A STUDY OF GIS-SD BASED TEMPORAL-SPATIAL MODELING OF WATER QUALITY IN WATER POLLUTION ACCIDENTS

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ABSTRACT:

In this paper, the one-dimension river quality system dynamics model was applied to the water quality simulation, and the conceptual GIS-SD frame was constructed. Based on the component GIS and system dynamics model, the experimental system of water quality simulation in water pollution accident was developed. The Songhua River water pollution accident which happened on November, 2005 was used as an example to show how the temporal-spatial change of nitrobenzene concentration can be dynamically simulated. The results showed that the simulation of temporal-spatial distribution of the pollutant in water pollution accident, the model regulation, and the scenario analysis can provide the decision-makers with scientific evidence to optimize the related emergency response measures.

1. INTRODUCTION

Water pollution accident is a major type of China's environmental accident. It not only causes water quality deterioration and ineffective use of water resource, but also affects the normal activities of economy and society and does serious harm to the water ecological environment. After a water pollution accident occurs, the pollutant enters the river and migrates with water current. During the transportation process, pollutant is influenced by hydraulics, hydrology, physics, chemistry, biology and other factors (Song, X. Sh., Deng, W., 2004), there is nonlinear relationship among these factors which is difficult to be expressed by conventional dynamics method. The migration and conversion of pollutants in the water pollution accident is typically a dynamic, complex, nonlinear system.

Dynamic systems are often hard to understand and difficult to model because of the interactions among the spatial elements, and the changes in the structure and function of the system over time. Traditional modelling approaches focus on either temporal or spatial variation, but not both (Ahmad, S., Simonovic, S. P., 2004). In order to better simulate dynamic, complex systems, we should be aware that the system performance in time is affected by the change of conditions in space. So we need to focus on both temporal and spatial variation. During the emergency response of water pollution accidents, the management department needs to understand the migration situation of pollution slick and the changes of pollutant concentration in both time and space as soon as possible to take effective emergency measures. Therefore, it is very important to construct a water quality model with the capability of simulating the pollutant concentration changes in both time and space simultaneously, and help decision-makers to grasp the change trends of accidents in two dimensional spaces (Zhang, B., 2007).

2. METHODOLOGY

System dynamics (SD) is a theory of system structure and a set of tools for representing complex systems and analyzing their dynamic behaviour (Forrester, J. W, 1961). The most important feature of system dynamics is to elucidate the endogenous structure of the system under study, to see how the different elements of the system actually relate to one another, and to experiment with changing relations within the system when different decisions are included. In system dynamics, the relation between structure and behaviour is based on the concept of information feedback and control (Simonovic, S. P., 2002). SD has advantage in water quality simulation due to the dynamic, complex and nonlinear characteristics of water pollution accident. It can be used to simulate and predict the water quality and model regulation in water pollution accidents (Zhang, B., 2007). Although SD models can represent temporal processes of system dynamic behaviour, it can not adequately represent and simulate the spatial elements and the state of the system. Moreover, the simulation results can only be expressed through charts, tables and other simple styles with low level of visualization (Pei, X. B., Zhao, D. Zh., 2000). Therefore, a simple SD model is clearly far from enough for a comprehensive temporal and spatial simulation of complex systems.

Geographic information system (GIS) is a computer system for collection, storage, analysis and display of spatial information, and a common technology for processing and analyzing geographic data (Chen, Sh. P., Lu, X. J., Zhou, Ch. H. 2000.).
During the integration process of water quality model and GIS, GIS is a powerful tool for spatial discretization, parameterization and visualization of water quality model (Liao, H., Tim., 1997; Ma, W. Ch., Chen, L. M., et al., 2003). Although GIS can effectively manage, query, express, analyze and process static information related to geospatial

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distribution, it is still difficult to describe and simulate the complex dynamic behaviour and process with time concept, and it can not express the dynamic characteristics of the space object. Therefore, GIS is not suitable for expressing dynamic change process in continuous time (Yu, J., Bian, F. L., et al, 2003).

