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Using the Backward Probability Method in contaminant source identification with a finite-duration source loading in a river

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Abstract

Violation of industries in discharging their effluents into rivers leads to river pollution, which endangers the environment and human health. Appropriate tools are needed to deal with violations and protect rivers. The Backward Probability Method (BPM) is one of the most recommended tools identifying the release time and location of the pollutant source. However, the BPM generally was developed for groundwater and spill injection. Since most industries inject their effluents with a constant rate for a finite-duration, the use of prevailing models will have some errors. In this study, a numerical model was developed that could simulate a source with either a finite-duration or spill injection. This model is verified for two hypothetical cases and one real case. The results show that the model can accurately identify the release time and location of the pollutant source.

Keywords: Pollution source identification, Backward Probability Method, Adjoint Model, Fintie-duration loading

1. Introduction

Water is one of the most important and fundamental factors for living organisms. Surface water resources, because of their availability and easy extraction, are widely used in industry, agriculture, and municipal services. Surface water plays a prominent role in human societies (Cheng and Jia, 2010; Jing et al., 2020; Lu et al., 2015; Mazaheri et al., 2015; Rasheed et al., 2019; Saha et al., 2017). Increasing the rate of using surface water resources led to increasing pollution of these resources and scarcity of them (Amiri et al., 2019). Scarcity in water resources affects human lives and threatens economic and social development (Duan et al., 2016; Jing et al., 2020). Therefore, protecting surface water resources has become a global and security issue (Mekonnen and Hoekstra, 2018).

Environmental contaminant transport problems are broadly categorized into two subgroups, source-based and receptor-based problems. In source-based problems, information about the source is available, and the goal is to determine the concentration downgradient from the source (Neupauer and Wilson, 1999). In order to respond to these problems, researchers use the solution of the transport model (forward model) in which the advection-dispersion equation (ADE) is the base for analysis (FISCHER et al., 1979; Runkel, 1996; Van Genuchten, 1981). In receptor-based problems, contaminants are observed at monitoring points. In these cases, the main point is identifying source location, release time, and injected mass. Researchers (Boano et al., 2007; Ghane et al., 2016; Neupauer and Wilson, 1999; Tong and Deng, 2015) have used the inverse methods In order to respond to these problems. The approaches that are used in the inverse methods can be classified into three categories: simulation-optimization approach, mathematical approach, and probabilistic approach (Mazaheri et al., 2015).

The simulation-optimization approaches use a combination of optimization algorithms and the forward model to solve the inverse problem. This method, despite its simple formulation, requires high computational power. Alapati and Kabala (2000) used the least-squares method without any regularization methods in order to reconstruct the released mass in groundwater aquifers. Mahinthakumar and Sayeed (2005) claimed that combination methods have a better performance than basic optimization, in which the goal is finding the relative minimum. They combined the genetic algorithm with the basic optimizations in order to identify the source location. Xing et al. (2019) proposed an ensemble surrogate model to identifying groundwater contaminant sources. This model was following three individual surrogate models: kriging, radial basis function, and Monte Carlo method. They could effectively identify not only conservative contaminants source but also contaminants containing chemical reaction.

Mathematical approaches solve inverse problems in a direct manner and reduce computational costs. However, complexity is considered a disadvantage of these approaches. Skaggs and Kabala (1994) applied a mathematical method to calculate the release rate of pollutant sources; actually, they solved the Fredholm integral equation. Thus, they used the Tikhonov regularization technique in a one-dimensional domain to solve the inverse form of the ADE for groundwater. Milnes and Perrochet (2007) used the concepts of transfer functions theory to find the location of pollutant sources in groundwater aquifers. They could simulate this phenomenon as an inverse problem by using concentration at the detection point. They showed that in the inverse solution, concentration contours start to gather until these contours become a point that represents source location. Mazaheri et al. (2015) tried to determine the release rate of pollutant sources in the river with non-steady non-uniform flow conditions. They tried to resolve the problem of ill-posed equations by using the least square, the Green's function, and the Tikhonov regularization method.

Probabilistic approaches use probabilistic distributions, and one of the important advantages of this approach is small simulations and computations (Amiri et al., 2019). Liu (1995) established a continuous inverse model that could identify the location of spill-releasing pollutants into groundwater aquifers. In order to produce a probability density function (PDF), he used Laplace transformations and inversed the flow velocity. Neupauer and Wilson (1999) tried to use the adjoint method to solve the inverse ADE and produced a PDF. They verified their model using the model that Liu (1995) presented. Neupauer and Wilson (2001) enhanced their method and showed that the adjoint method could be used for multi-dimensional problems. They showed how the numerical methods could be combined with the adjoint method in order to identify the release time and source (Neupauer and Wilson 2004). Cheng and Jia (2010) were one of the first to try to identify the release time and the source location in a river. They used the adjoint method under steady non-uniform flow conditions; also, they assumed that the pollutant source is an instantaneous point source of a contaminant. Ghane et al. (2016) realized the release time and the source location in a river using the adjoint method by assuming one dimensional, steady, non-uniform flow conditions and an instantaneous point of source contaminant. They used a hypothetical example and real river conditions in order to verify their backward model. Jing et al. (2020) tried to obtain the pollutant release mass in a river by using the adjoint method. They assumed that the pollutant source is a finite-duration source, not instantaneous; their model was established for one-dimensional, steady non-uniform flow conditions. They verified their model using two hypothetical examples and a real case study.

