Modelling and Simulation of Water Pollution Diffusion with Seasonal Unsteady Input Flows: A Case Study from China

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ABSTRACT: Because of its threats to public health and the ecology, water pollution is now recognized as one of the most crucial problems facing the environment, the main source of which is industrial waste. This paper examined the diffusion principle when industrial production activities are irregular and the input flows into the river are unsteady. Under a one-point pollution source with an unsteady input flow assumption, a one-dimensional diffusion model was developed that has an initial parabolic flow condition, for which a Jacobian-matrix-based finite-difference solution method was proposed. Finally, various practical scenarios were simulated, such as varying river flow velocities and degradation coefficients, to address the severe water pollution in the Tuojiang River Basin in the upper Yangtze River Basin in China, from which several useful managerial implications were elucidated to address complex real-life scenarios.

1. Introduction

Rapid urbanization and overpopulation have led to changes in the management and use of fresh water resources [1], with river water quality and load abilities being crucial indices for the safety of river water resources because of their effect on regional environments [2]. Economic development has also increased the conflict between wastewater discharge and regional water environment carrying capacities [3]. Globally, over 420 billion cubic meters of waste water are annually discharged into rivers and lakes, and over 5500 billion cubic meters of water, or 14% of the global runoff volume, has been found to be polluted. Water quality degradation has been found to impact public health and human welfare, with more than 300 million people worldwide experiencing daily water pollution problems, 25 million of which die each year from water-related diseases. Although water quality management plans have been developed by many governments to address water pollution and the related environmental and human health problems, the effect of these measures has so far been insufficient.

One important strategy has been to first assess the pollutant diffusions and then propose targeted, efficient interventions to address the possible water pollution sources, for which water pollution diffusion models have been developed to reveal the pollutant diffusion transport in rivers [4-7]. Recent studies have focused on the water-quality modeling of either point or non-point sources [8-11], for which one-dimensional diffusion models have been used as the foundation for the diffusion investigations. For example, Zhang et al. (2004) and James (2002) examined longitudinal pollutant diffusion using one-dimensional diffusion models to simulate the diffusion process [4-5]. Other studies have developed mathematical water quality models and found several meaningful properties. Lindstrom and Boersma (1989) and Jaiswal et al. (2009) conducted several one-dimensional model scenario simulations using different initial and boundary conditions to determine analytical solutions [12-13], and Yates (1992)
investigated a one-dimensional porous media diffusion problem and determined an analytical solution \cite{14}.

However, most one-dimensional models have been based on a steady flow state assumption \cite{15\textsuperscript{-}16}, which is somewhat unrealistic as water pollution diffusion tends to be variable and unsteady rather than non-changing and stable. Various factors, such as seasonal changes, production cycles, production methods and specific geographic basin conditions can have different impacts on water pollution diffusion. For example, the liquor production factories distributed along the Tuojiang River Basin in China produce pollution input flows that differ throughout the production cycle and the seasons.

Motivated by the need to improve the water quality management in the Tuojiang River Basin, this paper developed a general one-dimensional diffusion model to account for the unstable pollutant input flows and answer the following questions.

• What is the general principle governing the pollutant diffusion for unsteady input inflows?
• Which parameters have the most significant impact on diffusion rates?
• What managerial insights can be derived to assist policy decision-makers?

The remainder of this paper is organized as follows. Section 2 presents the fundamental assumptions driving this research, develops the one-dimensional diffusion model with unsteady input flows, and proposes a Jacobian-matrix-based finite-difference method to solve the model. In Section 3, the model is applied to a practical case in the Tuojiang River Basin in China to fully investigate the diffusion principle. Section 4 gives several managerial insights for policy decision-makers to assist them in developing more effective methods to improving river water quality, and Section 5, gives the conclusions and proposes future research directions.

2. Diffusion model with unsteady input flow

2.1 Assumptions

• As shown in Figure 1, contaminant diffusion is the diffusion processes driven by water movement, such as longitudinal diffusion and turbulent diffusion; however, this paper only considered turbulent diffusion.
• The model was bounded by an assumption of a continuous one-point pollution source with a parabolic flow.
• Other influencing factors such as chemical reactions and wind are not considered.
• Only one type of contaminant is considered in the following model.

