined by both its current methanol content at the source of emission and the value shifted for some time. [2,3]

3. Results and discussion

The industrial zone is a compact location of a complex of petrochemical enterprises, which include industries that use phenol and methanol as starting materials. In the air of the industrial zone, the phenol content is not recorded, and only the methanol content is recorded. In this regard, it seems interesting to carry out modeling of the phenol content in the atmosphere, based on its content in the residential area, taking into account the methanol content in the air of the industrial zone and weather conditions - temperature, humidity, wind direction and speed.

The industrial zone is located north of the residential area of the city. Therefore, the direction of the wind acquires a significance in the qualitative and quantitative chemical composition of the atmosphere of the residential area.

Using cross-correlation functions between the concentrations of phenol (residential zone) and methanol at the source of atmospheric pollution (industrial zone), it was found that in recorded weather conditions (north wind 2 - 3 m/s, temperature 8° C, humidity 80%), the phenol content is determined by the concentration methanol in the discharged gas mixture at a given time and in the previous hour (Fig. 1). Therefore, in the equation for modeling the concentration of phenol (lvl 1 and 2), in addition to meteorological parameters, the methanol concentration at the source at the initial moment and in the previous hour is included.

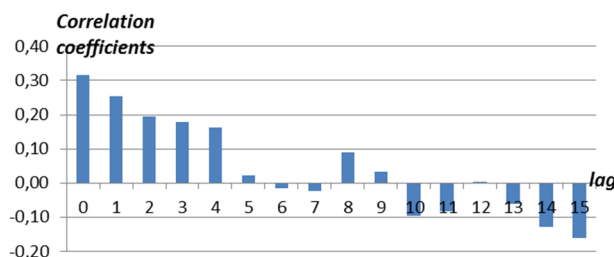


Figure 1. Correlation coefficients for cross-correlation functions linking the concentrations of methanol at the source of pollution and phenol at AAAMS (weather conditions: north wind 2 - 3 m/s, temperature 8°C, humidity 80%)

The obtained equations allow us to calculate the phenol content in the atmosphere as a function of methanol concentrations at the indicated time points and the values of the weather parameters:

$$q_{C_6H_5OH} = -0.14v - 0.002\varphi + 0.06I_0 + 0.04I_1 + 0.023vT - 0.012vI_0 - 0.004TI_0 - 0.0002\varphi I_0 - 0.0017vI_1 - 0.001TI_1 - 0.0003\varphi I_1 - 0.003I_0I_1 + 0.0008vTI_1 + 0.00002v\varphi I_0 - 0.0004vI_0I_1 + 0.000003\varphi TI_0I_1 \quad (1)$$

Coefficient of determination (correlation) 0.65 (0.8)

$$q_{C_6H_5OH} = -0.00004v - 0.00002T + 0.000005\varphi + 0.00014I_0 - 0.00008I_1 \quad (2)$$

Coefficient of determination (correlation) 0.11 (0.33) (2),

T - air temperature, °C;

v - wind speed, m/s;

φ - air humidity, %;

I_0 - methanol concentration at the source at time t, mg/m³;

I_1 - methanol concentration at the source at time t-1, mg/m³.

A comparison of the calculated (model) and recorded phenol concentration in the air of the residential area (Fig. 2) allows us to note a satisfactory coincidence of these parameters when using equation (1), the correlation coefficient is about 0.8. The calculation according to equation (2) does not transmit experimental data, the correlation coefficient is about 0.33 (Fig. 2).

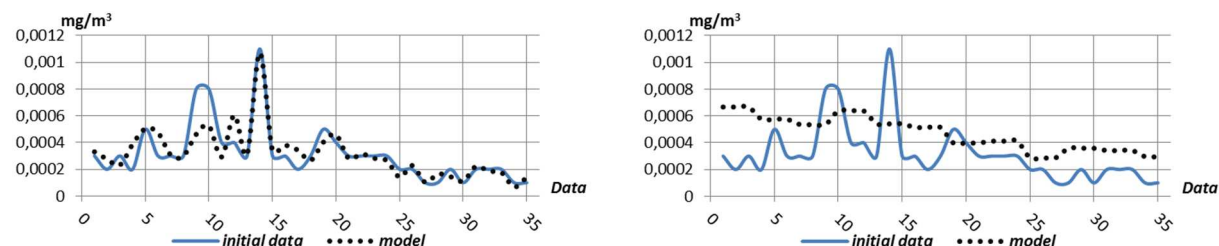


Figure 2. The phenol content in the air of the residential area recorded experimentally and calculated according to equations 1 and 2.

