Multi-parameter identification of a two-dimensional water-quality model based on the Nelder–Mead Simplex algorithm

Xiaodong Liu, Qile Tu, Zulin Hua, Wenrui Huang, Linghang Xing and Yuanyuan Zhou

ABSTRACT

To solve the multi-parameter identification problem of a two-dimensional river water-quality model, a new parameter identification method based on the Nelder–Mead Simplex algorithm coupled with the alternating direction implicit method has been constructed to determine hydraulic and water-quality parameters such as the longitudinal dispersion coefficient, the transverse mixing coefficient, and the pollutant degradation coefficient. Moreover, the influences of observation noise, observation location, and sampling frequency on the identified parameters were discussed for the given model. The method was validated using three numerical cases (two steady state and one dynamic), and one field experiment. The computational results indicated that the model provided good identification precision and showed good anti-noise capability. The longitudinal distribution of observed points made it possible to identify the contributions of the degradation coefficient K and the transverse distribution to the identification of the transverse dispersion coefficient E_y. Sampling frequency has a strong influence on the accuracy of the identified parameters. Generally, the higher the sampling frequency, the higher will be the accuracy obtained, but the convergence rate may be slow and the computational time lengthy. Therefore, when dealing with practical problems, a reasonable balance should be sought between the amount of calculation required and the parameter estimation accuracy.

Key words | alternating direction implicit, Nelder–Mead Simplex, optimization, parameter identification, water-quality model

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INTRODUCTION

Demands on watercourses for waste disposal, for water supply, as a leisure resource, and as an environmental habitat are increasing. It is therefore, imperative to understand the impact and fate of pollutants introduced into these watercourses. Research has been undertaken to improve the understanding of mixing processes in open-channel flows, so that the fate of pollutants can be predicted and hence the impact of contaminants effectively controlled and appropriate consent limits set. Most rivers have a high-width/depth ratio, and pollutants become mixed vertically within a short distance from the source. Vertical mixing is important only in the so-called near field and is often neglected when considering subsequent transverse and longitudinal mixing. When dealing with practical

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engineering problems, it is not computationally efficient to use three-dimensional (3D) models. Instead, researchers have used two-dimensional (2D) water-quality models to simulate pollutant transport in channels. There is, however, one troublesome point in the solution of these water-quality models. Whichever method is chosen, certain parameters in the model equations must be estimated. The importance of parameter estimation in model application has been widely recognized in engineering practice. Most previous studies of parameter estimation in river water-quality models have focused on the longitudinal dispersion coefficient (Fischer *et al.* 1979; Deng *et al.* 2002; Ho *et al.* 2002; Seyed & Roger 2002; Fan *et al.* 2003; Seo & Baek 2004; Gokmen 2009; Liu *et al.* 2011; Ahmad 2013). However, not only the longitudinal dispersion coefficient, but also the transverse mixing coefficient need to be determined when using 2D water-quality models. Only a small body of published research exists on the transverse mixing coefficient. The methods for calculating the transverse mixing coefficient include mainly theoretical methods (Fischer *et al.* 1979; Boxall & Guymer 2003; Duan 2004; Baek *et al.* 2006; Albers & Steffler 2007), empirical formulas (Yotsukura & Sayre 1976; Baek & Seo 2011), and tracer-test methods (Holley & Abraham 1973; Zeng & Huai 2008; Zhang & Zhu 2011). The tracer-test method is thought to be more accurate and reliable than the others, but it requires a tracer-test, which is very expensive. When analyzing pollutant mixing in streams, besides the longitudinal dispersion coefficient and the transverse mixing coefficient, certain other parameters, such as the degradation coefficient, must also be properly evaluated. For practical engineering problems, the most popular parameter selection method is the trial-and-error method, which adjusts parameters continuously until an optimal agreement between predicted values and measured concentration data is achieved. This method constitutes a subjective and laborious step in the water-quality model calibration process because water-quality state variables and model parameters are interrelated. Successful use requires high computational cost and expert practical ability. To overcome these difficulties and obtain reliable water-quality model performance, researchers have used many auto-calibration models to estimate unknown parameters. The optimization method has become the main way to determine parameters because of its advantages, such as low-sampling requirements and simple and convenient calculation. However, its optimization process largely ignores field measurement errors. The Gauss–Newton method is considered the most popular method because it does not require calculation of the Hessian matrix and its rate of convergence is faster than that of other methods (Bard 1970; Yeh 1986). However, because the Gauss–Newton method cannot converge under certain conditions, it requires an algorithm. To solve the convergence problem, the Nelder–Mead Simplex (NMS) method is another efficient direct search method that determines its search direction only by comparing the function values. It is insensitive to small inaccuracies or stochastic perturbations in function values (Chang 2012) and has become one of the most widely used methods for multidimensional non-linear unconstrained optimization (Lagarias *et al.* 1998). It is very easy to implement in practice because it does not require gradient computation (Peter & Terry 2011). Of the methods described above for solving parameter optimization problems, the NMS method was used in this study to determine the optimal parameters of the water-quality model because it is efficient and robust for estimating parameters in non-linear models and has been successfully used to estimate parameters of non-linear Muskingum models (Reza 2011).