Figure 1. Different diffusion processes
2.2 Indices

- \( C \): pollutant concentration (g/m³)
- \( t \): time (s)
- \( x \): distance from a point downstream to the pollution source (m)
- \( D \): longitudinal diffusion coefficient (m²/s)
- \( E \): turbulent diffusion coefficient (m²/s)
- \( u \): river flow velocity (m/s)
- \( u_c \): friction velocity (m/s)
- \( K \): degradation coefficient (s⁻¹)
- \( \theta \): temperature coefficient

2.3 Modelling

In Figure 2, the cube represents the contaminant movement by distance \( \Delta x \) during time interval \( \Delta t \), that is, a certain amount of pollution moves \( \Delta x \) along the river during \( \Delta t \). Generally, the contaminant changes are calculated as the contaminant input minus the dispersed contaminant output. The processes driving the contaminant level changes and the relevant relationship structures are summarized in Table 1.

![Figure 2. Contaminant movement during \( \Delta t \)](image)

### Table 1. Various diffusion process factors in the

| Influencing factor | Diffusion driven by water | Longitudinal diffusion | Turbulent diffusion | Contaminant degradation |
|--------------------|---------------------------|------------------------|---------------------|-------------------------|
| factor             | average river flow        | longitudinal river movement | river fluctuation | degradation coefficient self-purification capacity of the river |
| mechanism          | contaminant movement with the river's movement | longitudinal contaminant mixing | accelerated mixing |                          |
| Mathematical relation | \(-u\frac{\partial C}{\partial x}\) | \(D\frac{\partial^2 C}{\partial x^2}\) | \(-E\frac{\partial C}{\partial x}\) | \(-KC\) |

The one-dimensional diffusion model can be described as follows:

\[
\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - u\frac{\partial C}{\partial x} - E\frac{\partial C}{\partial x} - KC
\]
The initial and boundary conditions are:
\[ C(x, t) = 0; \quad \text{if } t = 0, x \geq 0 \]  
\[ \frac{\partial C(x, t)}{\partial x} = 0; \quad \text{if } x \to \infty, t \geq 0 \]  
Specifically, the unsteady input flow is not constant because of industrial production activity variations; for example, the pollution from a factory that produces seasonal products or multiple heterogeneous products may have an unsteady input flow. Generally, for a given company production during period \( \pi \), the initial conditions are:
\[ C(x, t) = -C_0 t^2 + C_1 \pi t; \quad x = 0, 0 \leq t \leq \pi \]  
or
\[ \begin{cases} \frac{\partial C(x, t)}{\partial t} = -C_0 t + C_1 \pi; \quad x = 0, 0 \leq t \leq \pi \\ C(x, 0) = 0 \end{cases} \]  
where \( \pi \) denotes the length of one production and emissions period.

The degradation coefficient also differs at different temperatures. The following function yields the value of \( K \).
\[ K_t = K_{20} \times (T^{T-20}) \]  
where \( T \) is the temperature. Because the focus is on a specific time period, \( K \) can be treated as a constant value.

\( D \) is the longitudinal diffusion coefficient, which is influenced by the temperature, the fluid viscosity, and the particle size in accordance with the Stokes-Einstein relation, with \( D \) being determined from the differences between them. In this paper, the following formula is used:
\[ D = \alpha h u_e \]  
\[ \alpha = 5.915 \left( \frac{W}{h} \right)^{0.62} \left( \frac{u}{u_e} \right)^{1.428} \]  
The shear velocity is determined using the following empirical formula:
\[ u_e = \frac{\mu \varepsilon}{\ln \left( \frac{z}{Z_0} \right)} \]  
where \( \varepsilon \) is the Karman coefficient, \( z \) is the height of the measured point from the bottom of the river, and \( Z_0 \) is the river course length.