Rivers are known as the main source of water for industry, irrigation, and domestic use. Therefore, they must be constantly monitored for quality; In this case, identifying the source of the pollutant in the rivers is important. Traditional pollutant source identification methods require a lot of data

monitoring, including water quality, topographic and hydrological data, while numerical models of water quality modeling can be more efficient. The backward probability method as a numerical model can identify contaminant sources with limited data. In previous researches, the backward probability method is used for source identification in groundwater with an instantaneous point source. It is clear that many industries discharge their pollutants into the river in a step-loading manner. Therefore, to identify the industries that violate, it is necessary to develop a numerical model appropriate to this type of injection. Furthermore, the instantaneous and finite-duration injection should be discriminated. In this study, the adjoint method is applied for a source with a finite-duration injection, and the adjoint equations for steady uniform flow conditions and conservative pollutants are derived. The proposed model is validated by hypothetical and experimental examples.

2. Study Area

In order to verify the proposed model, a hypothetical problem and a real case are considered.

2.1 Hypothetical Area

In the hypothetical case, a hydrodynamically acceptable example should be defined. In this case, river width, flow velocity, roughness coefficient, and river slope were assumed; with these assumptions, the water depth and dispersion coefficient were calculated using Manning's equation and Fisher's equation (Hessel et al., 2003), respectively. Suppose that there is a factory upstream of a straight river. This factory, which is located 21500 m upstream of the monitoring point, discharged its sewage continuously in the river for a finite duration. Figure 1 shows the factory and the monitoring point location in the river. Table 1 lists the flow and transport properties of this example.

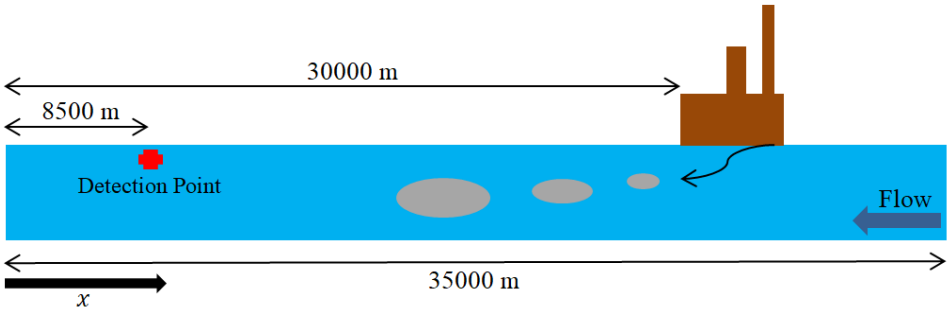

Figure 1. Stright river geometry for case 1

Table 1. Flow and transport properties in case 1

Parameter	Assumed values
Flow velocity (U)	1 *m/s*
Dispersion coefficient (D)	24 m^2/s
River width (b)	10 *m*
Water depth (y)	1 *m*
Initial concentration after mixing (C_0)	50 kg/m^3
Discharge start time (t_1)	0
Discharge completion time (t_2)	1 *hr*

112

113

114 2.2 Chicago Waterway Area

115 Jackson and Lageman (2013) did a field trace experiment in which Rhodamine WT (RWT) dye was
116 injected for a finite-duration source estimation to the Chicago Sanitary and Ship Canal (Figure 2). In
117 this canal, six stations measured the dye concentration, two of which, fluorometer FL291 located *9930*
118 *m* downstream of the source and FL293 located *7033 m* downstream of the source, are used in this
119 study. The US Geological Survey collected the data. Hydrodynamic parameters used in the proposed
120 model are the calibration results of Zhu et al. (2017). More information can be found in Jackson and
121 Lageman (2013) and Zhu et al. (2017). Table 2 summarizes the field tracer experiment information.

122 **3. Table 2. Flow and transport properties in Case 2**

Parameter	Assumed values
Flow velocity (U)	0.14 *m/s*
Dispersion coefficient (D)	4 m^2/s
River width (b)	49 *m*
Water depth (y)	8 *m*
Initial concentration after mixing (C_0)	10 $\mu g/L$
Discharge start time (t_1)	December 2, 2009, at 19:51
Discharge completion time (t_2)	December 3, 2009, at 04:47