In this study, a NMS algorithm combined with the alternating direction implicit (ADI) method was developed to predict parameters in natural streams. Moreover, the influences of noise, observation location, and sampling frequency on parameter estimation using this method were systematically analyzed. This work could offer guidance on parameter determination for model calibration.

MATERIALS AND METHODS

ADI method for 2D river water-quality model

In the 2D river water-quality model, the governing equation was generated by transforming the 3D advection-diffusion equation into the 2D advection-dispersion equation by integration with respect to depth. Pollutant concentrations were then obtained by solving the following

advection-dispersion equation:

$$\frac{\partial hC}{\partial t}+\frac{\partial(huC)}{\partial x}+\frac{\partial(hvC)}{\partial y}=\frac{\partial}{\partial x}\left(hE_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(hE_y\frac{\partial C}{\partial y}\right)-KhC, \quad (1)$$

where t is time, x is the longitudinal coordinate, y is the transverse coordinate, h is flow depth, C is the depth-averaged concentration of transported mass, u and v are depth-averaged velocities in the longitudinal and transverse directions, respectively, E_x and E_y are bulk dispersion coefficients in the longitudinal and transverse directions, respectively, and K is the bulk pollutant degradation coefficient.

Only under conditions of steady uniform flow can an analytic solution of this equation be obtained. Numerical methods must be used to solve the equation under other conditions. The ADI scheme, a well-known finite-difference method, has been used here to solve the vertically averaged flow equation. ADI is a two time-level method in which solutions of the x- and y-equations are staggered one-half time step apart and each is solved using the continuity equation. The computations are carried out using finite-difference approximations on a space-staggered grid in which water levels and velocities are described at different grid points (Leendertse & Gritton 1971; Adérito *et al.* 2014). The concentrations are described at the same locations as the water levels. Details of the flow and advective dispersive transport computations are presented in Leendertse & Gritton (1971). The method has been used in a water-quality study of Jamaica Bay (Leendertse 1970).

Parameter identification model based on ADI model and NMS algorithm

In parameter identification, the agreement between measured results and simulated values is one of the most important indicators of how well a model has been calibrated. The Parameter identification problem can be converted to an extremum problem by defining the following target function J

$$J(C,E)=\int_0^T\frac{1}{2}\|C-C^*\|^2\mathrm{d}t+\frac{1}{2}\alpha\|E-E_0\|^2 \quad (2)$$

