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*Proceedings of the 5th International Conference on Inverse Problems in Engineering: Theory and Practice, Cambridge, UK, 11-15th July 2005*

## SOME INVERSE CONTAMINANT FLUID FLOW PROBLEMS USING BOUNDARY ELEMENT METHODS

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**Abstract -** This study is concerned with the application of the boundary element method (BEM) and the dual reciprocity boundary element method (DRBEM) for solving inverse source problems that occur in water pollution. Based on the BEM or the DRBEM, the inverse problems are reduced to solving nonlinear systems of algebraic equations which are solved using an iterative sequential quadratic programming (SQP) method. The numerical results obtained are compared with the corresponding analytical solutions for several test examples considered.

### 1. INTRODUCTION

Among all the environmental concerns that have become the focus of both public and scientific interest over the last four decades, water pollution plays a very important role. This is because water is one of our most important natural resources and there are many conflicting demands upon it. Knowing the origin of the source of contamination is probably the most important aspect when attempting to understand, and therefore to control, the pollution transport process. Thus, the identification of the sources of pollution in waters is a challenging issue in numerous environmental problems. The aim of this study is to assist in the development of the necessary techniques to solve this practical problem.

Water contaminants arise from two categories of sources: point sources and distributed or non-point sources. Point sources of pollution occur when harmful substances are emitted directly into a body of water, e.g. domestic and industrial sewage pipelines, leaks or spills of industrial chemicals at manufacturing facilities, underground injection wells (industrial waste), municipal landfills, leaky sewage pipes, etc. A non-point source delivers pollutants indirectly through environmental changes. An example of this type of water pollution is when fertilizer from a field is carried into a stream by rain in the form of run-off which in turn affects aquatic life.

In general, the identification of one or more point sources of pollution is an easier task than the identification of non-point sources. However, there are many cases when many sewage pipelines could be responsible for discharging contaminant into the water, but only certain of them have caused the pollution in the given situation. Thus, their identification is required. Another example could be the case when the breakage of an offshore underwater outlet sewage pipeline occurs and this breakage has to be localised using only some measurements of the contaminant concentration taken at different locations.

In this study the governing equation for the pollution process is taken to be the steady-state convection-diffusion equation. Over the past 20 years or so, several attempts have been made to solve inverse source problems associated with this equation. As a result, several methods are currently available for contaminant source identification, which analyse the contaminant distribution to determine either the prior location of the observed contamination or the release history from a known source. One of the early methods used to backtrack the pollution source location is to run forward simulations and check the solutions with the measured/current spatial data observed. Owing to the non-uniqueness of the solution and the infinite number of plausible combinations, one needs to follow an optimisation method to obtain the best fit solution. In [9] a procedure based on least squares regression and linear programming for the least absolute error estimation was formulated, the pollution sources being identified by matching simulated and measured nonreacting solute concentration data. The multitude of approaches on the contaminant source identification problem can be divided in two categories. One subset of work focuses on determining the values of a number of parameters describing the source such as, for example, the location and the strength of a steady state point source, [9], [10]. Another subset of work uses a function estimate to characterize the source location or release history. In this case, the source characteristics are not limited to a small set number of parameters, but are instead free to vary in space and time. This last category includes methods that use a deterministic approach, [2], [3], [5], [15], [22] and others that offer a stochastic approach to the problem, [6], [13], [16], [23], [24]. Good literature reviews on contaminant source identification methods can be found in [4] and [13].

In this paper, the contaminant source identification problem is approached by developing a novel technique that combines either the BEM or the DRBEM with an iterative procedure based on the SQP method. This novel technique follows the work from [11] and [12] where the BEM for the heat diffusion equation has been combined with an iterative algorithm built to minimize a cost function in order to solve inverse problems for identifying point heat sources. The BEM [19] and the DRBEM [20] combined with Tikhonov regularisation or truncated singular value decomposition have been employed to solve Cauchy inverse problems associated to the convection-diffusion equation with constant and variable coefficients, respectively. However, BEMs have not as yet been employed in order to solve inverse source problems related with the convection-diffusion equation, thus the novelty of the present work.

## 2. MATHEMATICAL FORMULATION

We consider a bounded domain $\Omega \subset \mathbb{R}^d$ and we assume that its boundary $\Gamma$ consists of two parts, $S_1$ and $S_2$, such that $\Gamma = S_1 \cup S_2$, where $S_1, S_2 \neq \varnothing$ and $S_1 \cap S_2 \neq \varnothing$.