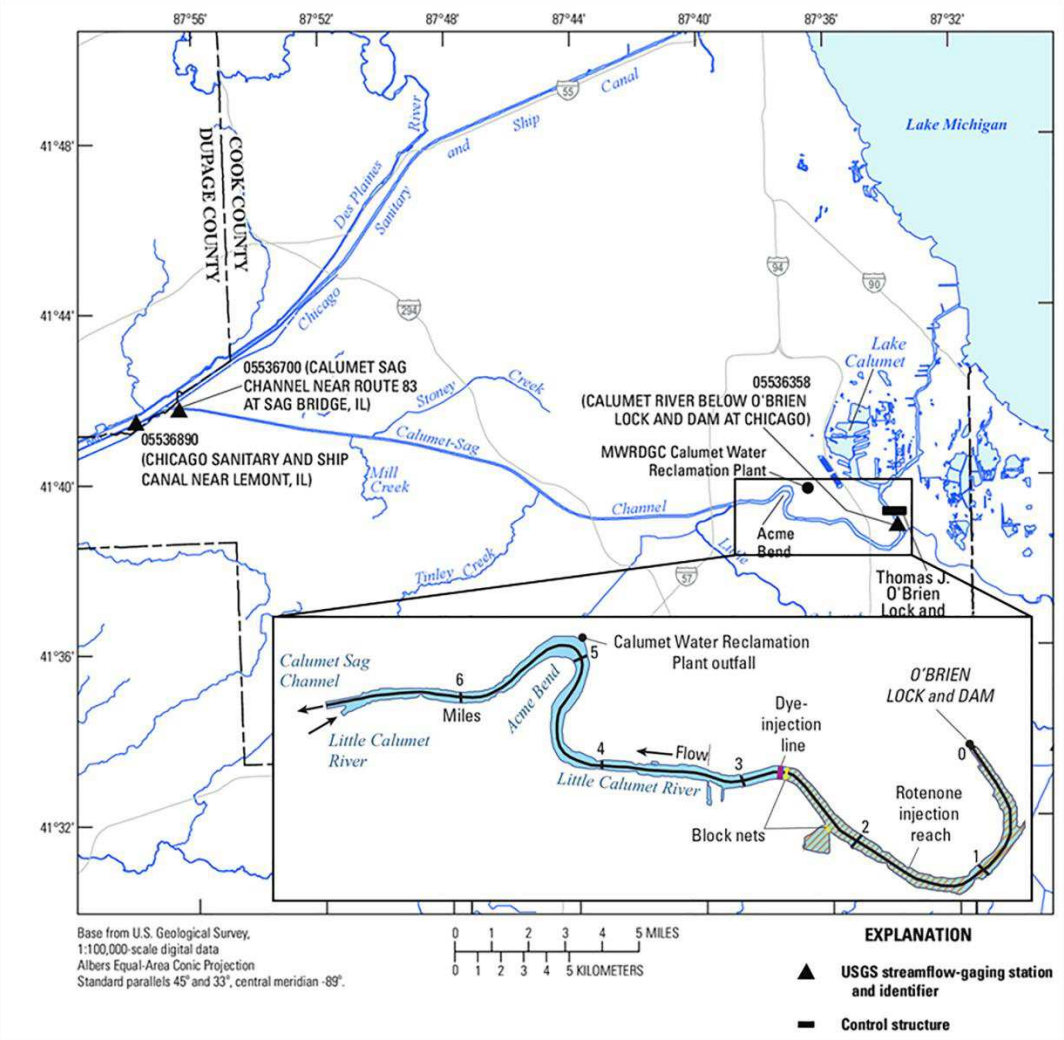

Figure 2. Map of Chicago waterway area

4. Methodology and Methods

In this section, the forward model and the backward model are described. The prerequisite of solving the backward model is the forward model results. It was stated that the ADE was the base equation in the forward model. In order to solve the ADE, hydrodynamic conditions must be known; thus, a hydrodynamic model is used. Series of inputs and outputs derived from the hydrodynamic model are used in the ADE. The forward model results are used as inputs to the backward model to find the release time and source location. Furthermore, the identification process, the numerical model, and the way that the proposed model was verified are described.

4.1 Forward model

The basic governing equation of contaminant transport is the ADE that is shown as Eq. (1). This equation is for one dimensional, steady, and uniform flow conditions (Chapra, 1997):

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} + S + KC \quad (1)$$

where C is the concentration, D is the longitudinal dispersion coefficient, U is the flow velocity, S is the source term, K is the first-order decay rate coefficient, t is the forward time, and x is the longitudinal coordinate. The source term defines the characteristics of the source and shows how pollutants discharge into the river. In this study, identifying the source of the pollutants in the river with a finite duration of injection (step loading, Figure 3) is the main idea. Therefore, the source term can be defined, as shown in Eq. (2):

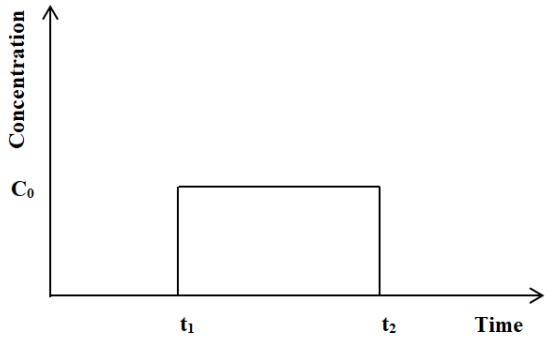

Figure 3. Step loading with a finite duration

$$S = C_0\delta(x - x_s)[H(t - t_1) - H(t - t_2)] \quad (2)$$

where C_0 is the initial concentration at the source location, δ is the Delta Dirac Function, H is the Heaviside Function, t_1 is the time that pollutant injection starts, and t_2 is the time that pollutant injection stops. Considering a conservative solute ($K=0$), and the ADE and its initial and boundary conditions became as shown in Eq. (3) (Cheng and Jia, 2010).