Meteorological conditions associated with the absence of wind - calm, 13°C, humidity 90%, are characterized by surface inversion of air masses. It can be assumed that the influence of industrial pollution sources is determined with a long delay. Observations show that the methanol content does not exceed established standards in the residential area, while its average concentration at the source was 7.9 mg/m³. In the atmosphere of the residential area, cases of exceeding the MPC of phenol were recorded.

Using cross-correlation ratios, it was found that the closest relationship between the phenol content in air and the methanol content at an industrial source corresponds to periods of 13 and 14 hours (Fig. 3).

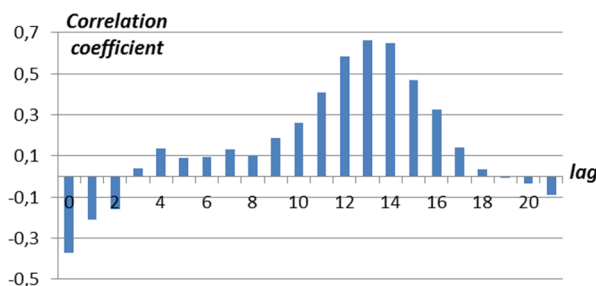


Figure 3. View of the cross-correlation function between the concentrations of methanol at the source of pollution and phenol at AAAMS under weather conditions: calm, temperature 13°C, humidity 90%.

$$q_{C_6H_5OH} = 0.02T - 0.0003\varphi + 0.18I_{13} - 0.0002T\varphi + 0.01TI_{13} - 0.002\varphi I_{13} - 0.09I_{14} + 0.0001I_{13}I_{14} - 0.006TI_{14} + 0.001\varphi I_{14} - 0.0001\varphi TI_{13} + 0.00007\varphi TI_{14} + 0.000007 TI_{13}I_{14} \quad (3)$$

Coefficient of determination (correlation) 0.71 (0.84)

$$q_{C_6H_5OH} = 0.0001T + 0.00003\varphi + 0.0006I_{13} + 0.0001I_{14} \quad (4)$$

Coefficient of determination (correlation) 0.44 (0.66)

T - air temperature, °C;

φ - humidity, %;

I_{13} - methanol concentration at the source at time t - 13, mg/m³;

I_{14} - methanol concentration at the source at time t - 14, mg/m³

These equations (3) and (4) describe the dependence of the phenol concentration on the selected parameters with a fairly high degree of coupling, having correlation coefficients of 0.84 and 0.66, which determine the similarity of the calculated and experimentally recorded values (Fig. 4).

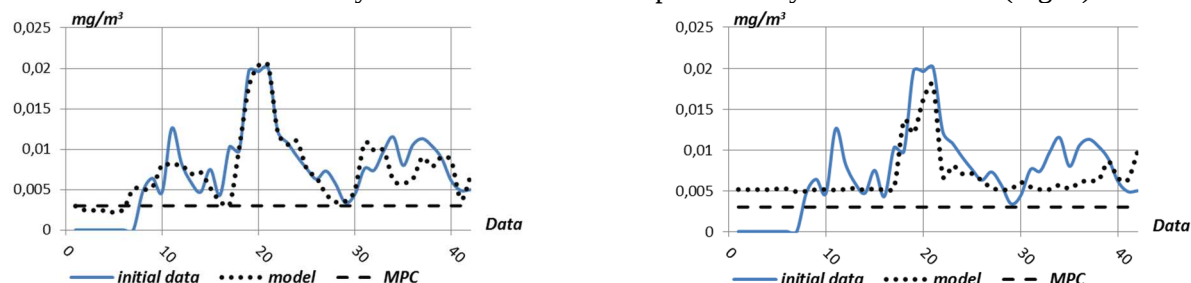


Figure 4. The phenol content in the air of the residential area recorded experimentally and calculated according to equations 3 and 4.