The water pollution process is assumed to be modelled by the following steady-state convection-diffusion equation:

$$\sum_{m=1}^{d} \frac{\partial^2 c}{\partial x_m^2}(\underline{x}) - \sum_{m=1}^{d} u_m(\underline{x}) \frac{\partial c}{\partial x_m}(\underline{x}) - k(\underline{x})c(\underline{x}) + \psi(\underline{x}) + \sum_{l=1}^{N_s} \phi_l \delta(\underline{x} - \underline{x}_l) = 0, \qquad \underline{x} \in \Omega, \tag{1}$$

where $c(\underline{x})$ is the concentration of the pollutant, the function $u_m(\underline{x})$ is the $x_m$ component of the fluid velocity, the function $k(\underline{x})$ is a decay parameter, $\psi(\underline{x})$ is a continuous source, $N_s$ is the number of point sources, $\delta$ is the Dirac delta function and $\phi_l$ and $\underline{x}_l \in \Omega$ are the $l^{th}$ source strength and location, respectively.

The inverse source problem under investigation requires finding the solution $(c, (\underline{x}_l)_{l=\overline{1,N_s}}, (\phi_l)_{l=\overline{1,N_s}})$ which satisfies eqn. (1) subject to the following boundary conditions:

$$c(\underline{x}) = \tilde{c}(\underline{x}), \qquad \underline{x} \in S_1, \tag{2}$$

$$\frac{\partial c}{\partial n}(\underline{x}) = \tilde{q}(\underline{x}), \qquad \underline{x} \in S_2, \tag{3}$$

where $\tilde{c}$ and $\tilde{q}$ are prescribed functions of $\underline{x}$. It can be seen that on $S_1 \cap S_2$ both $c$ and $\frac{\partial c}{\partial n}$ are specified.

The technique proposed in order to solve numerically the inverse problem given by eqns. (1)−(3) is based on reducing it to a system of algebraic equations which is then solved by an iterative SQP method. We mention that BEM is employed in the case when the coefficients $u_m(\underline{x})$ and $k(\underline{x})$ are constant and $\psi(\underline{x}) = 0$, while in the general case, when $u_m(\underline{x})$, $k(\underline{x})$ and $\psi(\underline{x})$ are variable functions, the DRBEM is employed.

## 3. THE BEM

In the constant coefficients case, i.e. $u_m(\underline{x})$ and $k(\underline{x})$ are constant and $\psi(\underline{x}) = 0$, following the idea from [21], based on the change of variable

$$c = v \exp\left(\frac{1}{2}\underline{u} \cdot \underline{x}\right), \tag{4}$$

where the vector $\underline{u}$ is defined as $\underline{u} = (u_1, u_2, ..., u_d)$, eqn. (1) recasts as follows:

$$\sum_{m=1}^{d} \frac{\partial^2 v}{\partial x_m^2}(\underline{x}) + \mu^2 v(\underline{x}) = -\exp\left(-\frac{\underline{u} \cdot \underline{x}}{2}\right) \sum_{l=1}^{N_s} \phi_l \delta(\underline{x} - \underline{x}_l), \tag{5}$$

where $\underline{x} \in \Omega$ and $\mu = j\left(k + \frac{1}{4}\sum_{m=1}^{d} u_m^2\right)^{1/2}$, with $j = \sqrt{-1}$. The boundary conditions (2) and (3) transform into

$$v(\underline{x}) = \tilde{c}(\underline{x}) \exp\left(-\frac{1}{2}\underline{u} \cdot \underline{x}\right), \qquad \underline{x} \in S_1, \tag{6}$$

$$\frac{\partial v}{\partial n}(\underline{x}) + \frac{1}{2}v(\underline{x})\left(\underline{u} \cdot \frac{\partial \underline{x}}{\partial n}\right) = \tilde{q}(\underline{x}) \exp\left(-\frac{1}{2}\underline{u} \cdot \underline{x}\right), \qquad \underline{x} \in S_2. \tag{7}$$

The standard BEM procedure is applied to eqn. (5) to obtain the following boundary integral equation for each boundary node $\underline{x}^i \in \Gamma$, $i = \overline{1,N}$:

$$\eta(\underline{x}^i)v(\underline{x}^i) + \int_\Gamma v(\underline{y})\frac{\partial E}{\partial n(\underline{y})}(\underline{x}^i,\underline{y})d\Gamma(\underline{y}) - \int_\Gamma \frac{\partial v}{\partial n(\underline{y})}(\underline{y})E(\underline{x}^i,\underline{y})d\Gamma(\underline{y}) = -\sum_{l=1}^{N_s}\exp\left(-\frac{\underline{u}\cdot\underline{x}_l}{2}\right)\phi_l E(\underline{x}^i,\underline{x}_l), \tag{8}$$

where $\eta(\underline{x}^i) = \vartheta_i/(2\pi)$, with $\vartheta_i$ the angle between the left and the right tangents on $\Gamma$ at the boundary node $\underline{x}^i$ for $i = \overline{1,N}$, and $n$ is the outward normal at the boundary $\Gamma$. In particular, if $\Gamma$ is smooth then $\vartheta_i = \pi$ for $i = \overline{1,N}$. The function $E(\underline{x},\underline{y})$ is the fundamental solution for the Helmholtz operator $\nabla^2 + \mu^2$, i.e. $E(\underline{x},\underline{y}) = \frac{i}{4}H_0^{(1)}(\mu r(\underline{x},\underline{y}))$, where $r(\underline{x},\underline{y}) = |\underline{x}-\underline{y}|$ is the geodesic distance and $H_0^{(1)}$ is the Hankel function of the first kind and of zero order, see for example [1] or [7].