3. THE ASSOCIATION AND INTEGRATION OF SD AND GIS

3.1 The requirement for the association between SD and GIS

Given the strength of SD in representing temporal processes with restricted spatial modelling capabilities, and the competency of GIS for spatial modelling with limited representation of temporal aspects, the association of SD and GIS will produce synergy effect of these two analysis technologies. Using GIS as pre-processing tool of SD model can significantly reduce data preparation and processing workload, enhance spatial data display capabilities and reveal hidden space relationship; Meanwhile, SD model can extend the spatial analysis functions of GIS, realize the dynamic simulation and trend prediction of system behaviour. By the integration of GIS and SD, the feedback based dynamic processes can be modelled in time and space (Ahmad, S., Simonovic, S. P., 2004).

3.2 The conceptual framework of SD-GIS association

The association of SD and GIS includes data association and semantic association. Data association is achieved by dynamic data exchange (DDE) through Excel, which is a two-way exchange of data and information between SD and GIS (Figure 1). Initially, GIS provides spatial information to the SD model through Excel. The SD model, through dynamic modelling, identifies changes in spatial features with time and returns them to GIS via Excel. Thus, data can be analyzed and processed in time and space in an integrated way with association of SD and GIS (Ahmad, S., Simonovic, S. P., 2001). Semantic association compares different manifestations for one variable within SD and GIS, which is realized by the spatial discretization of the calculation domain in GIS using array variables to represent level variables in SD.

If the spatial simulated object is a linear feature, the object of interest needs to be divided into sections (For example, river is divided into sections). The level variable is expressed in the form of one-dimensional array in SD. Each one-dimensional array element corresponds to the specific attribute value of each studied object sections in GIS；If the spatial simulated object is an area feature, the object of interest needs to be divided into cells (For example, lake is divided into cells). The level variable is expressed in the form of two-dimensional array in SD. Each two-dimensional array element corresponds to the specific attribute value of each studied object cells in GIS. In this way, the spatial distribution of SD level variables in GIS is determined.

Through establishing the association of SD and GIS, when SD model is running, it will calculate the value of level variables in each sections (or cells), then via dynamic data exchange (DDE), the value of level variables in each sections (or cells) can be displayed, analyzed and calculated in GIS (Zhang, B., 2007).

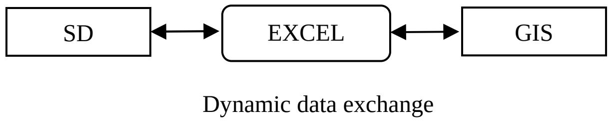

Figure 1. The data association of SD and GIS

3.3 The integration of component GIS and SD embedded software development kit

The integration of component GIS and SD embedded software development kit is one of the application based on the conceptual framework of SD and GIS association. It does not depend on specific programming language, to realize GIS functions (Song, G. F., Zhong, Er. Sh., 1998), while integrates component object of SD model as well as other auxiliary controls in a universal development environment (For example, Visual Studio 2005). In the universal development environment, data transfer between SD and GIS can be achieved without going through Excel. The attribution of the geographical object will be updated dynamically by calculating the results of the SD model through the programming language directly. The real-time display and analysis can be realized based on the updated value of the attribution in GIS.

The universal development environment is responsible for calling controls supplied by GIS component, calculating results of SD model, and interacting with the database; GIS is used for management of spatial data, and spatial visualization of model operation results; With the software development kit of SD software, SD model is called by model DLL to get the input data of simulation system. After model calculation, simulation results are called by universal development environment in the forms of tables, curves and thematic map through GIS control (Zheng, Z. M., Xia, B., Zhang, J.L., 2005), which is showed in Figure 2.

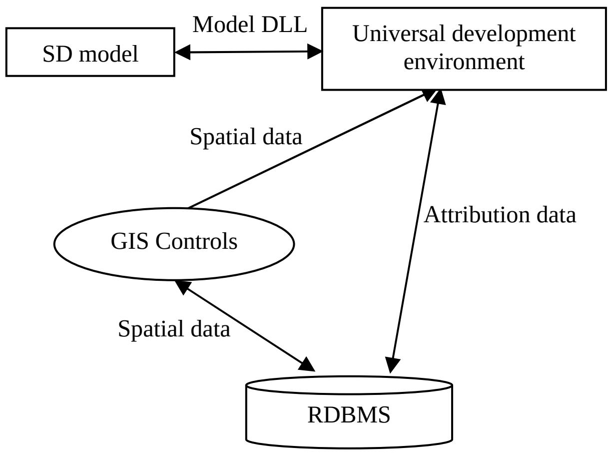

Figure 2. The integration framework of Component GIS and SD embedded software development kit