$$\begin{aligned} &\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - U\frac{\partial C}{\partial x} + S \\ &C(x,t) = 0 \qquad at \quad x = \infty \\ &\frac{\partial C}{\partial x} = 0 \qquad at \quad x = 0 \\ &C(x,0) = 0 \qquad at \quad x \geq 0 \end{aligned} \quad (3)$$

$$S = C_0\delta(x - x_s)[H(t - t_1) - H(t - t_2)] \quad (4)$$

The result of solving equation Eq. (3) is the concentration at time t and location x. Normalizing concentration by the total concentration entering the system defines the Forward Location Probability (FLP) from source to the detection point (Neupauer and Wilson, 1999). Equation Eq. (5) shows this expression:

$$f(x,t) = \frac{C(x,t)}{\int_0^\infty C(x,t)\,dt} \quad (5)$$

In this study, it is assumed to have a steady and uniform flow condition. Manning's equation and Fisher's equation are used in order to determine the hydrodynamic parameters (A, U, and D). Eq. (6) represents Manning's equation, and Eq. (7) represents Fisher's equation.

$$U = \frac{1}{n} R^{2/3} S^{1/2} \tag{6}$$

$$D = 0.011 \frac{U^2 B^2}{H U^*} \tag{7}$$

$$U^* = \sqrt{gHS} \tag{8}$$

where n is a Manning's roughness coefficient, R is the channel hydraulic radius, S is the channel slope, B is the average channel width, H is the average depth, and U^* is the shear velocity.

4.2 Backward model

The adjoint method is used in order to form the backward model. The adjoint of the ADE for the finite-duration of injection was developed by pursuing the steps that (Neupauer and Wilson, 1999) established. The performance measure, P, expresses the state of the system and is defined as Eq. (9):

$$P = \int_{x_1}^{x2} \int_0^{\infty} h(\alpha, C) dt\, dx \tag{9}$$

where $h(\alpha, C)$ is a function of the state of the system, and α is a vector of system parameters (*U, D, C_0*). The marginal sensitivity is obtained by differentiating the performance measure with respect to one of the system parameters Eq. (10) shows marginal sensitivity in which differentiation is with respect to *C_0*.

$$\frac{dP}{dC_0} = \int_{x_1}^{x2} \int_0^{\infty} \left[\frac{\partial h(\alpha, C)}{\partial C_0} + \frac{h(\alpha, C)}{\partial C} \psi \right] dt\, dx \tag{10}$$

where $^{dP}/_{dC_0}$ is defined as a marginal sensitivity, $\psi = {}^{\partial C}/_{\partial C_0}$ is a state sensitivity that indicates the measure of the change in the state of the system. The state sensitivity in Eq. (10) is unknown; thus, in order to calculate the marginal sensitivity, ψ from Eq. (10) must be eliminated by using the adjoint method. The first step in utilizing the adjoint method is differentiating the ADE, and its initial and boundary conditions respect to the *C_0*. Differentiating Eq. (3) respect to the *C_0* gives:

$$\begin{aligned} & -\frac{\partial \psi}{\partial t} + D \frac{\partial^2 \psi}{\partial x^2} - U \frac{\partial \psi}{\partial x} + \frac{\partial S}{\partial C_0} = 0 \\ & \psi(x, t) = 0 \quad at \quad x = \infty \\ & \frac{\partial \psi}{\partial x} = 0 \quad at \quad x = 0 \\ & \psi(x, 0) = 0 \quad at \quad x \geq 0 \end{aligned} \tag{11}$$

The next step is obtaining to an equation similar to the ADE in which ψ^*, an arbitrary function, is the main variable. It will be shown that $\psi^*$is the adjoint state. Therefore, the inner product of the adjoint state and each term in Eq. (11) is taken after defining the inner product of two functions.

$$\int_0^T \int_{x_1}^{x_2} \left[-\psi^* \frac{\partial \psi}{\partial t} + \psi^* D \frac{\partial^2 \psi}{\partial x^2} - \psi^* U \frac{\partial \psi}{\partial x} + \psi^* \frac{\partial S}{\partial C_0} \right] dx dt = 0 \tag{12}$$

where T is the final time (detection time), x_1, and x_2 are the downstream and the upstream boundaries, respectively. A similar form of the ADE for ψ^* is obtained by manipulating each term in Eq. (12).

$$\int_0^T \int_{x_1}^{x_2} -\psi^* \frac{\partial \psi}{\partial t} dx dt = \int_0^T \int_{x_1}^{x_2} -\frac{\partial}{\partial t}(\psi^* \psi) + \psi \frac{\partial \psi^*}{\partial t} dx dt \tag{13}$$

$$\int_0^T \int_{x_1}^{x_2} \psi^* D \frac{\partial^2 \psi}{\partial x^2} dx dt = \int_0^T \int_{x_1}^{x_2} D \frac{\partial}{\partial x}\left(\psi^* \frac{\partial \psi}{\partial x} \right) - D \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} dx dt \tag{14}$$

$$\int_0^T \int_{x_1}^{x_2} -D \frac{\partial \psi}{\partial x} \frac{\partial \psi^*}{\partial x} dx dt = \int_0^T \int_{x_1}^{x_2} -D \frac{\partial}{\partial x}\left(\psi \frac{\partial \psi^*}{\partial x} \right) + \psi D \frac{\partial^2 \psi^*}{\partial x^2} dx dt \tag{15}$$

$$\int_0^T \int_{x_1}^{x_2} -\psi^* U \frac{\partial \psi}{\partial x} dx dt = \int_0^T \int_{x_1}^{x_2} -U \frac{\partial}{\partial x}(\psi^* \psi) + U \psi \frac{\partial \psi^*}{\partial x} dx dt \tag{16}$$