After integrating over each boundary element, eqn. (8) can be written in terms of the nodal values as follows:

$$\eta_i v_i + \sum_{k=1}^{N} H_{ik}v_k - \sum_{k=1}^{N} G_{ik}q_k = -\sum_{l=1}^{N_s} I_{il}\phi_l, \qquad i = \overline{1,N}, \tag{9}$$

where $q = \partial v/\partial n$, $H_{ik}$ and $G_{ik}$ are the usual resultants of integration over the boundary elements, see [8], and

$$I_{il} = \exp\left(-\frac{\underline{u}\cdot\underline{x}_l}{2}\right)E(\underline{x}^i,\underline{x}_l), \qquad i = \overline{1,N}, \qquad l = \overline{1,N_s}. \tag{10}$$

After application to all the boundary nodes $\underline{x}^i$, $i = \overline{1,N}$ and incorporating the terms $\eta_i$ onto the diagonal of $\mathbf{H}$, eqn. (9) can be expressed in matrix form as follows:

$$\mathbf{H}\underline{v} - \mathbf{G}\underline{q} = -\mathbf{I}\underline{\phi}, \tag{11}$$

where $\mathbf{H}$ and $\mathbf{G}$ are the $N \times N$ matrices of the coefficients $H_{ik}$ and $G_{ik}$, $\underline{v}$ and $\underline{q}$ are two vectors of order $N$ containing the boundary values of $v$ and $\frac{\partial v}{\partial n}$, respectively, $\mathbf{I}$ is an $N \times N_s$ matrix of the coefficients $I_{il}$ and $\underline{\phi}$ is a vector of order $N_s$ containing the values of the strengths of the sources.

## 4. THE DRBEM

In the variable coefficients case, i.e. $u_m(\underline{x})$, $k(\underline{x})$ and $\psi(\underline{x})$ are variable functions, the BEM cannot be employed since the fundamental solution for eqn. (1) is not available. Thus a more general method, i.e. the DRBEM must be used.

The governing eqn. (1) is written in the following form:

$$\sum_{m=1}^{d}\frac{\partial^2 c}{\partial x_m^2}(\underline{x}) + \sum_{l=1}^{N_s}\phi_l\delta(\underline{x}-\underline{x}_l) = b(\underline{x},c,\nabla c), \qquad \underline{x}\in\Omega, \tag{12}$$

where

$$b(\underline{x},c,\nabla c) = \sum_{m=1}^{d} u_m(\underline{x})\frac{\partial c}{\partial x_m}(\underline{x}) + k(\underline{x})c(\underline{x}) - \psi(\underline{x}). \tag{13}$$

In this way the left-hand side of eqn. (12) is dealt with by using the fundamental solution of the Laplace equation and the proprieties of the Dirac delta function, whilst all the integrals corresponding to the right-hand side $b$ are taken to the boundary using the approximation

$$b \simeq \sum_{j=1}^{N+L}\alpha_j f_j \tag{14}$$

where $\alpha_j$ are initially unknown coefficients and $f_j$ are approximating functions. In the numerical results presented in Section 6, the thin plate spline (TPS) function $f = r^2\ln r$ was considered as the approximating function. However, we mention that other radial basis functions (RBFs) were also considered in our study, especially the augmented thin plate spline (ATPS) which involves the following approximation of the source term $b$:

$$b \simeq \sum_{j=1}^{N+L} \alpha_j (r_j^2 \ln r_j) + \beta_0 + \beta_1 x_1 + ... + \beta_d x_d, \tag{15}$$

with $\beta_0$, $\beta_1$,...,$\beta_d$ constants determined with the help of some equilibrium constraints. It should be noted that for the test examples investigated in this study the TPS and the ATPS approximating functions provided very similar results.

The DRBEM procedure, [14] and [17], is applied to give

$$\int_\Omega (\sum_{m=1}^{d} \frac{\partial^2 c}{\partial x_m^2}) G d\Omega + \int_\Omega (\sum_{l=1}^{N_s} \phi_l \delta(\underline{x} - \underline{x}_l)) G d\Omega = \sum_{j=1}^{N+L} \alpha_j \int_\Omega (\sum_{m=1}^{d} \frac{\partial^2 \hat{c}_j}{\partial x_m^2}) G d\Omega, \tag{16}$$

where $\hat{c}_j$ are particular solutions of eqn. (1) for $j = \overline{1,(N+L)}$ and $G$ is the fundamental solution of the Laplace equation.