expressed as the norm, where C is the vector of calculated values, C^* is the vector of observed values, E is the unknown parameter vector, E_0 is the initial parameter vector, and α is a regular coefficient. The first term is the distance between calculated and observed values. The second term is added to improve the well-posed characteristic of the optimization problem. The value of α is between 0 and 1. The value should be closer to one when the observed values are fewer or their precisions are lower, and vice versa. The value 0.01 is used in this paper. In parameter identification, the model parameters are adjusted to minimize $J(C,E)$ for all variables simultaneously. J is a non-linear function, and its extremum problem can be solved by multidimensional non-linear optimization methods. The NMS algorithm coupled with the 2D ADI model (ADI-NMS) was used here because of its high efficiency and robustness. The general steps in the ADI-NMS method are as follows:

1. Transform the parameter estimation problem into an extremum problem by defining the target function J.
2. Obtain observed data and other information at the measurement locations.
3. Assign to E an initial value E_0.
4. Based on the current E, calculate the concentrations at the measurement locations using the ADI method for the 2D river water-quality model.
5. Check the target function value J to determine whether it has satisfied the computational accuracy requirement.
6. If so, go to step (8); otherwise, go to step (7).
7. Change E to decrease the value of J using the NMS algorithm, then go to step (4).
8. Output the current value of E as the final parameter estimation results.

RESULTS AND DISCUSSION

Three cases of parameter identification for both steady state and dynamic flow were used to verify the method. Besides the computation method, other factors can influence the predictive value of the parameters in the water-quality model. The influence of noise, the distribution of observation points, and the richness of the data are discussed below.

Case 1

This case was a purely numerical experiment, not a real test. The river width B was 100 m, and the flow depth h was 2 m. The longitudinal velocity u was 0.5 m s^{-1}, and the transverse velocity v was 0 m s^{-1}. The tracer (10 kg) was released in the upper reaches of the river. Assuming that the longitudinal dispersion coefficient E_x was 50 $m^2 s^{-1}$, E_y was 0.1 $m^2 s^{-1}$, and the degradation coefficient K was 0.3 d^{-1}. Tracer concentrations at five different locations 500 m downstream were calculated (to three decimal places) by the water-quality model and are shown in Table 1 and Figure 1. By treating the data in Table 1 as observed data and u, E_x, E_y, and K as unknown parameters to be identified, this case can be used to verify the reliability of the parameter estimation method.

Table 1 | Tracer-test data from an instantaneous source (mgL^{-1})

	y (m)				
t (min)	−40	−20	0	20	40
2	0	0	0	0	0
6	0	0.007	0.119	0.007	0
10	0	0.040	0.212	0.040	0
12	0.001	0.054	0.215	0.054	0.001
14	0.002	0.062	0.203	0.062	0.002
16	0.003	0.065	0.184	0.065	0.003
20	0.005	0.062	0.142	0.062	0.005
24	0.006	0.052	0.104	0.052	0.006
36	0.006	0.024	0.038	0.024	0.006
40	0.005	0.017	0.026	0.017	0.005

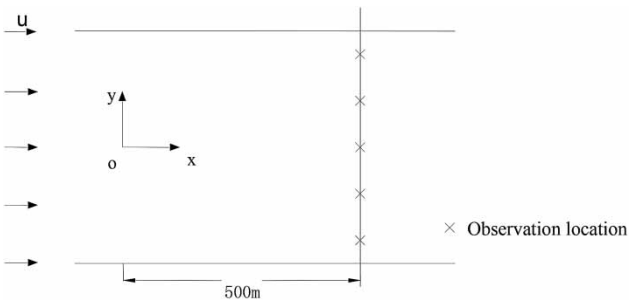

Figure 1 | Observation location.

Parameter estimation based on concentration data without noise

The initial values of u, E_x, E_y, and K were set to 1 ms^{-1}, 100 $m^2 s^{-1}$, 1 $m^2 s^{-1}$, and 0.5 d^{-1}, respectively. By entering the data in Table 1 directly into the model, the results shown in Table 2 can be obtained. The identified values are satisfactory except for K. The error in determining K is large compared to that for the other parameters. It is very difficult to estimate K because its assumed value was 0.3 d^{-1}, but the total length of time over which measurements were taken was only 40 minutes, which was a much shorter time scale.