2.4 Solution method
The finite-difference method was used to solve the proposed problem. First, the time layer, the initial conditions, and the boundary conditions were defined, after which layer by layer calculations were conducted, which allowed for the pollution level at any time in each section to be determined and the pollution diffusion process monitored. Equation (1) can therefore be discretized as follows:
\[ \frac{c_{i+1}^j - c_i^j}{\tau} = \left( \frac{D}{l^2} + \frac{u}{2l} \right) C_i^j + \left( \frac{-2D}{l^2} - K \right) C_i^j + \left( \frac{D}{l^2} - \frac{u}{2l} \right) C_{i+1}^j \]  
where \( 1 \leq i \leq M + N - j - 1 \) and \( 0 \leq j \leq N - 1 \), \( i \) is the index indicating the length increments along the river, \( M \) and \( N \) are the total length and time increments, and \( j \) is the index indicating the time increments. For the initial values,
\[ C_i^0 = 0 \quad (1 \leq i \leq M + N) \]
\[
C_i^j = \begin{cases} 
-C_i(\tau, j)^2 + C_i(\pi, j) & \text{if } N \geq \pi \text{ and } \pi \leq j \leq N \\
0 & \text{if } j \leq N
\end{cases}
\]

and
\[ C_i^j = -C_i(\tau, j)^2 + C_i(\pi, j) \quad \text{if } N \leq \pi. \]

In the above formulations, \( l \) and \( \tau \) are the length and time increments, that is, \( l = \frac{x}{M} \) and \( \tau = \frac{t}{N} \), the matrix form for which is:

\[
\begin{bmatrix}
C^0_{i+1} - C_i^0 \\
C^1_{i+1} - C_i^1 \\
\vdots \\
C^{M-1}_{i+1} - C_i^{M-1} \\
\end{bmatrix} = 
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{D_u^+}{l^2} & -2D & \frac{D_u^-}{l^2} & 0 & \ldots & 0 & 0 \\
0 & \frac{D_u^+}{l^2} & \frac{D_u^-}{l^2} & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \frac{D_u^+}{l^2} & -2D & \frac{D_u^-}{l^2} & K \\
\end{bmatrix} \begin{bmatrix}
C_i^1 \\
C_i^2 \\
\vdots \\
C_i^{M-1} \\
C_i^M \\
\end{bmatrix}
\]

Therefore, the Jacobian matrix is

\[
J = 
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{D_u^+}{l^2} & -2D & \frac{D_u^-}{l^2} & 0 & \ldots & 0 & 0 \\
0 & \frac{D_u^+}{l^2} & \frac{D_u^-}{l^2} & 0 & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & 0 & \frac{D_u^+}{l^2} & -2D & \frac{D_u^-}{l^2} & K \\
\end{bmatrix}
\]

With this formulation, the ODE15 function in MATLAB can be used to solve the problem and obtain the results.

3. Model implementation

3.1 Study area: Tuojiang River Basin

The Tuojiang River Basin part of the upper Yangtze River Basin in China has a total length of 712 km, an area of 3.29 million km\(^2\), a mean annual precipitation of 1200 mm, and an annual average runoff of 14.94 billion cubic meters. As shown in Figure 3, the Tuojiang River flows through more than ten large and medium-sized cities, including Chengdu, Chongqing, Deyang, Neijiang, Zigong, Ziyang, Mianyang, Suining and Luzhou, and several other small cities. There are thousands of large and medium-sized manufacturing plants located throughout the river basin, which is one of the most important industrial concentrations in Sichuan Province. However, the Tuojiang River also plays a crucial role in offering fresh drinking water to local residents, factories and cities in the basin. Currently, the river and the surrounding regions are suffering from severe soil erosion and water pollution, which has resulted in both economic and health problems. There are 33 functional areas and 181 sewage outlets on the main Tuojiang River stream, with the discarded water quantity in these functional areas being 201.79 million cubic meters per year, with a further 172.27 million cubic meters per year being introduced via the river inlets. The main contaminants found in the river are CODcr, NH3-N, and P, with the CODcr and NH3-N inputs into the river being respectively 20382 t/a and 4301 t/a.
To efficiently address the pollution problems in the Tuojiang River basin, the proposed model was implemented to explore the underlying pollution diffusion and develop effective policies. The study area was divided into four zones: Zone 1, the Neijiang Beidukou drinking and industrial water resource area; Zone 2, the Neijiang Shizhong landscape and industrial water resource area; Zone 3, the Tuojiang Neijiang Pimu pollution control area; and Zone 4, the Tuojiang Neijiang Chenjiaba transition area. Table 2 shows the yearly sewage data for the Tuojiang River Neijiang segment.