On applying Green's second identity and the proprieties of the Dirac delta function to expression (16) the following boundary integral equation for each source node $i = \overline{1,(N+L)}$, is obtained:

$$\eta_i c_i + \int_\Gamma c G' d\Gamma - \int_\Gamma q G d\Gamma + \sum_{l=1}^{N_s} \phi_l G(\underline{x}^i, \underline{x}_l) = \sum_{j=1}^{N+L} \alpha_j \left( \eta_i \hat{c}_{ij} + \int_\Gamma \hat{c}_j G' d\Gamma - \int_\Gamma \hat{q}_j G d\Gamma \right), \tag{17}$$

where $G' = \partial G/\partial n$ and $\hat{q} = \partial \hat{c}/\partial n$. The coefficients $\eta_i$ are defined as

$$\eta_i = \begin{cases} \vartheta_i/(2\pi), \text{for} & i = \overline{1,N} \\ 1, \quad\quad \text{for} & i = \overline{(N+1),(N+L)}. \end{cases} \tag{18}$$

Equation (17) is then written in discretised form, with summations over $\Gamma_k$ boundary elements for $k = \overline{1,N}$ replacing the integrals. $(N+L)$ DRBEM collocation nodes are used for the discretisation and the following equation for a source node $i$ is obtained:

$$\eta_i c_i + \sum_{k=1}^{N} H_{ik} c_k - \sum_{k=1}^{N} G_{ik} q_k + \sum_{l=1}^{N_s} I_{il} \phi_l = \sum_{j=1}^{N+L} \alpha_j \left( \eta_i \hat{c}_{ij} + \sum_{k=1}^{N} H_{ik} \hat{c}_{kj} - \sum_{k=1}^{N} G_{ik} \hat{q}_{kj} \right), \tag{19}$$

where $i = \overline{1,(N+L)}$ are the source nodes, $k$ are the boundary elements and $j$ are the DRBEM collocation points. $H_{ik}$ and $G_{ik}$ are the usual resultants of integration over the boundary elements, see [8], and the coefficient $I_{il}$ is the following:

$$I_{il} = G(\underline{x}^i, \underline{x}_l), \qquad i = \overline{1,N}, l = \overline{1,N_s}. \tag{20}$$

After application to all boundary nodes $\underline{x}^i$, $i = \overline{1,N}$ and incorporating the terms $\eta_i$ onto the diagonal of $\mathbf{H}$, eqn. (19) can be expressed in matrix form as follows:

$$\mathbf{H}\underline{c} - \mathbf{G}\underline{q} + \mathbf{I}\underline{\phi} = \sum_{j=1}^{N+L} \alpha_j (\mathbf{H}\underline{\hat{c}}_j - \mathbf{G}\underline{\hat{q}}_j), \tag{21}$$

where $\mathbf{H}$ and $\mathbf{G}$ are $(N+L) \times (N+L)$ matrices, $\underline{c}$ and $\underline{q}$ are two vectors of order $(N+L)$, $\mathbf{I}$ is an $(N+L) \times N_s$ matrix of the coefficients $I_{il}$ and $\underline{\phi}$ is a vector of order $N_s$.

If each of the vectors $\underline{\hat{c}}_j$ and $\underline{\hat{q}}_j$ is considered to be a single column of the matrices $\hat{\mathbf{C}}$ and $\hat{\mathbf{Q}}$, respectively, then eqn. (21) can be written without summation to produce

$$\mathbf{H}\underline{c} - \mathbf{G}\underline{q} + \mathbf{I}\underline{\phi} = (\mathbf{H}\hat{\mathbf{C}} - \mathbf{G}\hat{\mathbf{Q}})\underline{\alpha}. \tag{22}$$

The DRBEM expansion for every term of $\underline{b}$, [18], is employed and the following expression is obtained:

$$\mathbf{H}\underline{c} - \mathbf{G}\underline{q} + \mathbf{I}\underline{\phi} = \mathbf{S} \left[ \sum_{m=1}^{d} \mathbf{U}_m \frac{\partial \mathbf{F}}{\partial x_m} \mathbf{F}^{-1} + \mathbf{K} \right] \underline{c} - \mathbf{S}\underline{\psi}, \tag{23}$$

where $\mathbf{S} = (\mathbf{H}\hat{\mathbf{C}} - \mathbf{G}\hat{\mathbf{Q}})\mathbf{F}^{-1}$. The matrices $\hat{\mathbf{C}}$, $\hat{\mathbf{Q}}$, $\mathbf{F}^{-1}$ and $\frac{\partial \mathbf{F}}{\partial x_m}$ are all known since $f$ is defined. The other matrices, namely $\mathbf{U}_m$ and $\mathbf{K}$, and the vector $\underline{\psi}$ are also known, as the coefficients $u_m(\underline{x})$, $k(\underline{x})$ and $\psi(\underline{x})$ of eqn. (1) are known.