Parameter estimation based on concentration data with noise

Regardless of the accuracy of the measuring instruments, measurement noise cannot be avoided. Because this noise is usually random, some random noise was added to the values in Table 1. The observed data with noise can be expressed as

$$C_j^{\delta} = C_j^{*}(1 + \beta * \delta), \tag{3}$$

where C_j^{*} is the true concentration, β is a random number between −1 and 1, and δ is the noise (disturbance) level. By running the model for 100 iterations, the statistical results shown in Table 3 can be obtained. These results show that the ADI-NMS-based parameter estimation method has high accuracy and good anti-noise properties, except for the parameter K.

Case 2

This numerical test was performed to test the parameter identification approach for steady-state flow and continuous

Table 2 | Inversion results under no noise

Parameter	u (ms^{-1})	E_x ($m^2 s^{-1}$)	E_y ($m^2 s^{-1}$)	K_1 (d^{-1})
True value	0.5	50	0.1	0.3
Identified value	0.4999	50.1609	0.1004	0.6563
Relative deviation (%)	0.02	0.32	0.40	118.77

Table 3 | Results under different noise levels

Parameter	Noise level (%)	Mean value	Standard deviation	Relative standard deviation (%)
u (ms^{-1})	$\delta = 1\%$	0.4999	0.0001	0.02
	$\delta = 5\%$	0.4996	0.0044	0.88
	$\delta = 10\%$	0.5002	0.0091	1.82
	$\delta = 30\%$	0.5017	0.0280	5.60
E_x (m^2s^{-1})	$\delta = 1\%$	50.1621	0.1757	0.35
	$\delta = 5\%$	50.1353	0.9324	1.86
	$\delta = 10\%$	50.0243	1.6994	3.40
	$\delta = 30\%$	49.6833	5.6331	11.27
E_y (m^2s^{-1})	$\delta = 1\%$	0.1004	0.00003	0.03
	$\delta = 5\%$	0.1004	0.0013	1.30
	$\delta = 10\%$	0.1004	0.0027	2.70
	$\delta = 30\%$	0.1010	0.0080	8.00
K (d^{-1})	$\delta = 1\%$	0.3226	0.2544	84.80
	$\delta = 5\%$	0.3225	0.4538	151.27
	$\delta = 10\%$	0.5615	0.7203	240.10
	$\delta = 30\%$	0.8383	0.8420	280.67

pollutant release. The river width B was 100 m, and the depth h was 2 m. The tracer was released continuously at a rate of 100 gs^{-1} in the upper reaches of the river. The longitudinal velocity u was 0.5 ms^{-1}, and the transverse velocity v was 0 ms^{-1}. The effect of the longitudinal dispersion coefficient E_x can be neglected in this case. With E_y set to 0.1 m^2s^{-1} and the degradation coefficient K to 0.3 d^{-1}, the tracer concentration downstream can be calculated by the water-quality model. Treating the calculated data as observed data and u, E_y, and K as unknown parameters to be identified, this case can be used to verify the reliability of the parameter estimation method and to investigate the effect of observation location on the parameter estimation results.

Parameter estimation based on data located on the transverse distribution

Assuming five sampling points located on the transverse distribution in the 500 m downstream section shown in Figure 1, data for (500,40), (500,20), (500,0), (500, −20), and (500, −40) were calculated by the water-quality model. Treating these data as observed data, the parameter estimation results using the parameter identification model are shown in Table 4. As in Case 1, the results show that u and E_y have high accuracy, but that the identified value of K is unsatisfactory.