4. THE CASE STUDY OF WATER QUALITY SIMULATION IN WATER POLLUTION ACCIDENT

4.1 The study background and general situation

The Songhua River basin of 920 km long and 1070 km wide is located in the north of northeastern China, with drainage area of 556,800 km^2. The river is the largest tributary of the Heilong

River, flowing about 1,927 km from Changbai Mountains through the Heilongjiang and Jilin provinces, ending in the Amur at the town of Tongjiang. On November 13th, 2005, an explosion happened in the aniline unit of the Bi-Benzene Factory under PetroChina Jilin Petrochemical Company. The blast created an 80 km long toxic slick in the Songhua River, a tributary of the Heilong River. The slick, predominantly made up of benzene and nitrobenzene, passed through the Songhua River over the subsequent weeks, converged into the Heilong River at the mouth of the Songhua River on the border between China and Russia, then entered the Russian region and eventually into the sea.

The Songhua River has many tributaries. As the accident occurred in the winter, the tributaries had entered the period of freeze-up. So only the mainstream of the Songhua River was considered as the generalized study area. The water flow increase in mainstream of the Songhua River caused by the inflow of tributaries can be simplified by increasing the river velocity of simulated river segments. The river reach between Sujiatun section in Haerbin city and Huachuan section was selected as the study area which had five sections (Which are Sujiatun, Bayangang, Yilandalianhe, Jiamusi and Huachuan section respectively, see Figure 3) with relatively complete monitored data. The initial section is Sujiatun, and basic information of each section is shown as Table 1.

Figure 3. The distribution of study sections

No	Sections Name	Distance to Sujiatun (km)	Period of monitored data
1	Sujiatun	0	Nov 23, 21:00-Nov 27, 8:00
2	Bayangang	120	Nov 27, 6:00-Dec 2, 8:00
3	Yilandalianhe	330	Dec 2, 20:00-Dec 9, 20:00
4	Jiamusi	440	Dec 7, 20:00-Dec 12, 18:00
5	Huachuan	480	Dec 9, 12:00-Dec 14, 6:00

Table 1. The information of research sections

4.2 One-dimension SD model of river quality

SD is an approach to describe, explore and analyze the procedure, information and the boundary of organizations in complex systems. Quantitative model simulation and analysis are helpful for understanding the structure and behaviour of a system, and suitable for solving dynamic complex problems with non-linearity, causal circulation, information feedback and time-delay (Wang, Q. F., 1995).

The on-site monitored data of the Songhua River water pollution accident showed that the nitrobenzene pollutant had basically evenly mixed into the entire cross-section of the river after downstream of Harbin. It was assumed that there was no more nitrobenzene discharged into the river after the downstream of Harbin. So one-dimension water quality model can be used to forecast. The basic equation of one-dimensional water quality model is shown as follows (Peng, Z. Zh., Yang, T. X., et al, 2007):

$$\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + E_x\frac{\partial^2 C}{\partial x^2} - kC \quad (1)$$

where C (mg/L) = average concentration of pollutant
u (km/h) = vertical current velocity
E_x (km^2/h) = vertical diffusion coefficient
x (km) = distance that the river current has flowed
k (h^{-1}) = decay rate coefficient

From the explicit finite difference approach, forward difference method is used to express the first-order partial derivative of C to t, and C to x, central difference method is used to express the second-order partial derivative of C to x at moment j. Therefore, the equation (1) can be expressed as following difference equation (Fu, G. W., 1987):

$$\frac{C_i^{j+1} - C_i^j}{\Delta t} = -u_i\frac{C_{i+1}^j - C_i^j}{\Delta x} + E_i\frac{C_{i+1}^j - 2C_i^j + C_{i-1}^j}{\Delta x^2} - k_i C_i^j \quad (2)$$

where E_i = vertical diffusion coefficients of section i
u_i = vertical current velocity of section i
Δx = step in the x direction
Δt = step of the time
C_i^j = pollutant concentration of section i
k_i = decay rate coefficient of section i

The following equation can be derived:

$$C_i^{j+1} = C_i^j + (E_i\frac{C_{i+1}^j + C_{i-1}^j}{\Delta x^2} + u_i\frac{C_i^j}{\Delta x})\Delta t - (E_i\frac{2C_i^j}{\Delta x^2} + u_i\frac{C_{i+1}^j}{\Delta x}k_i C_i^j)\Delta t \quad (3)$$