## 5. AN ITERATIVE SQP METHOD

As in Sections 3 and 4, the inverse source problem is reduced to a system of algebraic equations of the form (11) and (23) after the application of the BEM and the DRBEM, respectively. As these systems of equations are non-linear, special care must be taken when solving them.

In the following we present an iterative SQP proposed in order to solve the system of eqns. (11) and we mention that the same technique, with very few and straightforward modifications, is employed to solve the system of eqns. (23).

In the two-dimensional case, and when all the boundary values for $v$ and $q$ are specified ($S_1 = S_2 = \Gamma$), then the system of eqns. (11) contains $N$ eqns. and $3N_s$ unknowns, namely $x_l$, $y_l$ and $\phi_l$ for $l = \overline{1, N_s}$. When some of the boundary values for $v$ and $q$ are not known ($S_1 \neq S_2$), then those values will act as unknowns in the system of eqns. (11), making the number of unknowns greater than $3N_s$.

It is observed that only the strengths of the sources appear linearly in the system of eqns. (11), while the locations of the sources appear as nonlinear unknowns. The iterative SQP method employed in this study consists in solving at each iteration a system of linear algebraic eqns. that results from a direct problem. Briefly, the method used to solve the nonlinear system of eqns. (11) in the two-dimensional case is the following:

(i) Choose an initial guess for the locations $(x_l^0, y_l^0)$ and the strengths $\phi_l^0$ of the sources of pollution, where $l = \overline{1, N_s}$. This initial guess should be made in such a way that some bounds on the unknown variables are satisfied, namely $(x_l^0, y_l^0) \in \Omega$ and $\phi_l^0 \geq 0$, for $l = \overline{1, N_s}$, as the location of the source should be inside the solution domain and the strength of the source a non-negative number.

(ii) Separate the boundary conditions into two categories. The first set of boundary conditions contains the minimum number of boundary conditions which generate a well-posed direct problem when combined with the Helmholtz equation (5) and the initial guesses for the unknown variables made in the first step. This set of boundary conditions is used to form a vector $\underline{v}^A$. The second set of boundary conditions contains the information that is not necessary for solving the direct problem. These boundary conditions form a vector, denoted by $\underline{v}^B$, that is used in the stopping criterion of the iterative procedure. It should be noted that the vector $\underline{v}^B$ contains the observed values of $v$ at the sampling locations, which are usually all situated on the boundary in order to benefit from the advantage of the BEM, i.e. the possibility of using only boundary values. However, internal sampling points can easily be accomodated in the iterative BEM without reducing the performance of the method.

(iii) A positive real function of $3N_s$ variables, called the objective function, is defined as follows:

$$F((x_l, y_l, \phi_l), l = \overline{1, N_s}) = \|\underline{v}^{(num)} - \underline{v}^B\|^2, \tag{24}$$

where the vector $\underline{v}^{(num)}$ contains some of the numerical results for $v$ and $q$ obtained by solving the direct problems considered at each iteration, chosen such that the difference from the definition of the function $F$ given in the expression (24) is relevant.

(iv) Solve the nonlinear programming problem that is the minimisation of the smooth function $F$ subject to some bounds on the variables using a sequential quadratic programming (SQP) method. This minimisation problem is stated in the following form:

$$\text{Minimise } F \qquad \text{subject to} \qquad \begin{cases} (x_l, y_l) \in \Omega \\ \phi_l \geq 0 \end{cases}, \qquad l = \overline{1, N_s}. \tag{25}$$

This problem is solved using the NAG Fortran subroutine $E04UCF$, see NAG Fortran Library Manual, Mark 20. The numerical solution of the problem (25) is obtained iteratively by this subroutine containing both the value of the function $F$ and the values of the variables $x_l$, $y_l$ and $\phi_l$ for $l = \overline{1, N_s}$, where the function $F$ reaches its minimal value. These last values also represent the numerical solution for the inverse source problem. This subroutine allows the user to change the accuracy of the numerical solution by modifying an optimality tolerance parameter. Broadly speaking, this parameter indicates the number of correct figures desired in the objective function $F$ at the solution. For example, if the optimality tolerance parameter is $10^{-7}$ and $E04UCF$ terminates successfully, the final value of the objective function $F$ should have approximately seven correct figures. We mention here that in all the test examples considered, the optimality tolerance parameter was taken to be the same as the machine precision, namely $10^{-16}$.