Table 4 | Parameter results under transverse distribution

Parameter	u (ms^{-1})	E_y (m^2s^{-1})	K_1 (d^{-1})
True value	0.5	0.1	0.3
Identified value	0.5018	0.1003	1.0340
Relative deviation (%)	0.36	0.30	244.67

Parameter estimation based on data located on the longitudinal distribution

Assuming five sampling points located on the longitudinal distribution, three different conditions were designed and are shown in Figure 2 and Table 5. The parameter estimation results obtained from the parameter identification model are shown in Table 6. As in Case 1, the results show that u and E_y have higher accuracy than K. Of the three conditions, parameter identification under condition 3 was more accurate than under conditions 1 and 2, which shows that increasing the value of y can lead to better results. However, increasing the value of y also leads to lower concentrations, which may be more difficult to observe. When working with real-world observation distributions, this balance needs to be considered.

A comparison of the parameter results under the longitudinal and transverse distributions shows that the longitudinal distribution is well suited for identification of K and the transverse distribution for subsequent identification of E_y.

Case 3

This numerical test was performed to test the parameter identification approach under dynamic flow. The length of river studied was 2 km, and the river width B was 100 m. The upstream discharge was 60 m^3s^{-1}. The variation in downstream water level with time can be expressed as follows:

$$z = z_0 + A \sin(2\pi t/T), \tag{4}$$

where the wave amplitude A is 0.1, z_0 is 1.0 m, and the cycle time T is 12 h. A point source released pollutants continuously at a rate of 15 gs^{-1}. The upstream concentration and the initial concentration in the river were assumed to be 0 mg L^{-1}. Two hundred meshes were distributed in the

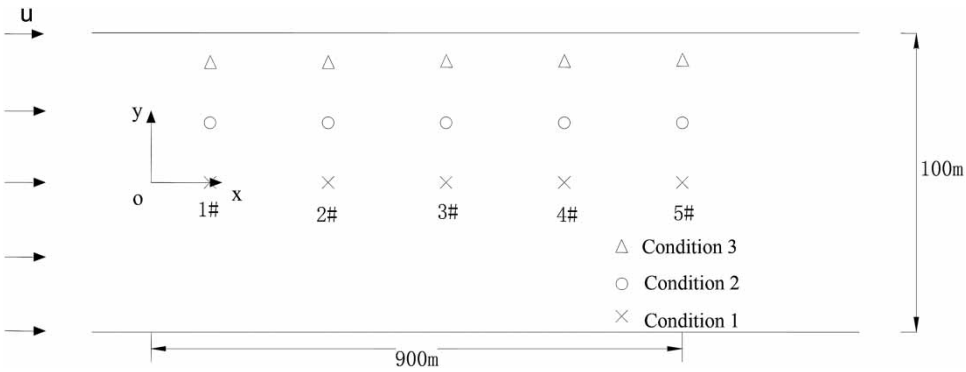

Figure 2 | Observation locations on the longitudinal distribution.

Table 5 | Coordinates of observation locations under different conditions

		Observation location				
Condition	**Y-coordinate**	**1#**	**2#**	**3#**	**4#**	**5#**
1	$y = 0$	(100,0)	(300,0)	(500,0)	(700,0)	(900,0)
2	$y = 20$	(100,20)	(300,20)	(500,20)	(700,20)	(900,20)
3	$y = 40$	(100,40)	(300,40)	(500,40)	(700,40)	(900,40)

Table 6 | Parameter results under longitudinal distribution for different conditions

	u (ms^{-1})		E_y (m^2s^{-1})		K (d^{-1})	
Condition	**Value**	**Relative deviation (%)**	**Value**	**Relative deviation (%)**	**Value**	**Relative deviation (%)**
1	0.6917	38.34	0.0726	27.40	0.8612	187.07
2	0.503	0.60	0.1009	0.90	0.7301	143.37
3	0.5039	0.78	0.1008	0.80	0.475	58.33

study area, as shown in Figure 3. With E_x set to 1.0 m^2s^{-1}, E_y to 0.1 m^2s^{-1}, and K to 0.3 d^{-1}, the pollutant concentrations at five points every hour 1,000 m downstream were calculated (to three decimal places) using the water-quality model, with the results shown in Table 7 and Figure 4. By treating these data as observed data and u, E_x, E_y, and K as unknown parameters to be identified, this case can be used to verify the reliability of the parameter estimation method and to investigate the effect of observed data richness on the parameter estimation results.