Substituting Eq. (13), Eq. (14), Eq. (15), and Eq. (16) into Eq. (12) gives:

$$\int_0^T \int_{x_1}^{x_2} \left[-\frac{\partial}{\partial t}(\psi^* \psi) + \psi \frac{\partial \psi^*}{\partial t} + D \frac{\partial}{\partial x}\left(\psi^* \frac{\partial \psi}{\partial x} \right) - D \frac{\partial}{\partial x}\left(\psi \frac{\partial \psi^*}{\partial x} \right) + \psi D \frac{\partial^2 \psi^*}{\partial x^2} - U \frac{\partial}{\partial x}(\psi^* \psi) + U \psi \frac{\partial \psi^*}{\partial x} + \psi^* \frac{\partial S}{\partial C_0} \right] dx dt = 0 \tag{17}$$

The left side of Eq. (17) is equal to zero; thus, it can be added to the right side of Eq. (10) without a change in results. Equation Eq. (18) shows the new expression of the marginal sensitivity. It is obtained by rearranging terms after adding the left side of Eq. (17) to the right side of Eq. (10).

$$\frac{dP}{dC_0} = \int_0^T \int_{x_1}^{x_2} \left\{ \frac{\partial h(\alpha, C)}{\partial C_0} + \psi \left[\frac{h(\alpha, C)}{\partial C} + \frac{\partial \psi^*}{\partial t} + D \frac{\partial^2 \psi^*}{\partial x^2} + U \frac{\partial \psi^*}{\partial x} \right] + \frac{\partial}{\partial x}\left[D \psi^* \frac{\partial \psi}{\partial x} - D \psi \frac{\partial \psi^*}{\partial x} - U \psi^* \psi \right] - \frac{\partial}{\partial t}(\psi^* \psi) + \psi^* \frac{\partial S}{\partial C_0} \right\} dx dt \tag{18}$$

The current goal is to eliminate ψ from Eq. (18). Therefore, it can be assumed that $\partial h(\alpha, C) / \partial C_0 = 0$, because the system parameters (e.g., U, and D) are independent of C_0. The coefficient of ψ in the second term of integration in Eq. (18) is equal to zero (the adjoint equation). The third and fourth terms are divergence terms and represent initial and boundary conditions for the adjoint equation after integration. These assumptions are shown in Eq. (19), Eq. (20), and Eq. (21).

$$\frac{h(\alpha,C)}{\partial C}+\frac{\partial\,\psi^*}{\partial t}+D\frac{\partial^2\,\psi^*}{\partial x^2}+U\frac{\partial\,\psi^*}{\partial x}=0 \tag{19}$$

$$\int_0^T\int_{x_1}^{x_2}\frac{\partial}{\partial x}\left[D\psi^*\frac{\partial\psi}{\partial x}-D\psi\frac{\partial\psi^*}{\partial x}-U\psi^*\psi\right]dxdt=0$$

$$\int_0^T\left[D\psi^*\frac{\partial\psi}{\partial x}-D\psi\frac{\partial\psi^*}{\partial x}-U\psi^*\psi\right]\Big|_{x_1}^{x_2}dt=0 \tag{20}$$

188 Substituting conditions that represented in Eq. (9) into Eq. (17) gives:

$$D\psi^*\frac{\partial\psi}{\partial x}|x=\infty+D\psi\frac{\partial\psi^*}{\partial x}|x=0+U\psi^*\psi|x=0 \tag{21}$$

189 As previously indicated, the adjoint state, ψ^*, is an arbitrary function and can be defined to
190 eliminate ψ. Therefore, the initial and boundary conditions for the adjoint equation are shown in Eq.
191 (22) and Eq. (23):

$$\psi^*(x,t)=0 \qquad at \quad x=\infty$$

$$D\frac{\partial\psi^*}{\partial x}+U\psi^*=0 \quad at \quad x=0 \tag{22}$$

$$\int_{x_1}^{x_2}\int_0^T-\frac{\partial}{\partial t}(\psi^*\psi)dtdx=0$$

$$\int_{x_1}^{x_2}(\psi^*\psi)\Big|_0^T dx=0 \tag{23}$$

$$\psi^*(x,T)=0 \qquad at \quad x\geq 0$$

192 The final time in the forward model, T, is determined arbitrarily, and $t\leq t_d$ is essential; thus, the
193 detection time can be determined as the final time. In the backward model, backward time is used, τ,
194 which defined as $\tau=T-t=\ t_d-t$. The definition of the function of the state, $h(\alpha,C)$, is related to
195 the performance measure. When the performance measure was considered as a concentration at a
196 known time and location, i.e., the detection point, the function of the state should be defined in a way
197 that the integration over the time and space domain results in the measured concentration at the
198 detection point. Therefore, the function of the state can be defined as Eq. (24). ${}^{h(\alpha,C)}/_{\partial C}$ is a Frechet
199 derivative (Saaty, 1981) of $h(\alpha,C)$ with respect to the *C.* take the derivative of both sides of Eq. (24)
200 gives Eq. (25). Eq. (26) represents the marginal sensitivity. Eq. (27) shows the adjoint equation and its
201 initial and boundary conditions.