## 6. NUMERICAL RESULTS AND DISCUSSION

We investigate some examples in order to test the method proposed for solving the inverse source problem associated with the two-dimensional steady-state convection-diffusion equation. The solution domain for all the examples presented herein is chosen to be the rectangular domain $\Omega = \{(x, y) : -2 < x < 2, -1 < y < 1\}$ bounded by the rectangle $\Gamma = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3 \cup \Gamma_4$, where $\Gamma_1 = \{2\} \times [-1, 1)$, $\Gamma_2 = ([-2, 2] \times \{1\})$, $\Gamma_3 = \{-2\} \times [-1, 1)$ and $\Gamma_4 = ((-2, 2) \times \{-1\})$. This geometry is intended to approximate a region of a polluted river from one or more pollutant point sources. We consider several examples whose analytical solution is known, such that a comparison between the numerical results obtained by the method and some exact solutions can be made.

**Example 1.** We present the results obtained using the BEM and the iterative SQP method for the constant-coefficients case when the method correctly assumes the existence of three point sources of pollution. The governing convection-diffusion equation is taken to be the following:

$$\nabla^2 c(x, y) - \frac{\partial c}{\partial x}(x, y) - \frac{1}{2}c(x, y) + \frac{3}{2}\delta\left((x, y), (-1.5, 0.7)\right) + \delta\left((x, y), (-1, -0.5)\right) + \frac{6}{5}\delta\left((x, y), (1, 0.5)\right) = 0, \tag{26}$$

where $(x, y) \in \Omega$. As presented in Section 3, the convection-diffusion eqn. (26) corresponds to the following equation:

$$\nabla^2 v(x, y) - \frac{3}{4}v(x, y) = -\exp\left(-\frac{x}{2}\right)\left[-\frac{3}{2}\delta\left((x, y), (-1.5, 0.7)\right) - \delta\left((x, y), (-1, -0.5)\right) - \frac{6}{5}\delta\left((x, y), (1, 0.5)\right)\right]. \tag{27}$$

| | Exact solution | Initial guess | 0% noise | 1% noise | 3% noise | 5% noise | 10% noise |
|---|---|---|---|---|---|---|---|
| $x_1$ | $-1.5$ | 0 | $-1.5 + \mathbf{O}(10^{-8})$ | $-1.49968$ | $-1.49916$ | $-1.49896$ | $-1.49853$ |
| $y_1$ | 0.7 | 0 | $0.7 + \mathbf{O}(10^{-8})$ | 0.70170 | 0.70524 | 0.70708 | 0.71901 |
| $\phi_1$ | 1.5 | 0 | $1.5 + \mathbf{O}(10^{-8})$ | 1.50515 | 1.51439 | 1.51847 | 1.53569 |
| $x_2$ | $-1$ | 0 | $-1 + \mathbf{O}(10^{-9})$ | $-0.99995$ | $-1.00009$ | $-1.00024$ | $-1.00151$ |
| $y_2$ | $-0.5$ | 0 | $-0.5 + \mathbf{O}(10^{-8})$ | $-0.51384$ | $-0.54109$ | $-0.55442$ | $-0.62843$ |
| $\phi_2$ | 1 | 0 | $1 + \mathbf{O}(10^{-8})$ | 0.98489 | 0.95599 | 0.94229 | 0.87157 |
| $x_3$ | 1 | 0 | $1 + \mathbf{O}(10^{-9})$ | 0.99780 | 0.99348 | 0.99138 | 0.98017 |
| $y_3$ | 0.5 | 0 | $0.5 + \mathbf{O}(10^{-9})$ | 0.49573 | 0.48709 | 0.48276 | 0.45741 |
| $\phi_3$ | 1.2 | 0 | $1.2 + \mathbf{O}(10^{-9})$ | 1.20673 | 1.22012 | 1.22670 | 1.26307 |
| $F((\underline{x}_l, \phi_l), l = \overline{1, 3})$ | | | $7.80537E-16$ | $2.15E-4$ | $1.92E-3$ | $3.42E-3$ | $2.12E-2$ |
| Number of iterations | | | 67 | 71 | 64 | 80 | 102 |

Table 1: The numerical results obtained using 60 CBEs and input data with 0%, 1%, 3%, 5% and 10% noise, for Example 1.

