Modeling and forecasting the dynamics of wastewater contaminant pollution by manganese (II) ions

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Abstract. Modeling and forecasting of the dynamics of wastewater contaminant pollution by manganese (II) ions is carried out. The informational basis of the technique is statistical indicators of changing in the chemical composition of raw materials and change in the mass concentration of manganese (II) ions in river water used for washing the process gas obtained by calcining limestone. The purpose of the modeling is to detect the relationship between the independent values (change in the compounds of bivalent manganese in limestones as well as change in the mass concentration of manganese (II) ions in river water) and the dependent factor (change in the volume of wastewater contaminant pollution by manganese (II) ions. For modeling, it is proposed to use the mathematical apparatus of correlation and regression analysis, in particular multiple regression. According to calculations, there is a relationship between the change in the volume of environmental pollution and the parameters of the model, that is between the change in the amount of bivalent manganese compounds in the raw material and the change in the content of manganese (II) ions in river water.

Modern society has developed a number of special measures aimed at the rational use of natural resources and environmental protection. These include environmental forecasting, environmental management, environmental legislation, environmental monitoring etc. At present, forecasting is one of the basic principles of rational nature management and environmental protection. Environmental forecasting is the prediction of changes in natural systems under natural conditions or under the influence of humans on them.

The degree of environmental pollution is closely related to a number of significant factors. During the study of the process of calcining limestone raw materials for the production of soda ash, when cleaning process gas in wet scrubbers and electrostatic precipitators, a tendency to increase in the amount of manganese compounds in wastewater was revealed. The study revealed that the reason for the appearance of manganese compounds is river water used for gas washing as well as change in the quality of limestone raw materials [1,2]. The purpose of modeling is to find a relationship between two independent factors (change in the proportion of impurities in natural raw materials and water used for washing process gas (river water)) and the dependent factor (change in the volume of environmental pollution). For modeling, it is proposed to use the mathematical apparatus of correlation and regression analysis, in particular multiple regression.

In the general case, the resulting indicator \( y \) is a function of significant \( (x_1, …, x_k) \) and insignificant \( (\varepsilon_1, …, \varepsilon_n) \) factors.
In the case of linear multiple regression, the model looks like this:

$$y = \beta_0 + \sum \beta_i x_i + \epsilon, \quad y' = y' + \epsilon,$$

where

$$G_{ij}(T) = G_{ij}(R_i \cdot V_j, T) + \epsilon,$$

$$G'_{ij}(R_i \cdot P_j, T) = \alpha_0 + \alpha_1 R_i(T) + \alpha_2 P_j(T),$$

$$G_{Mn}(T) = G_{Mn}(R_{Mn}, P_{Mn}, T) + \epsilon,$$

$$G'_{Mn}(R_{Mn}, P_{Mn}, T) = \alpha_0 R_{Mn}(T) + \alpha_2 P_{Mn}(T)$$

Table 1. Average content of bivalent manganese compounds in limestone, %.

| Period | Production volume on the i-th horizon, % | $R_{Mn}(T), \%$ |
|--------|----------------------------------------|-----------------|
| 1      | 0.59 0.59 0.59                       | 0.34            |
| 2      | 0.42 0.42 0.42                       | 0.36            |
| 3      | 0.33 0.33 0.33                       | 0.39            |
| 4      | 0.24 0.24 0.24                       | 0.42            |
There is no need to approximate the time series $R_{Mn}(T)$ since on the basis of simplified limestone mining scheme, the values of the analyzed parameter have already been obtained in the forecast periods. In addition to dynamics of the change in the amount of the impurity component in the initial natural raw material $R_{Mn}(T)$ which affects the change in the volume of waste generation, in order to describe the desired model it is necessary to know how the composition of the river water used for washing the process gas changed. Table 2 shows data for modeling changes in the volume of environmental pollution.

| No. | Values                                      | 1      | 2      | 3      | 4      |
|-----|---------------------------------------------|--------|--------|--------|--------|
| 1   | Content of bivalent manganese compounds in limestone, $R_{Mn}(T)$, t | 70.95  | 96.08  | 81.95  | 89.58  |
| 2   | Change in $R_{Mn}(T)$ to the previous period, % | -      | 108.33 | 107.69 | 107.14 |
| 3   | Change in $R_{Mn}(T)$ to the base period, %   | 100    | 108.33 | 116.66 | 125.00 |
| 4   | The content of manganese compounds in river water, $P_{Mn}(T)$, t | 0.094  | 0.027  | 0.074  | 0.047  |
| 5   | Change in $P_{Mn}(T)$ to the previous period, % | -      | 28.72  | 264.28 | 63.51  |
| 6   | Change in $P_{Mn}(T)$ to the base period, %   | 100    | 28.72  | 78.72  | 50.00  |
| 7   | The amount of manganese $\Delta G_{Mn}$ in wastewater, t | 0.120  | 0.056  | 0.112  | 0.085  |
| 8   | Change $\Delta G_{Mn}$ to the previous period, % | -      | 46.66  | 200.00 | 75.89  |
| 9   | Change in $\Delta G_{Mn}$ to the base period, % | -      | 46.66  | 93.33  | 70.83  |

The calculation of coefficients of the regression line and additional regression statistics based on the data given in the table below was carried out using the LINEST function of the MS Excel analysis package. The calculation results are shown in table 3.

Table 3. The results of calculating the coefficients of the regression equation and additional regression statistics of the LINEST function.

|   | 1       | 2       | 3       |
|---|---------|---------|---------|
| 1 | $\alpha$ | $\alpha$ | $\alpha$ |
|   | 1.0795  | 0.00058 | 0       |
| 2 | $S_{e_2}$ | $S_{e_1}$ | $S_{e_1}$ |
|   | 0.1089  | 0.00015 | 0       |
| 3 | $R^2$   | $S_y$   |         |
|   | 0.961   | 0.012   |         |
| 4 | $F$     | $D_f$   | 2       |
|   | 25.10   | 2       |         |
| 5 | $SS_{reg}$ | $SS_{res}$ |         |
|   | 0.0074  | 0.00029 |         |

The equation will take the form:
\[ G_{Mn}(R_{Mn}, P_{Mn}, T) = 0.00058 R_{Mn}(T) + 1.079 P_{Mn}(T) \] (8)

R^2 (coefficient of determinateness) is close to one (1) which means there is a complete correlation with the model, i.e. there is no difference between actual and estimated y values.

The value of the Fisher criterion calculated in MS Excel (table), F = 25.10 is greater than the tabular value of the F-distribution (k_1 =2, k_2 =3) for the significance level \( \alpha =0,05 \) (F=9.55). Thus, according to Fisher's criterion, the equation is significant. There is a relationship between the change in the volume of environmental pollution and the parameters of the model, i.e. between the change in the amount of bivalent manganese compounds and the change in the content of manganese compounds in river water [3-6].

References
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