![Figure 3. Tuojiang River Basin](image)

Table 2. Sewage per year in the Tuojiang River Neijiang segment

| First-level water functional areas | Second-level water functional areas | Sewage outlets | Quantity of discarded water (million m$^3$) | Inlets into river (million m$^3$) | COD into river (t) |
|------------------------------------|------------------------------------|----------------|---------------------------------------------|----------------------------------|-------------------|
| Tuojiang Neijiang development and utilization area | Zone 1 | 7 | 5.298 | 4.328 | 615.5 |
| | Zone 2 | 21 | 27.82 | 22.74 | 4007 |
| | Zone 3 | 1 | 0.5 | 0.42 | 60 |
| | Zone 4 | 1 | 0.09 | 0.072 | 50 |

Table 3 gives the relevant coefficients and their variations in the different seasons. Each year is divided into two periods based on the precipitation in the rainy season (k = 1) and the dry season (k = 2).

![Table 3. Coefficient Variations in the different seasons](image)

| k = 1  | Q   | W   | h   | u   | u *  |
|--------|-----|-----|-----|-----|------|
| 615    | 250 | 2.5 | 1.8 | 0.06 |
| 80.3   | 160 | 4   | 1.15| 0.06 |
3.2 Results and analysis

3.2.1 General situation

Figure 4. Concentration profile as a function of time; each line represents a different position

Figure 5. Concentration profile as a function of position; each line represents a different position

In Figure 4, the horizontal ordinate represents the time and the vertical ordinate represents the contaminant level, with each line showing a different situation for the different distance layers. It can be concluded from Figure 4 that: (1) at a given position in the river, the contaminant level increases over time and eventually reaches a steady level; and (2) at a given time, the contaminant level at each point is different, that is, the further from the source, the lower the contaminant level. The red line denotes the curve in the steady state, and the blue lines denote the concentration curves at the different positions, each of which gradually approaches the red line as the concentration at every point on the river that is
involved in this diffusion process gradually approaches a steady state, that is, the concentrations at the different positions remain constant over time.

In Figure 5, the horizontal ordinate represents the different points along the river in terms of the distance from the source point, with each line indicating a different situation in a different time layer, from which it can be seen that: (1) at a given point in the river, the contaminant level increases over time; and (2) at a given time, the contaminant level at each point in the river is different as the further from the source, the lower the contaminant level.

3.2.2 Dry season and rainy season

Because of the obvious changes in the river data (river flow, river width and river height) between the dry season and the rainy season, these seasons were independently considered. From the results in Figures 6 and 7, the following conclusions were made: (1) the overall tendencies were the same, that is, a steady-state situation was attained in both cases; (2) during the dry season, there is a slow river flow, which means that the contaminant diffusion does not go as far as in the rainy season over the same time; and (3) during the dry season, the contaminant concentration is higher at close distances because the diffusion process is slower.
3.2.3 Different degradation coefficients

Figure 8 shows the results for $K=0.1$ and Figure 9 shows the results for $K=0.5$. Comparing the above results, it can be seen that a higher $K$ value gives rise to a faster diffusion process and the steady-state reached varies for different values of $K$, that is, when the value of $K$ is higher, the steady-state contaminant level is lower and the steady state is more quickly attained.

4. Managerial implications

Use either SI (MKS) or CGS as primary units. (SI units are The application of the diffusion model to the Tuojiang River Basin indicated that it is possible to effectively manage the water contamination using various technologies and control methods; therefore, the following actions are proposed.

4.1 Make use of degradation coefficient

The data analysis revealed that the value of $K$ significantly affected contaminant levels. Therefore, if the $K$ value were enlarged, it would be possible to accelerate the diffusion and degradation processes and more quickly reduce the influence of the emitted pollution.
4.1.1 Different temperatures
To manage the industrial polluted water discharges, different actions could be implemented for different K conditions. For example, during the warmer rainy season, there could be a strict emissions limit, which during the colder dry season could be appropriately relaxed.

The temperature could be increased to increase the value of K. Because K can be determined that is \(K_i = K_{20} \theta^{(T-20)}\), the temperature could be increased to achieve a higher K value and maximize the self-purification of the river. However, as higher temperature water could be seen to be another form of pollution, this approach is only recommended in an emergency to reduce high contaminant concentrations.