In the time series of observations, there are periods that are characterized by relatively low concentrations of phenol in the air of the residential part of the city. For example, under weather conditions: calm, 11° C, humidity 71%, the average concentration of phenol in the air in the residential area is 33% of the MPC, while in the previous observation period it exceeds the MPC by 230%.

In the period under consideration, there is no movement of air masses, therefore, there is a delay in the influence of pollution sources on the quality of atmospheric air in residential neighborhoods. The time for phenol to reach the residential part of the city is 12 - 13 hours (Fig. 5).

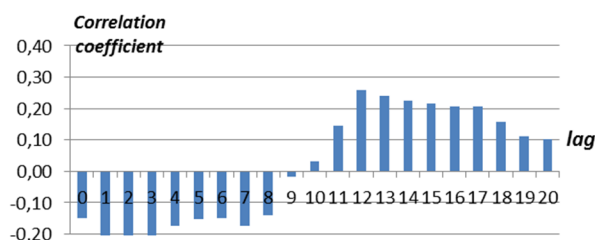


Figure 5. View of the cross-correlation function between the concentrations of methanol at the source of pollution and phenol at AAAMS under weather conditions: calm, temperature 11°C, humidity 71%.

Therefore, when constructing a model of phenol concentration changes, the methanol content at the source with a lag of 12 and 13 hours is used as parameters.

$$q_{C_6H_5OH} = -0.135T - 0.03\varphi - 0.026I_{12} - 0.0006T\varphi + 0.026TI_{12} + 0.006\varphi I_{12} + 0.009I_{13} + 0.028TI_{13} + 0.006\varphi I_{13} + 0.003I_{12}I_{13} + 0.0001\varphi TI_{12} + 0.0001\varphi TI_{13} - 0.005TI_{12}I_{13} - 0.001\varphi I_{12}I_{13} - 0.00003\varphi TI_{12}I_{13} \quad (5)$$

Coefficient of determination (correlation) 0.92 (0.96)

$$q_{C_6H_5OH} = 0.00012T + 0.00006\varphi - 0.0005I_{12} + 0.0001I_{13} \quad (6)$$

Coefficient of determination (correlation) 0.30 (0.54)

T - air temperature, °C;

φ - humidity, %;

I_{13} - methanol concentration at the source at time t - 13, mg/m³;

I_{14} - methanol concentration at the source at time t - 14, mg/m³

Comparison of the calculated phenol concentration values according to equation 5 with the experimentally obtained results allows us to obtain a correlation coefficient of 0.96, which indicates a high bond strength. According to equation 6, the correlation coefficient is 0.54.

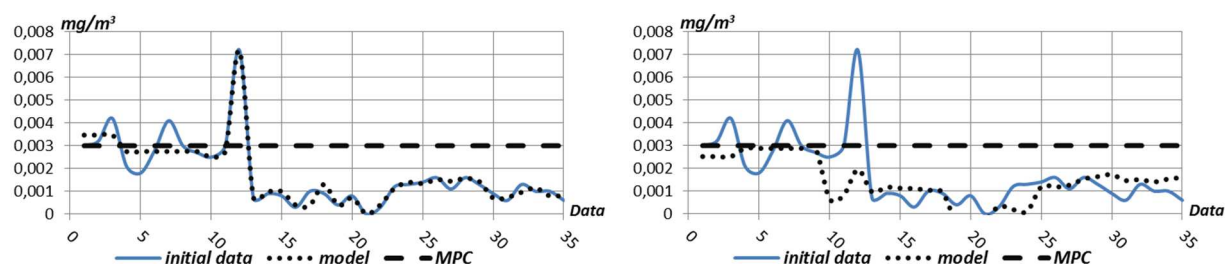


Figure 6. The phenol content in the air of the residential area recorded experimentally and calculated according to equations 5 and 6.

The south wind provides the movement of air masses from the residential area of the city towards the industrial one. In this case, there is no direct effect of methanol and phenol emissions on the formation of the atmosphere composition of the residential area. Indeed, the average concentration of methanol at the source is 5.48 mg/m³, and the phenol in the residential area is 0.003 mg/m³. However, observations of a change in the phenol content at AAAMS show that even in such periods, the phenol concentration in the residential area may exceed the MPC (Fig. 7).

