IOP Conf. Series: Materials Science and Engineering **775** (2020) 012092 doi:10.1088/1757-899X/775/1/012092

Method for predicting trihalomethanes content in drinking water (by the example of surface type water intake)

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Abstract. The search for predicting the concentration of trihalomethanes in drinking water equations of the surface water intake was carried out. The turbidity, chromaticity, permanganate oxidation of the water source and the dose of chlorine are taken as dependent parameters.The listed parameters are an indirect reflection of the gunim substances presence in the water source. These substances are precursors for the formation of trihalomethanes. In addition, it was found an equation by which it is possible to predict the dose of chlorine depending on the unlisted generalized indicators of water quality. The coefficients of determination of the obtained equations vary between 0.78 - 0.96, and the average relative forecast error is 6.5 - 19.3%.

1. Introduction

The quality of drinking water often does not meet the standards adopted in the Russian Federation. High anthropogenic pressure on water bodies leads to a deterioration in the water source quality.

One of the most important requirements for water quality is the absence of pathogens of infectious, parasitic diseases and helminthic invasions.Therefore, there is a need for their disposal. Chlorination is the most common and reliable method of drinking water disinfection. However, this method leads to the formation of chlorination products — organohalogen compounds — most of which are trihalogenomethanes (THMs). This group of compounds includes chloroform $CHCl_3$ (CF), bromodichloromethane $CHBrCl_2$ (BDCM), dibromochloromethane $CHBr_2Cl$ (DBCM) and bromoform $CHBr_3$ (BF)[1-10].

THMs components can have a significant negative effect on public health. They have a toxic polymorphism and the ability to cause long-term effects, such as carcinogenesis. The great interest in the qualitative and quantitative content of THM in drinking water is due to two reasons. The first reason is related to the specific effects of the substances of this group on the human body. The second reason is related to the mass population in Russia and abroad, consuming and using drinking water for many years, the technological disinfection process of which included the stage of chlorination [4-6,11,12].

It seems appropriate to conduct a study to find the existence of a relationship between the content of TGM in drinking water from some indicators of water quality. In particular,

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generalized indicators can serve as such indicators: turbidity, chromaticity, and permanganicoxidizability of the water source. Turbidity of water is an indicator characterizing a water transparency decrease due to the presence of inorganic and organic finely dispersed suspensions, as well as the development of planktonic organisms. Chromaticity is an indicator that characterizes the intensity and degree of color of water. Chromaticity is a natural property of water, which is due to the fact that humic substances and complex compounds of iron are present in it. Permanganate oxidizability is an indicator of the content in water of organic and mineral substances that hold the conversion of iron from divalent to trivalent, which can be oxidized with oxygen, and allows judging the pollution of water in general. The choice of indicators is justified by the fact that they indirectly reflect the content in the water source of the main precursors of THMs - humic and fulvic acids. We used a correlation and regression analysis to obtain an equation linking the CF content in drinking water with a dose of chlorine (D_{Cl}) and some generalized indicators of water quality of the water source: turbidity (T), chromaticity (C), permanganate oxidizability (PO) at the surface type water intake. In addition to the concentration of CF, dependent parameters are the total concentration of THMs (THM) components and the total concentration of THMs, calculated from the content of atomic chlorine (THM (Cl)) [13,14].

2.Materials and research methods

When searching for equations, we used correlation and regression analysis.

The multiple regression equation can be represented as:

$$Y = f(\beta, X) \tag{1}$$

where X - the vector of independent variables,
β -the vector of parameters (to be determined),
Y -a dependent (explained) variable.

The linear equation of multiple regression has the form [15]:

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \ldots + \beta_m X_m \tag{2}$$

where β_0- the free term that determines the value of Y, in the case when all the variables X_j are equal to 0.

The initial data were the analytical control of these indicators, calculated as the average monthly (1997-2016).

