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Control Method of Environmental Pollution Caused by Chemical Elements Based on Computer Simulation Method

Jixiang Luo^{a,b}

^aThe Faculty of Civil Engineering and Architecture, Nanchang Institute of Technology, Nanchang 330099, China ^bJiangxi Provincial Key Laboratory of Hydraulic & Civil Engineering Infrastructure security, Nanchang Institute of Technology, Nanchang 330099, China 48260308@qq.com

The environmental pollution caused by chemical elements not only exerts adverse impact on agricultural production and livestock and poultry raising, but also endangers the health of the human beings, which must be taken seriously. It is of great practical significance to study the environmental pollution caused by chemical elements. Based on the computer model method, this paper uses nitrogen as an example to establish a model of pollution process simulation and study the environmental pollution caused by chemical elements and the control methods. The results show that the environmental pollution caused by nitrogen can be divided into natural sources and human sources. For the Yellow River Basin, the biggest source of pollution is rural life and the application of nitrogen fertilizers; the export coefficient of applied nitrogen fertilizer is the highest while the export coefficient of soli nitrogen pool is the lowest; the key control period of different pollution sources in the Yellow River Basin is different and the key control period of natural sources is the rainy season while the key control period of human sources is the emission period. The control effect of reducing pollution sources of equal quantity on environmental quality is different. When the pollution source is reduced by 40% and 60% respectively, the most significant response of river nitrogen concentration is the atmospheric sedimentation. The research results provide a scientific theoretical basis and effective countermeasures for the treatment of environmental pollution caused by chemical elements.

1. Introduction

With the continuous development of economy in China and the accelerating industrialization process, China's environmental pollution problems are increasing and have become more severe. China is a big agricultural country and environmental pollution caused by the abuse of chemical fertilizers and chemical feeds in rural areas is particularly serious (Gluhoi et al., 2004). The environmental pollution caused by chemical elements not only exerts adverse impact on agricultural production and livestock and poultry raising, but also endangers the health of the human beings, which must be taken seriously. It is not easy to perceive the environmental pollution caused by chemical elements at the moment, but once it occurs, the consequences will be extremely serious (Gu et al., 2012). It is of great practical significance to study the environmental pollution caused by chemical elements and propose targeted control measures (Wolterbeek and Verburg, 2004).

At present, domestic and foreign scholars have carried out a large quantity of analysis and research on the environmental pollution and control of chemical elements and have formed a series of fruitful research achievements. Some scholars have studied the types and manifestations of pollution caused by chemical elements (Radford et al., 2000; Zhao et al., 2014); some scholars have studied the harm and negative impact of chemical elements (Fang et al., 2007; Rautio and Huttunen, 2003); scholars have studied how to reduce the environmental pollution caused by chemical elements and the control of environmental pollution. Research (Ettler et al., 2008). Based on the computer model method, this paper uses nitrogen as an example to study the environmental pollution caused by chemical elements and the control methods, which provides a scientific theoretical basis and effective countermeasures for the treatment of environmental pollution caused by chemical elements.

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2. Introduction of Relevant Theories

2.1 Computer Simulation Method

With the continuous development of science and technology, computers have been widely applied in various fields. Among them, computer simulation is a very important computer application. It can stimulate various situations in the real world and analyze these situations, which can facilitate people's understanding of the real world (Świergosz et al., 1998).

The objects of computer simulation can be all-encompassing and the simulation methods are also very different. But no matter what kind of simulation method is used, the most important thing is to build a model for the simulated object, relying on more specific mathematical or physical models to simulate the model trough model programming (Cabeza and Rodriguez, 1996). In general, the following two methods are included:

The first is the determinate method, which is to establish a determinate model for a specific simulation object.

The second is the random method, also known as the Monte Carlo method. The basic idea is that if the problem to be solved is the probability of occurrence or the expected value of a random variable, the probability of this random event can be estimated by the frequency of such occurrence through some kind of "trial" method or some numerical characteristics of the random variable can be obtained as the solution to the problem (Giordano et al., 2005).