We take the analytical solution for the the partial differential eqn. (27) the following:

$$v(x, y) = \frac{1.5}{2\pi}\exp\left(\frac{1.5}{2}\right)K_0\left(\frac{\sqrt{3}}{2}\sqrt{(x + 1.5)^2 + (y - 0.7)^2}\right) + \tag{28}$$

$$\frac{1}{2\pi}\exp\left(\frac{1}{2}\right)K_0\left(\frac{\sqrt{3}}{2}\sqrt{(x + 1)^2 + (y + 0.5)^2}\right) + \frac{1.2}{2\pi}\exp\left(\frac{1.2}{2}\right)K_0\left(\frac{\sqrt{3}}{2}\sqrt{(x - 1)^2 + (y - 0.5)^2}\right)$$

where $K_0$ is the modified Bessel function of the second kind and order zero, see [1], and we assume that $v$ is specified on $S_1 = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ and $q$ is specified on $S_2 = \Gamma_2 \cup \Gamma_4$. In practical problems, the flux $q$ on the banks of the river is equal to 0 and therefore it is natural to consider the values of $q$ on $S_2$ as known. This example also assumes that the concentration can be measured at some points upstream (on $\Gamma_3$) and downstream (on $\Gamma_1$) of the source of pollution and at some points on one side of the river (on $\Gamma_2$).

The domain is discretised using 60 constant boundary elements (CBEs), i.e. 10 elements on $\Gamma_1$, 20 on $\Gamma_2$, 10 on $\Gamma_3$ and 20 on $\Gamma_4$, and the initial guesses are chosen to be $x_1^0 = 0$, $y_1^0 = 0$, $\phi_1^0 = 0$, $x_2^0 = 0$, $y_2^0 = 0$,

$\phi_2^0 = 0$, $x_3^0 = 0$, $y_3^0 = 0$ and $\phi_3^0 = 0$. In order to simulate the measurement error, random noisy variables are added to the exact values of the concentration input data at each nodal point. Therefore we perturb the input data $v$ on $S_1 = \Gamma_1 \cup \Gamma_2 \cup \Gamma_3$ as follows: $v_i^\delta = v_i + \delta v_i$, $\delta v_i = G05DDF(0, \sigma_i)$, $\sigma_i = |v_i| \frac{p}{100}$, where $\delta v_i$ is a Gaussian random variable with mean zero and standard deviation $\sigma_i$, generated by the NAG subroutine G05DDF (see NAG Fortran Library Manual, Mark 19) and $p$ is the percentage of noise.

Table 1 presents the numerical results obtained when both exact and noisy input data is used. We observe that all three sources are found very accurately. Also, the results for the cases when 1%, 3%, 5% and 10% noise is added indicate the stability of the method, as less noise in the input data generates more accurate numerical solutions.

**Example 2.** We investigate the use of the DRBEM combined with the iterative SQP method in the case of pollution caused by two point sources which are *a-priori* correctly estimated. The governing convection-diffusion equation with variable coefficients is considered to be the following:

$$\nabla^2 c(x,y) - (1-y^2)\frac{\partial c}{\partial x}(x,y) - \frac{1}{2}c(x,y) + \psi(x,y) + 7\delta\left((x,y)-(-1,-0.5)\right) + 5\delta\left((x,y)-(-1.5,0.7)\right) = 0, \tag{29}$$

where $(x, y) \in \Omega$ and

$$\psi(x,y) = y^2 \frac{\partial c_1}{\partial x}(x,y) - \frac{\partial c_2}{\partial x}(x,y) + \frac{1}{16}c_2(x,y), \tag{30}$$

with

$$c_1(x,y) = \frac{7}{2\pi}\exp\left(\frac{x+1}{2}\right)K_0\left(\frac{\sqrt{3}}{2}\sqrt{(x+1)^2+(y+0.5)^2}\right) + \frac{5}{2\pi}\exp\left(\frac{x+1.5}{2}\right)K_0\left(\frac{\sqrt{3}}{2}\sqrt{(x+1.5)^2+(y-0.7)^2}\right) \tag{31}$$

and

$$c_2(x,y) = \exp\left(-\frac{1}{4}x + \frac{1}{4}y^2\right). \tag{32}$$

| | Exact solution | Initial guess | 0% noise | 1% noise | 3% noise | 5% noise | 10% noise |
|---|---|---|---|---|---|---|---|
| $x_1$ | $-1$ | 0 | $-1.0004$ | $-1.0015$ | $-1.0038$ | $-1.0062$ | $-1.0120$ |
| $y_1$ | $-0.5$ | 0 | $-0.4986$ | $-0.4985$ | $-0.4984$ | $-0.4983$ | $-0.4981$ |
| $\phi_1$ | 7 | 0 | 7.0157 | 7.0290 | 7.0558 | 7.0826 | 7.1504 |
| $x_2$ | $-1.5$ | 0 | $-1.5001$ | $-1.4994$ | $-1.4982$ | $-1.4970$ | $-1.4939$ |
| $y_2$ | 0.7 | 0 | 0.7005 | 0.7004 | 0.7004 | 0.7003 | 0.7001 |
| $\phi_2$ | 5 | 0 | 4.9904 | 4.9883 | 4.9840 | 4.9798 | 4.9695 |
| $F((\underline{x}_l, \phi_l), l = 1, 2)$ | | | $2.2 \cdot 10^{-3}$ | $4.8 \cdot 10^{-3}$ | $2.8 \cdot 10^{-2}$ | $7.5 \cdot 10^{-2}$ | $2.9 \cdot 10^{-1}$ |
| Number of iterations | | | 48 | 68 | 43 | 41 | 44 |

Table 2: The numerical results obtained using the distribution $60-48$ and input data with 0%, 1%, 3%, 5% and 10% noise, for Example 2.