It can be drawn that the concentration of section i at moment (j+1) can be iteratively calculated from the concentration of section (i+1), i, (i-1) at its previous moment j, and other parameters such as E_i, u_i, Δx, Δt. Therefore, if C_i^0 (the initial concentration of each section at moment j when j=0) and C_0^j (the concentration of the initial section at each moment) are decided, and denotes $C_{-1}^j = C_0^j$, $C_{n+1}^j = 2C_n^j - C_{n-1}^j$, then C_i^j (the concentration of each section at each moment) can be calculated iteratively.
According to the above SD theory and the equation (3), the SD model of one-dimension water quality can be constructed. The complex relationship of variables can be expressed by SD

model in graphical way, and Figure 2 is the structure of SD model using the Stella software.

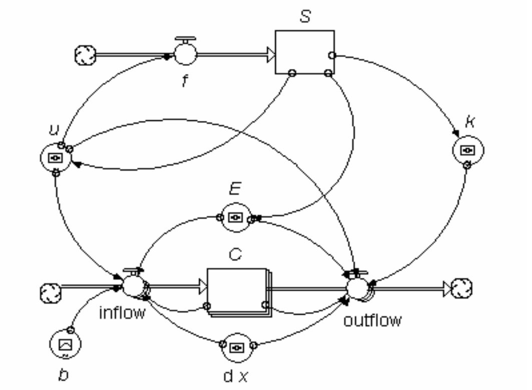

Figure 4. The structure of SD model

In Figure 4, *C*, the level variable, represents the nitrobenzene concentration in the river; Inflow and outflow are the rate variables controlling the change rate of level variable *C*; *S*, the level variable, represents the distance that river current has flowed, and *f*, which is equal to the vertical current velocity *u*, is the rate variable controlling the *S*; The auxiliary variable *b*, which is the pollutant concentration of initial section, represents the boundary conditions of the model; The auxiliary variable *k*, represents the decay rate coefficient of nitrobenzene during its migration and transformation in the river; The auxiliary variable *E*, is the vertical diffusion coefficients of simulated river sections, and the auxiliary variable d*x*, represents the length of the river sections, that is the space step of the simulation process.

4.3 The experimental system development of the water quality temporal and spatial simulation

The experimental system of the water quality temporal and spatial simulation was developed in Windows system environment, and based on the component GIS technology, SD embedded software development kit and API technology. It realized the integration of component GIS and SD model. Microsoft Visual Studio 2005 was used as the universal development environment. STELLA 9.0 and isee.NET Framework, its software development kits, were used as SD software. SuperMap Object 5 was used as component GIS. Figure 5 is the main interface of experimental system.

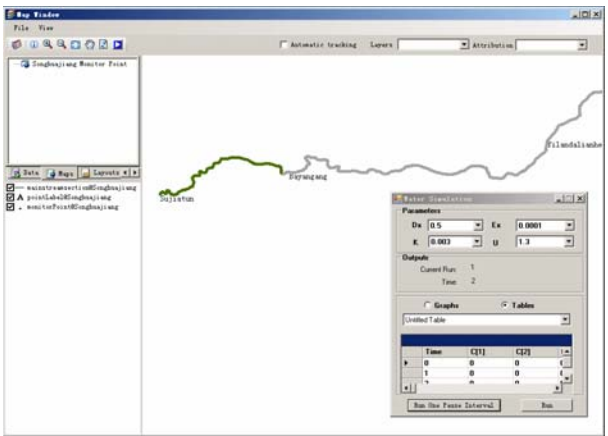

Figure 5. The main interface of experimental system

The interface mainly consists of the windows such as map display, water quality simulation, workspace management, legend management, as well as menus and toolbars and so on. The map display window is used to show the spatial distribution of study area and sections; Water quality simulation interface is mainly used for the adjustment of model parameters, the running of SD model, and the display of simulation results in forms of table and curve.