$$h(\alpha,C)=C(x,t)\delta(x-x_d)\delta(t-t_d) \tag{24}$$

$$\frac{h(\alpha,C)}{\partial C}=\delta(x-x_d)\delta(t-t_d) \tag{25}$$

$$\frac{dP}{dC_0} = \int_0^T \int_{x_1}^{x_2} \psi^* \frac{\partial S}{\partial C_0} dxdt = \int_0^T \int_{x_1}^{x_2} \psi^* \delta(x - x_s)[H(t - t_1) - H(t - t_2)]dxdt \quad (26)$$

$$\frac{\partial \psi^*}{\partial \tau} + D\frac{\partial^2 \psi^*}{\partial x^2} + U\frac{\partial \psi^*}{\partial x} = -\delta(x - x_d)\delta(t - t_d)$$

$$\psi^*(x, \tau) = 0 \qquad at \quad x = \infty$$
$$D\frac{\partial \psi^*}{\partial x} + U\psi^* = 0 \qquad at \quad x = 0 \quad (27)$$
$$\psi^*(x, 0) = 0 \qquad at \quad x \geq 0$$

Results of Eq. (27) are the adjoint state at every point in the time and space domain. Using these results in Eq. (26) gives the marginal sensitivity. Eq. (28) shows Backward Location Probability (BLP).

$$f(x, \tau) = \frac{1}{(t_2 - t_1)}\frac{dP}{dC_0} \quad (28)$$

4.3 Identification process

The FLP demonstrates the probability of the existence of a contaminant that has been released from the source at a particular location (detection point) after passing the specific time. However, the BLP determines the prior location of a contaminant that has been observed at the detection point (Neupauer and Wilson, 2001). Based on the backward probability method, BLP and FLP density functions are equal only at the source location (Wagner et al., 2015). The Root Mean Square Error (RMSE) have been used to compare the BLP and FLP density functions (Cheng and Jia, 2010; Ghane et al., 2016), which Eq. (29) shows:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(FLP - BLP)^2}{n}} \quad (29)$$

where n is the number of data entry points to be compared, the source location will be identified when the RMSE is minimized. Figure 4 shows the overall identification process.

4.4 Numerical Modeling

A numerical model has been developed to compute the forward and backward probabilities. This numerical model is based on the Finite Volume Method with the upwind and fully implicit scheme in space and time. The applied numerical model can solve Eq. (3) and Eq. (27). The Delta Dirac Function in Eq. (27) and Eq. (3) estimated and applied using the scheme proposed by Neupauer and Wilson (2004).

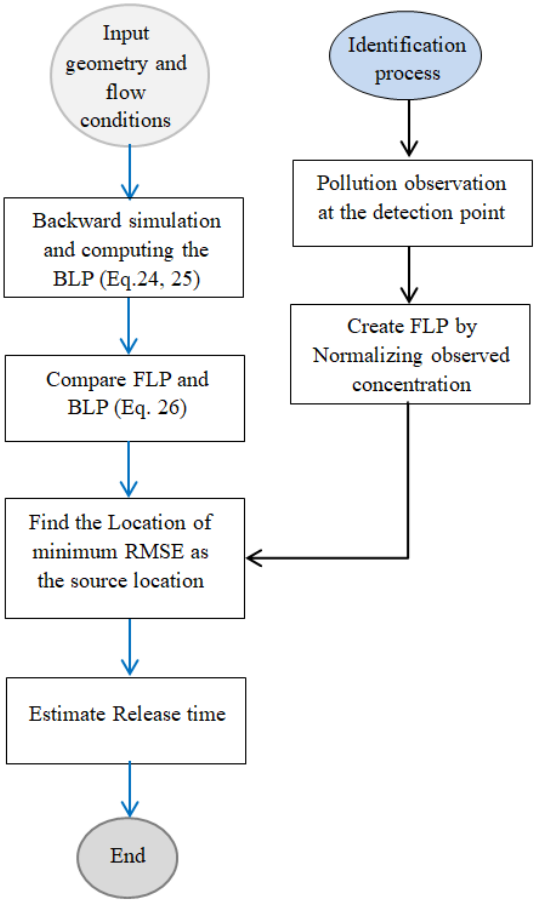

Figure 4. Flow chart of the identification process.

5. Results and discussion

The proposed model is verified for a hypothetical case and a real case. Also, it is expected that this model could simulate an instantaneous source since, in the step loading source, when the difference between the time that source starts and stops to inject contaminant becomes zero, t_1-t_2=0, the source becomes an instantaneous source. Therefore, this ability was verified by using a hypothetical case.

5.1 Finite-duration source (Case 1)

After injection, the monitoring point records concentration over time (Figure 5a), and the numerical model uses Eq. (5) to produce the FLP. The proposed model calculates the BLP for every possible source location and compares it with FLP (Figure 4b). However, the minimum RMSE between BLP and FLP shows source location. In this case, the model determined $x = 30000\,m$ as a contaminant source location since it has the minimum RMSE = $1.89 * 10^{-5}$. Figure 5a shows that *6.475 h* after injection, peak concentration reaches to the monitoring point. The peak concentration was considered as the presence of a contaminant at a specific location (Neupauer and Wilson, 1999). Figure 5b shows the best match between BLP and FLP, and the highest probability for the release time from the detected source location is *6.475 h* before observing contaminants in the monitoring point. As it is clear, the model could identify the release time and location with the least error.