This paper mainly establishes the SWTA model for computer simulation. The specific formula is as follows:

$$R_e = \frac{Q_s - Q_m}{Q_m} \times 100\% \tag{1}$$

$$R^{2} = \frac{(\sum_{i=1}^{n} (Q_{m} - Q_{avgm})(Q_{s} - Q_{avgs}))^{2}}{\sum_{i=1}^{n} (Q_{m} - Q_{avgm})^{2} \sum_{i=1}^{n} (Q_{s} - Q_{avgs})^{2}}$$
(2)

$$E_{ns} = 1 - \frac{\sum_{i=1}^{n} (Q_m - Q_s)^2}{\sum_{i=1}^{n} (Q_m - Q_{avgm})^2}$$
(3)

In this formula, Q_m and Q_{avgm} represent the observation value and the average value respectively; Q_s and Q_{avgs} represent the analog value and the average value respectively; and n is the observation frequency. If $R_e > 0$, it means that the predicted value of the model is rather large; if $R_e < 0$, it means that the predicted value of the model is rather large; if $R_e < 0$, it means that the predicted value of the model is rather large; if $R_e < 0$, it means that the predicted value of the model is rather small; if $R_e = 0$, it means that the simulation result of the model is exactly the same as the actual measured value (Adamo et al., 2006). If $R^2=1$, it indicates that the analog value is consistent with the observed value; when $R^2<1$, the smaller R^2 is, the lower the fitting degree. E_{ns} is less than or equal to 1. The larger the E_{ns} , the higher the simulation efficiency. If $E_{ns}<0$, it indicates the simulation result is invalid (Hernout et al., 2016).

2.2 Chemical Reaction of Nitrogen

Taking soil as an example, the nitrogen forms in the soil are mainly divided into organic nitrogen and inorganic nitrogen. Among them, inorganic nitrogen mainly includes ammonium nitrogen (NH_4^+), nitrate nitrogen (NO_3^-) and nitrite nitrogen (NO_2^-).

The nitrification of soil mainly refers to the process that the microorganisms in the soil oxidize NH_4^+ to NO_3^- . The ammonia volatilization refers to the conversion of nitrogen into NH3 into the atmosphere (Awasthi, A. K., et al. 2016). The main reaction chemical formula is:

$$(NH_2)_2CO + 2H_2O \leftrightarrow (NH_4)_2CO_3 \tag{4}$$

$$(NH_4)_2CO_3 \leftrightarrow 2NH_3 + CO_3 + H_2O$$

The loss of nitrogen in the soil mainly refers to the process of chemical denitrification, which is a chemical reaction under certain special environmental conditions. For example, in terms of the volatilization of ammonia nitrogen, the reaction formula is:

$$\mathrm{NH}_4^+ + \mathrm{OH}^- \to \mathrm{NH}_3 \uparrow + H_2 O \tag{6}$$

Another example is the nitrous acid decomposition reaction, the reaction formula is:

 $3HNO_2 \rightarrow HNO_3 + 2NO \uparrow +H_2O$

(7)

(5)

3. Research on the Control Methods of Environmental Pollution Caused by Nitrogen

In this paper, the Yellow River Basin is selected as the research object and the simulation model of nitrogen pollution process in the Yellow River Basin is established. Based on this, the nitrogen pollution in different time periods and of different land types is analyzed and corresponding pollution control measures are proposed.

3.1 Identification and Analysis of Nitrogen Pollution Sources

Firstly, the pollution sources are analyzed. The environmental pollution caused by nitrogen can be derived from many aspects. In general, it can be divided into natural sources and human sources. Figure 1 shows the contribution rate of different pollution sources to the total nitrogen pollution. It can be seen from the Figure that the biggest source of pollution in the Yellow River Basin is rural life, accounting for one-third of the total. Followed by the application of nitrogen fertilizers, accounting for 26.67%. Livestock and poultry raising accounts for the smallest proportion and the main reason is that livestock and poultry farming in the Yellow River Basin is rather dispersed and not the main pollution source. Thus, it can be seen that rural life and the application of nitrogen fertilizers are the key pollution sources in the Yellow River Basin.