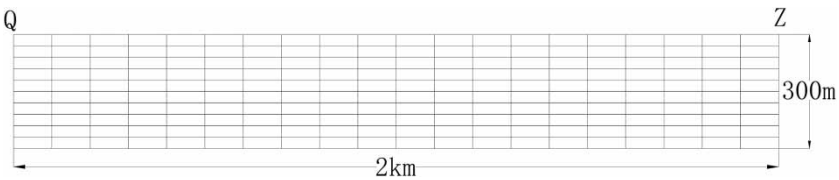

Figure 3 | Mesh distributions.

Table 7 | Tracer-test data from an instantaneous source (mgL^{-1})

	Observation station				
Sampling time/h	**1#**	**2#**	**3#**	**4#**	**5#**
1	0.0005	0.0042	0.0305	0.1546	0.4229
2	0.0050	0.0274	0.1363	0.4976	1.0651
3	0.0065	0.0329	0.1556	0.5465	1.1366
4	0.0073	0.0362	0.1672	0.5746	1.1732
5	0.0079	0.0380	0.1727	0.5842	1.1785
6	0.0081	0.0386	0.1725	0.5757	1.1483
7	0.0077	0.0367	0.1640	0.5480	1.0950
8	0.0071	0.0338	0.1523	0.5139	1.0356
9	0.0063	0.0308	0.1411	0.4835	0.9874
10	0.0057	0.0284	0.1326	0.4628	0.9602
11	0.0053	0.0270	0.1286	0.4559	0.9582
12	0.0052	0.0268	0.1289	0.4625	0.9815

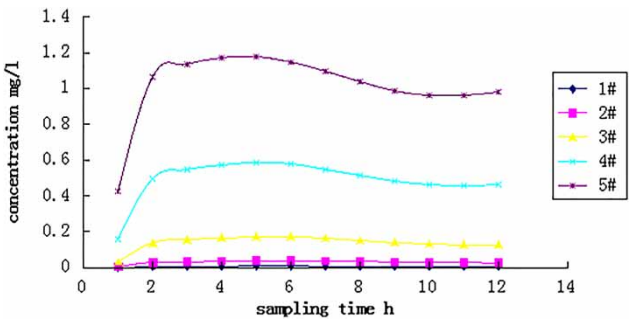

Figure 4 | Concentration profile at five points.

When the flow is dynamic, the concentration will vary with time. If the sampling frequency is inadequate, the accuracy of parameter identification will be affected by the insufficient richness of the observed data. However, the increased number of sampling times will also lead to a heavy workload. Therefore, the influence of sampling frequency on parameter identification was studied here. Using the target function $J \leq 0.000001$ as a termination condition, the parameter estimation results using the parameter identification model under different sampling time scales are shown in Table 8. Using a maximum of 100 iterations as a termination condition, the parameter estimation results are shown in Table 9. The parameter evolution process is illustrated in Figure 5.

These results show that the sampling frequency, which is directly related to the sampling time scale, has a great influence on the precision of the identified parameters. Generally, the more frequent the sampling, the higher will be the precision obtained, but the convergence rate may be slow and the computational time lengthy. Therefore, when dealing with practical problems, a reasonable balance should be determined between the amount of calculation and the parameter estimation accuracy. In this case, 12 is a reasonable number of sampling times which can reflect the processes of change within one hydraulic cycle.