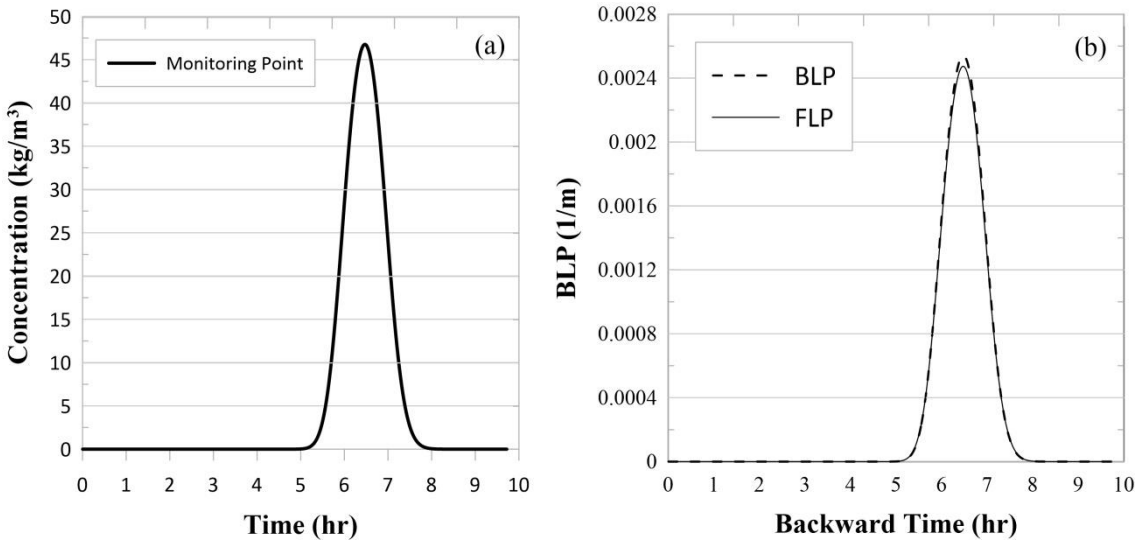

Figure 5. a) Concentration time series at monitoring point, b) Comparison between BLP and FLP

5.2 Field tracer experiments (Case 2)

Figure 6a shows a comparison between measured concentrations at two stations and the numerical results. As shown, the peak arrival time in both numerical and measured concentrations for FL291station is 24.3 hours after injection. The peak arrival time for FL293 station in the numerical model is 18.6 hours after injection, and in the field tracer experiment is 17.67 hours. Figure 6b and 6c show a best match between the FLP and BLP. The best match with minimum RMSE shows that the model can identify the source location in both tests. The source location that have minimum RMSE (0.002 for FL291 and 0.0024 for FL293) based on the observations at stations FL291 and FL293.