Figure 1: The ratio of total nitrogen output from different nitrogen source

Secondly, the annual average export coefficient is different of different pollution sources. Table 1 shows the export coefficient of each pollution source in the Yellow River Basin. According to the data in the Table, the order of export coefficient of different pollution sources is: application of chemical fertilizers (18.44%), rural life (15.48%), livestock and poultry raising (7.14%), atmospheric sedimentation (4.26%) and soil nitrogen pool (0.058%).

	Soil nitrogen pool	Atmospheric sedimentation	Rural life	Livestock and poultry breeding	Application of nitrogen fertilizer
Nitrogen input into river (t)	732.75	68.74	924.82	248.54	896.75
Nitrogen emission (t)	1265873.24	1594.61	5974.35	3482.19	4863.24
River entry coefficient (%)	0.058	4.26	15.48	7.14	18.44

Table 1: River entry coefficient of each pollution source in the Yellow River

3.2 Identification of Key Control Periods for Nitrogen Sources

Figure 2 shows the monthly nitrogen influx of different pollution sources. As can be seen from the Figure, the maximum nitrogen influx is in August and the minimum is in January.

The relationship between the nitrogen influx caused by natural sources (soil nitrogen pool and atmospheric sedimentation) and precipitation is significant, indicating that the rainy season is a critical period for the control of natural sources. In addition to the close relationship with precipitation, the nitrogen influx caused by human sources (rural life, livestock and poultry raising and the application of chemical fertilizers) is also affected by the amount and time of emissions. The growth period of crops is from March to September, during which the influx of nitrogen fertilizers can account for more than 90% of the total annual amount.

Therefore, the key control periods of different pollution sources in the Yellow River Basin are different. It is necessary to formulate plans for different pollution sources when developing pollution control measures.





3.3 Prediction of Nitrogen Concentration in the Case of Reducing Nitrogen Emissions

(1) Scenario setting of the application of chemical fertilizers. Based on the current application amount of chemical fertilizers, three scenarios are set: the application amount of chemical fertilizers is reduced by 20%, 40% and 60%, respectively. The simulation results are shown in Table 2 and Table 3.

There is a significant relationship between the influx of nitrogen in the farmland and the application amount of chemical fertilizers. With the reduction of the application of nitrogen fertilizers, the reduction of the influx of nitrogen in the farmland is the quickest.

	Primitive nitrogen fertilizer	N-20%		N-40%		N-60%	
	River intake	River intake	Reduction rate	River intake	Reduction rate	River intake	Reduction rate
Dry land	80.32	65.76	0.192	60.15	0.267	58.94	0.293
Habitat	49.75	49.75	0.000	49.75	0.000	49.75	0.000
Woodland	16.38	16.38	0.000	16.38	0.000	16.38	0.000
Garden plot	71.59	56.75	0.251	43.57	0.427	34.58	0.596
Paddy field	44.43	39.68	0.117	37.54	0.257	31.74	0.304
Whole basin	54.96	46.32	0.169	38.57	0.274	38.41	0.395

Table 2: Nitrogen status in different nitrogen application scenarios

Table 3:	Relationship) between i	nitroaen i	input amount	t and fertil	izer application

	Relationship betweer	n nitrogen input amount and fertilizer application
Dry land	Y=0.2358x+174.38	R ² =0.8758**
Garden plot	Y=0.3192x+58.671	R ² =0.9075**
Paddy field	Y=0.1096x+396.84	R ² =0.9836**
Whole basin	Y=0.2584x+1352.75	R ² =0.9527**

(2) Scenario setting of atmospheric sedimentation. Based on the current atmospheric sedimentation in the Yellow River Basin, three scenarios are set: the nitrogen deposition is reduced by 20%, 40% and 60%, respectively. The simulation results are shown in Tables 4 and 5.

The influx of nitrogen of all land utilization types will decrease significantly with the atmospheric nitrogen sedimentation, of which the change of forest land is the quickest. There is vast area of forestland in the Yellow River Basin and the effective control of the atmospheric sedimentation in the forestland can effectively control the environmental pollution caused by nitrogen.