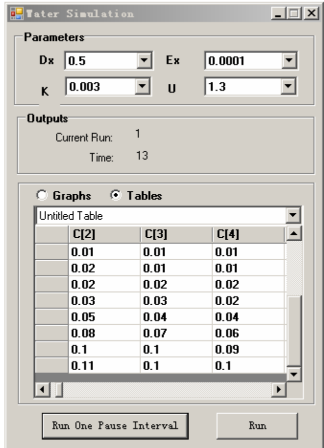

Figure 6. The water quality modelling interface of the experimental system

The Figure 6 is the water quality simulation interface of experimental system, including model parameters selection, display of model simulation calculation number, display of model simulation calculation results, and buttons. In the area of model parameters selection, the value of four parameters such as *u*, *k*, *E*, d*x* can be easily selected through a drop-down list box; The area for display of model simulation calculation number is used for displaying the running number of simulation calculation (Current Run), and the time step of each simulation (Time); The area for display of model simulation calculation results is used for showing the model calculation results, which is the nitrobenzene concentration, of different sections through a grid control; The button area is composed of two buttons: single-step running (Run One Pause Interval) and direct running (Run).

5. MODEL APPLICATION

5.1 Temporal and spatial distribution forecast of the pollutants

The temporal and spatial distribution forecast of the pollutants can be realized by simulating the change of pollutant concentration with time through the SD model, and the display the spatial distribution of concentration change in GIS. For example, the decision-makers would like to know the location and the temporal-spatial distribution of pollutant after the pollutant transfers 20 hours later. This can be achieved by selecting the button of "Run One Pause Interval" to begin simulation (Figure 6). After the model runs 20 steps, we can suspend it. The thematic maps of pollutant spatial distribution can be acquired (Figure 7).

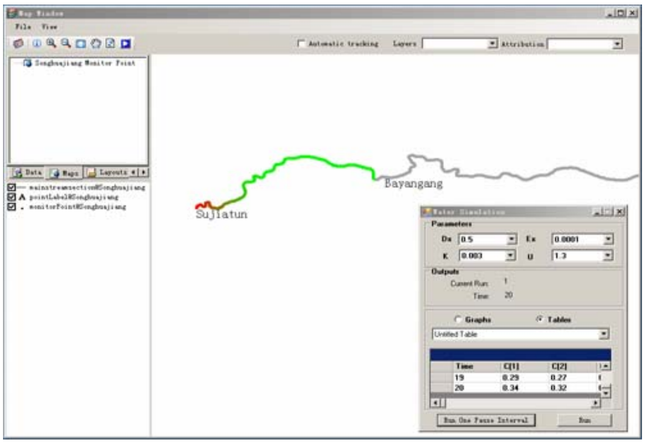

Figure 7. The spatial distribution theme map after the pollution moving twenty hours

5.2 The forecast of pollutant concentrations change over time in specific section

During the emergency response of water pollution accidents, we need to predict the pollutant concentration change over time in some important sections. Since the linear river is divided into sections, the forecast of pollutants concentration in a section can be achieved by choosing the element which represents the section of river in the state variable of SD model (Figure 8). (For example, the distance from Dalai section to the initial section is 385 km, if each section is 0.5 km long after the discretization of the river, the element of C[771] will represent the pollutant concentration of this section.)

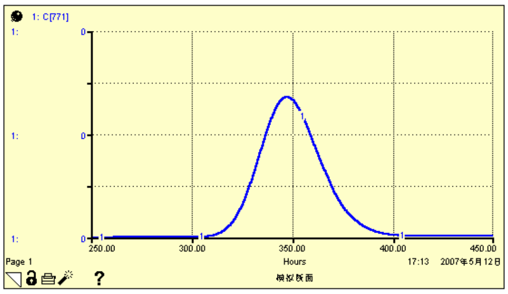

Figure 8. The pollutant concentration changes with time at Dalai section

5.3 The trend analysis of pollutant concentration change

During water pollution accidents, besides the forecast of pollutant concentrations in specific section, it is equally important to quantitatively identify the migration and transfer trend of pollutant. If lacking real-time monitoring data, the SD model may not accurately simulate of the pollutant concentration. However, in this circumstance, the model can still simulate the overall behaviour and the trend of the change of pollutants migration and transformation. Figure 9 shows the change curve of pollutant concentration over time in a certain section (Curve 1 and 2 is the simulation curve before and after adjustment of u respectively), when the velocity u decreased 50%. It can be seen from the figure that as the velocity decreases, the time when the pollutants peak passes through the certain section was 200 hours later than before, and the peak concentration will be reduced by about 50 percent.