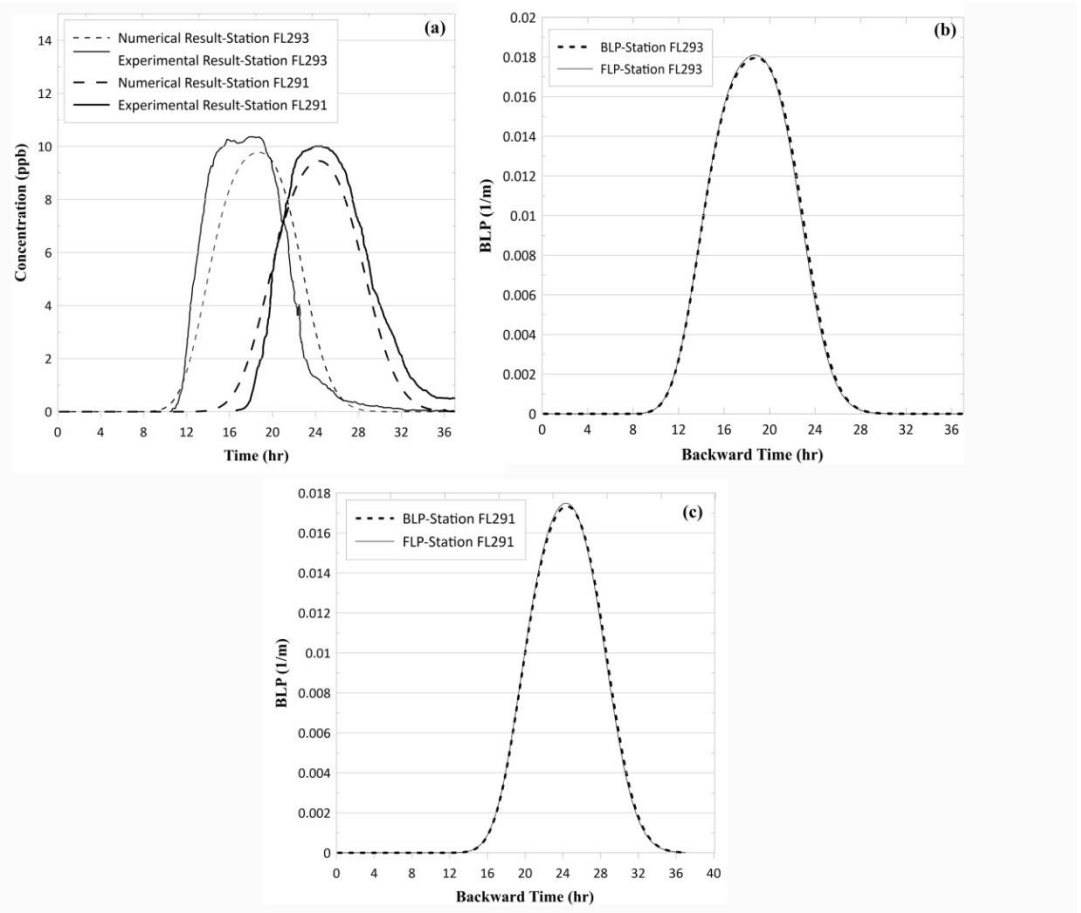

Figure 6. a) Comparison of concentration between numerical model and field tracer experiment at two stations b) Comparison between the BLP and FLP at station FL293, and c) Comparison between the BLP and FLP at station FL291

5.3 Instantaneous source (case 3)

Case 3 is defined to show that the proposed model can identify the release time and location of the contaminant source when the injection happens as an instantaneous source. In Case 3, the hypothetical example that is represented in Case 1 is used. However, If the model is used for simulating an instantaneous source, the difference between the time that the source starts and stops injection must be zero, $t_2 - t_1 = 0$. Figure 7a shows the concentration time series at the monitoring point; based on the results in Figure 7a the FLP became accessible. The peak concentration reaches the monitoring point *5.96 h* after injection. Figure 7b shows the comparison between the FLP and BLP at the source location, which has the minimum RMSE (1.22×10^{-5}). Based on Figure 7b the highest probability for release time is *5.96 h* before the injection.

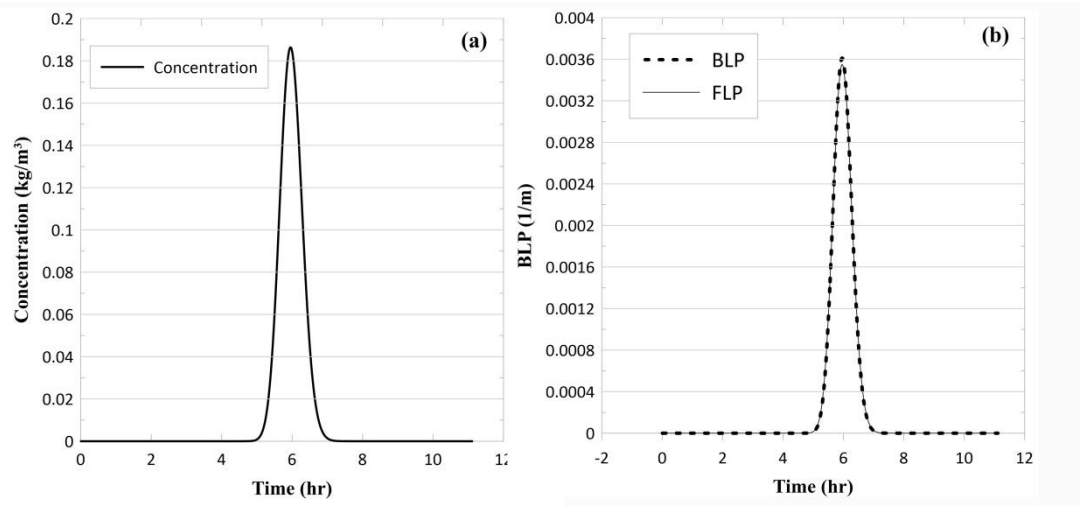

Figure 7. a) Concentration time series at the monitoring point for an instantaneous source b) Comparison between the FLP and the BLP

The proposed model has been validated by the three examples. The results show that this model can properly identify source location and release time. Most of the previous studies simulate instantaneous injection. With this in mind, in the third example, the proposed model could simulate instantaneous injection and determine the release time and source location. Furthermore, a sensitivity analysis for hydrodynamic parameters was done, and the results indicated that the model could identify the release time and source location correctly, and changing hydrodynamic parameters does not significantly affect the results.

6. Conclusions

In this study, an adjoint method was developed for a finite-duration injection to a river in order to expand previous studies. The proposed model successfully simulated steady uniform flow conditions and conservative pollutants. The results showed that when conservative pollutants exist, a monitoring point is sufficient for determining the release time and source location. Furthermore, the model performance in a real case was examined, and it was concluded that the model works accurately. The maximum error for release time and source location, in some cases, was 6%. Also, this model can be used for large-scale rivers and instantaneous sources. The adjoint method identifies the source location and release time by simulating the backward model once which is a beneficial ability compared to other methods in the literature.

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Ethical Approval

This manuscript is our original, unpublished paper, which we did not submit to another journal before.

Consent to Participate and Publish

It is our great pleasure to submit to you my manuscript entitled “Using the Backward Probability Method in contaminant source identification with a finite-duration source loading in the river” to be published in your admired journal.

Authors Contributions

Hossein Khoshgou is an M.Sc. student, and this paper originated from his thesis, and Seyed Ali Akbar Salehi Neyshabouri is his supervisor and corresponding author.

Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Availability of data and materials

There is no availability for data and materials.

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