4.1.2 Different technologies
There are many ways to increase K using technologies such as aeration, artificial hydraulic circulation and infiltration purification, which for COD, can respectively increase K by 34.4%, 47.8% and 57.8%. In comparative experiments on the effectiveness of different treatment technologies to improve river water quality, percolation purification technology, which improves the assimilative capacity of water bodies, introduces no secondary pollution and has a longer term effect, has been found to be the most efficient means of enhancing the K value. Therefore, this method is highly recommended.

Specifically, percolation purification technology focuses on promoting microbial purification. Experimental results have found that microbial purification has the greatest impact on on pollutant attenuation coefficient improvements, which indicates that microbes can play a very important role in the migration and transformation of water pollutants.

4.2 Targeted pollution solutions
The simulation results indicated that the proposed model could be used to simulate a specific pollutant diffusion distance at a given time and enable a determination of the optimal location from which to release the anti-pollutant inputs (microbes, activated carbon, etc.) to economically control the pollution. Therefore, there is no need to implement all possible extensive treatments as this is a waste of resources and often leads to less than ideal results.

4.2.1 Emergency water pollution
Sudden water pollution incidents are generally defined relative to conventional pollution incidents, such as accidents (transportation accidents, destruction of pollutant storage facilities, breaks in sewer lines, disruptions at sewage treatment plants and other accidental discharges) and pollution leakage incidents caused by vandalism or extreme natural phenomena (earthquakes, heavy rains, etc.) that result in the emission of a huge amounts of pollutants into the water causing the water quality to significantly deteriorate within a very short time. Sudden water pollution incidents influence the efficient use of water resources, which in turn can damage the economy, disrupt daily resident life, and cause excessive ecosystem damage.

When pollutant concentrations are too high, the diffusion is faster and the stable concentration is higher; therefore, in these situations, the self-degradation contribution is often negligible as the contaminant level exceeds the river’s self-purification capacity. Therefore, mitigating actions need to be immediately applied. Theoretical analysis, laboratory research and many pilot studies have been conducted to develop palliative measures based on the pollutants involved, for which six main emergency water purification technologies have been suggested: powdered activated carbon adsorption; chemical precipitation; oxidation/reduction; strengthened disinfection; aeration stripping; and integrated treatment. Therefore, it is suggested that a specialized pollution monitoring system based on the the special industry features in the Tuojiang River Basin in Neijiang be established for the most probable contamination types.
4.2.2 Pollution control plans for different districts
The Tuojiang River Basin is divided into several different zones, each of which has multiple sewage outlets. First, the overall pollution emissions limits in each zone need to be established as a single standard is not efficient, that is, if there are fewer firms located in a certain zone, the limitations in that zone should be less. Second, because the diffusion process depends on distance, sewage outlets should be placed at appropriate locations not too close to each other as the degradation process would not be effective and the diffusion process would not be sufficiently rapid to lower the concentrations, which means that there would be higher pollution levels near the outlets, which would severely harm the environment in these local regions. Third, because the Tuojiang River is surrounded by many residential areas, it is important to manage the pollution and the outlet locations to allow for local living environments to be improved and especially safeguard the quality of the drinking water resources.

5. Conclusions
A one-dimensional pollution diffusion model that incorporated parabolic input flow was developed to address complex real-life scenarios. Generally, because industrial production activities are irregular, the model was built under the assumption of one-point pollution sources with parabolic discharges. Then, a practical case in the Tuojiang River Basin was considered to demonstrate the effectiveness of the proposed model, from which it was found that: 1) the pollution concentration during the dry season was lower than that during the rainy season at distant locations, but higher at closer distances; and 2) when the degradation coefficient was higher, the steady-state concentration was lower and the steady state could be more easily attained. Finally, several managerial implications were given based on the analysis of the considered scenario.

However, as the proposed model only considered one possible type of unsteady input flow, there are still several other scenarios that could be investigated for real-life problems, such as exponential input flows and stochastic input flows. In addition, multiple-point sources with unsteady input flows could also be considered to address more complicated problems in the future.

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