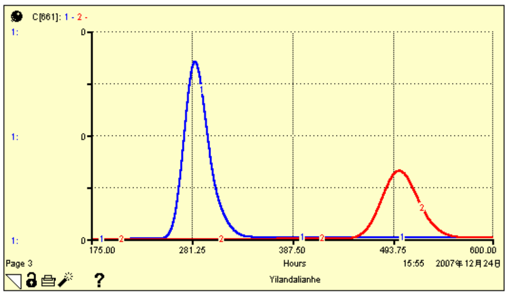

Figure 9. The change tendency of pollutant concentration after the adjustment of parameter u

5.4 The model regulation and scenario analysis

The characteristics of SD make the users to freely study the sensitivity of river system to factors or parameters and the system stability, and make multi-scheme simulation and comparison according to various conditions, in order to get the behaviour and the trend of system dynamic change with different parameters and strategies. In this paper, simulation results of two scenarios are contrasted (Zhang, B., 2007).

Scenario 1：increase the velocity u between Yilandalianhe and Huachuan section by 10%, that is, from 1.25 km/h to 1.375 km/h; meanwhile, decrease k, the decay rate coefficient, by 50%, that is, from $0.003h^{-1}$ to $0.0015h^{-1}$. The simulation result of scenario 1 is shown as Figure 10. It is shown that the time when the nitrobenzene concentration peak of Huachuan section appears decreases from 427 hours to 421 hours. In other word, the peak of nitrobenzene arrives the Huachuan section six hours earlier, and the peak concentration approximately increases by 12%. In reality, increase of velocity u can be achieved through the increased discharging of water from the reservoir, and if the temperature drops, the volatile and chemical reactions of nitrobenzene will be weakened, which will lead to the decrease of k.

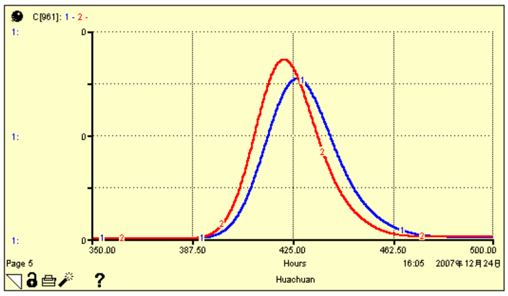

Figure 10. The simulated results of scenario 1

Scenario 2：decrease the velocity u between Yilandalianhe and Huachuan section by 10%, that is, from 1.25 km/h to 1.125 km/h; meanwhile, increase k, the decay rate coefficient, by 50%, that is, from $0.003h^{-1}$ to $0.0045h^{-1}$. The simulation result of scenario 2 is shown as Figure 11. It is shown that the time when the nitrobenzene concentration peak of Huachuan section appears increases from 427 hours to 433 hours. In other word, the peak of nitrobenzene arrives the Huachuan section six hours later, and the peak concentration approximately decreases by 15%. In reality, decrease of velocity u can be achieved through water storage of reservoir for decreasing water quantity, and if the temperature increases, the volatile and chemical reactions of nitrobenzene will be strengthened, which will lead to the increase of k.

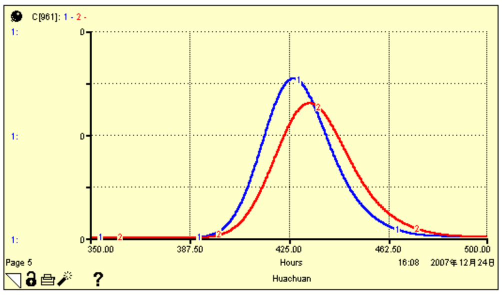

Figure 11. The simulated results of scenario 2

6. CONCLUSIONS

In this paper, system dynamics was applied to the water quality simulation of sudden water pollution accident, and the system dynamics model of one-dimension water quality simulation was constructed. The case of the Songhua river pollution accident proves that the system dynamics can be used to construct water quality model with good precision. Because the water flow and water quality are continuous in space, the temporal and spatial change of pollutants concentration can be simulated by building a one-dimension SD model using the array function of STELLA software with the river divided into many sections. This overcomes the difficulty of using a general system dynamics model to express the spatial change. The dynamic trend of change of pollutants concentration in time and space can be realized by constructing the data association and semantic association of SD and GIS. It can provide decision-makers with scientific basis to make more effective emergency response strategies in water pollution accident.

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