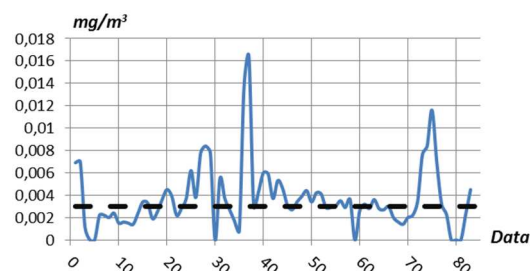


Figure 7. The phenol content in the air of the residential area recorded experimentally under weather conditions: south wind 2-4 m / s, temperature 1°C, humidity 63%

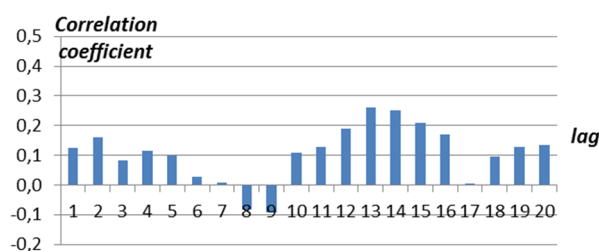


Figure 8. Type of cross-correlation function between the concentrations of methanol at the source of pollution and phenol at AAAMS under weather conditions: south wind 2-4 m / s, temperature 1°C, humidity 63%

Using the cross-correlation function between the concentrations of methanol at the source of pollution and phenol at AAAMS, it is not possible to establish the delay time for the appearance of phenol in the residential area of the city (Fig. 8). Similar results for similar weather conditions were obtained: south wind 3–5 m/s, temperature 9°C, humidity 79% (Fig. 9 and 10)

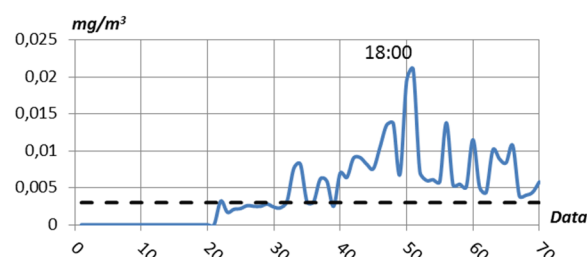


Figure 9. The phenol content in the air of the residential area recorded experimentally under weather conditions of south wind 3 - 5 m/s, temperature 9°C, humidity 79%

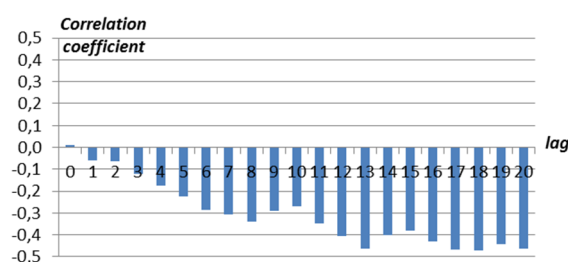


Figure 10. View of the cross-correlation functions between the concentrations of methanol at the source of pollution and phenol at AAAMS under weather conditions: south wind 3–5 m/s, temperature 9°C, humidity 79%

In this case, it is not possible to formulate equations that adequately describe the observed changes in the phenol concentration in the residential area, and judging by the cross-correlation function (Fig. 8, 10), the industrial source of atmospheric phenol pollution should not affect the change in the concentration of the substance in the air living area in the south wind. In these cases, the presence of phenol in the air of the residential area and the excess of its concentration compared with the MPC may be due to several reasons. Firstly, due to the presence of sources of atmospheric air pollution with phenol located south of the AAAMS station. Secondly, due to the presence of stagnant zones, in which the previously received air masses containing phenol are concentrated and redistributed over the urban area when the wind direction changes.

4. Conclusion

Thus, even in the absence of experimental monitoring of the phenol content in the air of the industrial zone, it is possible to simulate this parameter in the air of the residential zone, when the methanol concentration in the industrial zone is recorded, if both compounds are raw materials in the production of petrochemical products. The adequacy of the model is ensured by taking into account weather conditions (temperature, humidity, wind direction and its strength). On the other hand, meteorological conditions can be limiting parameters when choosing models that provide the greatest degree of adequacy of calculated and experimental data.

5. Acknowledgment

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