(3) Scenario setting of soil nitrogen pool. Based on the nitrogen content of the initial soil, three scenarios are set: the nitrogen pool is reduced by 20%, 40% and 60%, respectively. The simulation results are shown in Table 6 and Table 7. The influx of nitrogen of all land utilization types will decrease significantly with the 10cm nitrogen pool.

	Original nitrogen deposition	N deposition-20%		N deposition-40%		N deposition-60%	
	River intake	River intake	Reduction rate	River intake	Reduction rate	River intake	Reduction rate
Dry land	76.31	70.24	0.0769	62.74	0.1527	58.06	0.2318
Habitat	40.25	39.87	0.0612	33.05	0.2617	27.41	0.3725
Woodland	14.68	12.06	0.1895	10.27	0.3643	7.68	0.5418
Garden plot	84.02	72.54	0.0806	65.84	0.2153	60.15	0.2905
Paddy field	67.95	57.96	0.1537	49.15	0.2904	40.06	0.4257
Whole basin	57.32	50.91	0.0968	43.27	0.2361	37.94	0.3341

Table 4: Nitrogen annual River entry under different atmospheric settlement scenarios

Table 5: Relationship between nitrogen intake and atmospheric settlement

	Relationship between nitrogen intake and atmospheric settlement				
Dry land	Y=0.4308x+199.87	R ² =0.9887**			
Habitat	Y=0.4728x+78.925	R ² =0.9776**			
Woodland	Y=0.1924x+53.483	R ² =0.9937**			
Garden plot	Y=0.4381x+528.64	R ² =0.9824**			
Paddy field	Y=0.3684x+284.39	R ² =0.9795**			
Whole basin	Y=0.3724x+859.46	R ² =0.9916**			

Table 6: Nitrogen status in different nitrogen storage scenarios

	Original nitrogen library	N library-20%		N library-40%		N library-60%	
	Pivor intoko	River	Reduction	River	Reduction	River	Reduction
	River Intake	intake	rate	intake	rate	intake	rate
Dry land	76.05	72.18	0.0357	70.68	0.0644	69.14	0.0948
Habitat	41.93	41.65	0.0134	40.96	0.0249	41.85	0.0374
Woodland	15.82	15.07	0.0186	15.03	0.0352	15.04	0.0525
Garden plot	84.06	82.34	0.0171	79.98	0.0327	80.31	0.0486
Paddy field	67.97	65.19	0.0395	62.87	0.0815	60.16	0.1408
Whole basin	56.91	55.04	0.0258	54.19	0.0524	52.85	0.0784

Table 7: Relationship between nitrogen input amount and 10CM soil nitrogen pool

	Relationship between nitrogen input amount and nitrogen pool content
Dry land	Y=0.0012x+286.45 R ² =0.9989**
Habitat	Y=0.0008x+193.57 R ² =0.9989**
Woodland	Y=0.00006x+486.19 R ² =0.9999**
Garden plot	Y=0.0002x+846.37 R ² =0.9992**
Paddy field	Y=0.0004x+574.16 R ² =0.9998**
Whole basin	Y=0.0003x+2874.94 R ² =0.9999**

It can be seen from the above three different scenarios that the control effect of reducing pollution sources of equal quantity on environmental quality is different. When the pollution source is reduced by 40% and 60% respectively, the most significant response of river nitrogen concentration is the atmospheric sedimentation.

4. Conclusion

(1) The environmental pollution caused by nitrogen can be divided into natural sources and human sources. For the Yellow River Basin, the biggest source of pollution is rural life and the application of nitrogen fertilizers. Because livestock and poultry raising is rather dispersed, it is not the main pollution source; the order of the influx coefficient of different pollution sources is: application of chemical fertilizers (18.44%)> rural life (15.48%)> Livestock and poultry raising (7.14%)> atmospheric sedimentation (4.26%)> Soil nitrogen pool (0.058%).

(2) The key control periods of different pollution sources in the Yellow River Basin are different. The key control period for natural sources is the rainy season and the key control period for human sources is the emission period.

(3) The control effect of reducing pollution sources of equal quantity on environmental quality is different. When the pollution source is reduced by 40% and 60% respectively, the most significant response of river nitrogen concentration is the atmospheric sedimentation.

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