The contribution of TGM (Cl) is calculated by the formula:

$$\text{THM (Cl))} = m_{DBCM}\cdot(M_{DBCM})^{-1}\cdot 35{,}5\cdot 1 + m_{BDCM}\cdot(M_{BDCM})^{-1}\cdot 35{,}5\cdot 2 + m_{CF}\cdot(M_{CF})^{-1}\cdot 35{,}5\cdot 3 \tag{3}$$

where m - the content of the THMs component, μg / dm^3;
M -the molar mass of the THMs component, g / mol;
1,2,3 - the number of Cl atoms in the molecules $CHBr_2Cl$, $CHBrCl_2$, $CHCl_3$, respectively.

This calculation allows determining how much total atomic chlorine is contained in the components that make up the THMs.

3. Results and discussion

The calculation of the correlation coefficients reveals a high bond strength between the chlorine dose and the concentrations of CF, THM, THM (Cl), which confirms the determining effect of the chlorine dose on the formed THM amount (table 1).A moderate relationship was found between the time series of average monthly concentrations of D_{Cl} and T, C, and PO. The remaining bonds are weak.

The calculation of the correlation coefficient between the independent parameters showed a noticeable relationship between the time series «C - D_{Cl}», «PO - D_{Cl}», a high relationship between the series «T - C», «T - PO» and a very high relationship between the parameters «C - PO» (table 2).

Table 1. Results of paired calculating correlation coefficients between the mean monthly values THM, THM (Cl), D_{Cl}, and T, C, PO on the surface intake

Parameter	D_{Cl}	T	C	PO
CF	0,82	-0,37	0,04	0,19
THM	0,82	-0,37	0,04	0,19
THM (Cl)	0,81	-0,38	0,03	0,18
D_{Cl}	-	0,57	0,68	0,68

Table 2. Calculation results of paired correlation coefficients between the independent parameters D_{Cl} and M, C, O at the surface water intake

	D_{Cl}	T	C	PO
D_{Cl}				
T	0,11			
C	0,57	0,72		
PO	0,68	0,71	0,98	

Using correlation and regression analysis, there were found the equations that relate the concentration of trihalomethanes, chloroform, and the dose of chlorine with generalized indicators of water quality. The obtained result allows identifying high values of the coefficient of determination of 0.83 - 0.91 and low values of approximation errors (6-11%) (Table 3).The equation for chloroform was found because chloroform has a greater value of the true concentration of THM in comparison with organobromine THM.

Table 3. Main results of the correlation and regression analysis between the monthly average values of the parameters TCM, TGM, TGM (Cl), DSl, M, C, O on the surface water intake

Equation	R^2	F	S	A,%
CF = -13,45 + 23,04 D_{Cl} - 0,67 T - 2,18 C + 18,34 PO	0,96	38,6	3,8	10,6
THM = -9,88 + 22,93 D_{Cl} - 0,77 T -2,59 C + 21,78 PO	0,94	33,4	4,4	10,5
THM (Cl)= -11,22 - 20,52 D_{Cl} -0,62 T -2,01 C + 16,87 PO	0,78	12,9	7,6	19,3
D_{Cl} = 0,57- 0,03 T - 0,08 C + 1,04 PO	0,90	25,9	0,2	6,5

R^2- the coefficient of determination;
S -the estimate of standard deviation;
F - F-statistics of the Fisher distribution;
A -the average relative error of approximation;

The equations are significant at values of T - 0.5 - 60 mg / dm^3, C - 5 - 83^{0}C, PO - 0.9-8.2 mg / dm^3, D_{Cl} - 0.6 - 3.5 mg / dm^3.

The analysis of the equations for predicting the concentration of chloroform and the THMs total concentration in drinking water shows that the chlorine dose is the determining parameter of the choice environment.Analysis of the equation obtained for predicting the chlorine dose from the generalized indicators of the water source water quality shows that the free term of the equation is decisive.In the equation for predicting the total content of THM calculated by chlorine, the dominant parameter is permanganate oxidation.

4. Conclusion

The obtained equations have a high determination coefficient and a low approximation error. Thus, high values of the determination coefficients and low values of the approximation error allow using the obtained regression equations for long-term prediction of the concentration of

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THMs and components, as well as the dose of chlorine. This is important from a technological point of view for water treatment enterprises.

5. Acknowledgments

The work was performed within the framework of the State Task No. 5.12863.2018 / 8.9 "Development of a system for identification and quantitative analysis of environmental risks arising from the water supply of a large urban agglomeration".

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