Case 4

Field observation data (Fischer 1966) were used to determine the dispersion coefficient in the Green River, Washington. Two gallons of Rhodamine B dye were injected as a tracer from the Orillia Bridge. After the tracer was released, water was sampled downstream at Renton Junction. Lateral stations were located starting from the right end of the bridge. Concentration samples were taken at 10-minute intervals at stations 65, 75, 85, 95, 105, 115, 125, and 135. The concentrations measured at each lateral

Table 8 | Parameter results under different sampling time scales (termination condition $J \leq 0.000001$)

		E_x (m^2s^{-1})		E_y (m^2s^{-1})		K_1 (d^{-1})	
Sampling time	**Iterations**	**Value**	**Relative deviation (%)**	**Value**	**Relative deviation (%)**	**Value**	**Relative deviation (%)**
1	24	0.918604	8.14	0.11823	18.23	0.096869	67.71
3	124	0.992958	0.70	0.099024	0.98	0.37772	25.91
6	95	1.001411	0.14	0.100498	0.50	0.259421	13.53
12	106	0.999645	0.04	0.099987	0.01	0.302697	0.90

position are shown in Figure 6. The measured average velocity was approximately 0.35 ms^{-1}. For the investigated reach of the Green River, the calculated E_x was 8.3 m^2s^{-1} and the calculated E_y was 0.02 m^2s^{-1} by the proposed method. This value of E_x is very close to the result of 7.8 m^2s^{-1} obtained by integration of the theoretical profile with the velocity distribution.

CONCLUSIONS

To avoid the shortcomings of traditional optimization algorithms, a new multi-parameter estimation model based on the NMS algorithm coupled with the ADI method was proposed in this paper. Computational results for three numerical cases indicated that the proposed

Table 9 | Parameter results under different sampling time scales (termination condition 100 iterations)

	E_x (m^2s^{-1})		E_y (m^2s^{-1})		K_1 (d^{-1})	
Sampling time	**Value**	**Relative deviation (%)**	**Value**	**Relative deviation (%)**	**Value**	**Relative deviation (%)**
1	0.975934	2.41	0.109948	9.95	0.055047	81.65
3	0.97641	2.36	0.095401	4.60	0.648486	116.16
6	1.000929	0.09	0.100136	0.14	0.28819	3.94
12	0.999145	0.08	0.100108	0.11	0.291787	2.74

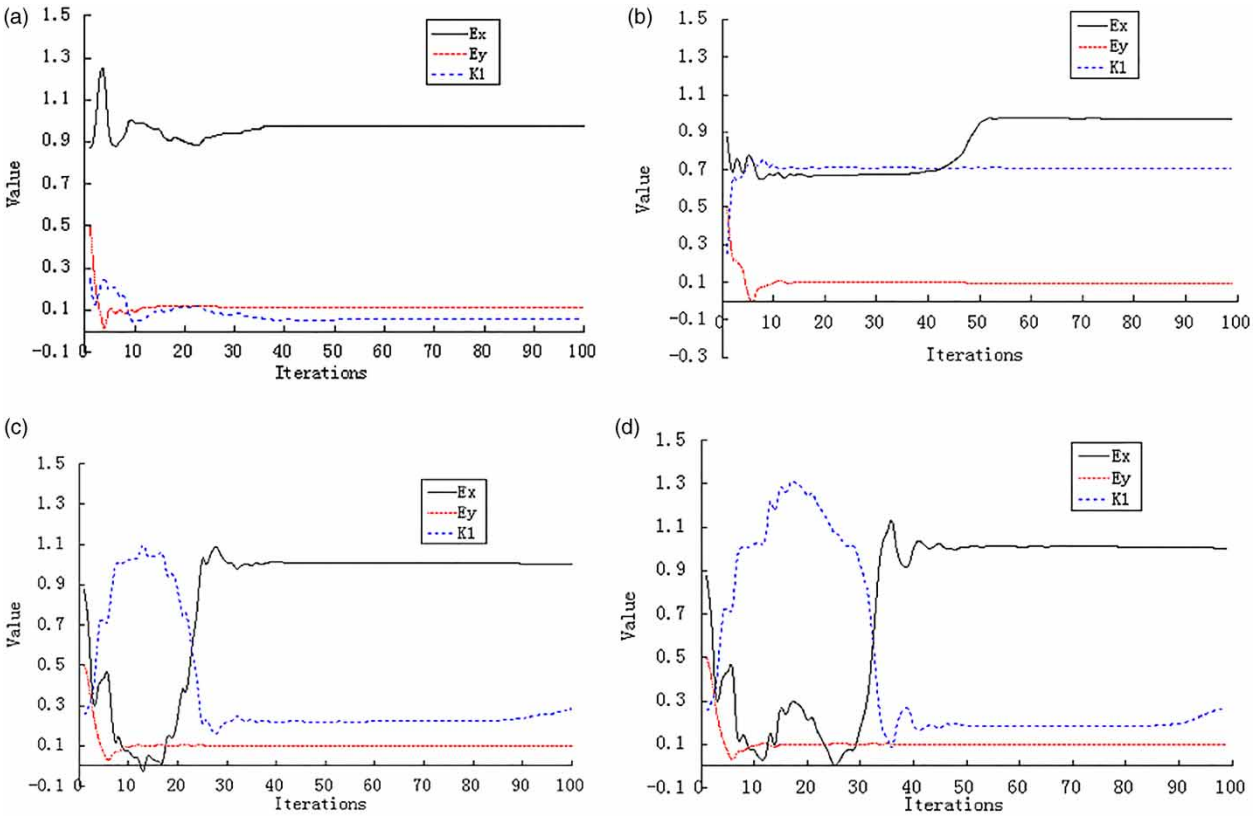

Figure 5 | Parameter evolution process: (a) one sampling time, (b) three sampling times, (c) six sampling times, (d) 12 sampling times.

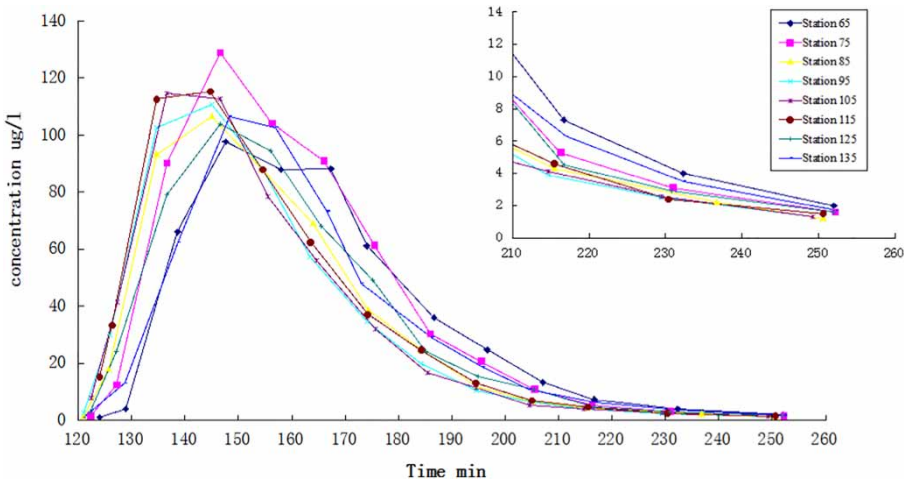

Figure 6 | Dye concentrations at Renton Junction.

parameter estimation model has high accuracy and good anti-noise properties. It can give precise results under both steady state and dynamic flow and can be used for both single-parameter and multi-parameter identification, including hydrodynamic parameters and water-quality parameters. The proposed method has a simple and easily understood theoretical basis, lower dependence on field data, and higher accuracy compared to previous methods.

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