The inverse source problem under investigation is defined by considering the following boundary conditions: it is assumed that, from measurements, the concentration $c$ is known on all the boundary $\Gamma$. Also, the flux on $\Gamma_2$ and $\Gamma_4$ is assumed to be known, as in a practical situation the flux is zero on the banks of the river. With these premises, the inverse source problem requires the identification of the locations and strengths of the two source of pollution. The analytical solution for the concentration $c$ is known and it is given by $c(x, y) = c_1(x, y) + c_2(x, y)$, where $c_1$ and $c_2$ are those defined in (31) and (32), respectively.

The iterative DRBEM with the distribution $60-48$ using discontinuous linear boundary elements (DLBEs) is employed when both exact and noisy input data is considered. The distribution $60-48$ means that 60 DLBEs are considered on the boundary with the following distribution: 10 on $\Gamma_1$, 20 on $\Gamma_2$, 10 on $\Gamma_3$ and 20 on $\Gamma_4$. Also, four small rectangles are considered, having the following widths and lengths: 0.2 and 0.4, 0.4 and 0.8, 0.6 and 1.2, and 0.8 and 1.6, and 12 uniformly distributed points are taken on each of these rectangles. The approximating function chosen is the TPS. Table 2 presents the numerical results obtained in this case, which show a very high accuracy and indicate the stability of the method.

**Example 3.** The constant-coefficient case is investigated when two point sources are expected to be found, but the real situation corresponds to the pollution being caused by only a single point source. We wish to present the way in which the method deals with this type of situation. Therefore the process of pollution is considered to be governed by the following convection-diffusion equation:

$$\nabla^2 c(x,y) - \frac{\partial c}{\partial x}(x,y) + \delta\left((x,y),(-1,-0.5)\right) = 0, \tag{33}$$

where $(x,y) \in \Omega$. Using the change of variable $c = v \exp\left(\frac{x}{2}\right)$, eqn. (33) can be recast as follows:

$$\nabla^2 v(x,y) - \frac{1}{4} v(x,y) = -\exp\left(-\frac{x}{2}\right) \delta\left((x,y),(-1,-0.5)\right) \tag{34}$$

and the same boundary conditions as in Example 1 are considered. The analytical solution for eqn. (34) has the following form:

$$v(x,y) = \frac{1}{2\pi} \exp\left(\frac{1}{2}\right) K_0\left(\frac{1}{2}\sqrt{(x+1)^2+(y+0.5)^2}\right). \tag{35}$$

The initial guesses are taken to be $x_1^0 = 0$, $y_1^0 = 0$, $\phi_1^0 = 0$, $x_2^0 = 0$, $y_2^0 = 0$ and $\phi_2^0 = 0$, and 60 CBEs are used for the discretisation. The problem is solved using both exact and noisy input data and the numerical results obtained are presented in Table 3. It is observed that although we wish to identify only one source, the numerical method assumes the existence of two sources. However, these two sources are found to be virtually at the same location, each of them having virtually the same strength, which is equal to approximately half the strength of the source we want to identify. The numerical results indicate the accuracy, convergence and stability of the method.

| | Exact solution | Initial guess | 0% noise | 1% noise | 3% noise | 5% noise | 10% noise |
|---|---|---|---|---|---|---|---|
| $x_1$ | $-1$ | 0 | $-1+\mathbf{O}(10^{-8})$ | $-1.00002$ | $-1.00008$ | $-1.00014$ | $-1.00029$ |
| $y_1$ | $-0.5$ | 0 | $-0.5+\mathbf{O}(10^{-9})$ | $-0.50121$ | $-0.50365$ | $-0.50611$ | $-0.51238$ |
| $\phi_1$ | 1 | 0 | $0.5+\mathbf{O}(10^{-8})$ | 0.49988 | 0.49963 | 0.49939 | 0.49877 |
| $x_2$ | none | 0 | $-1+\mathbf{O}(10^{-8})$ | $-1.00002$ | $-1.00008$ | $-1.00014$ | $-1.00029$ |
| $y_2$ | none | 0 | $-0.5+\mathbf{O}(10^{-9})$ | $-0.50121$ | $-0.50365$ | $-0.50611$ | $-0.51238$ |
| $\phi_2$ | none | 0 | $0.5+\mathbf{O}(10^{-8})$ | 0.49988 | 0.49963 | 0.49939 | 0.49877 |
| $F((\underline{x}_l,\phi_l), l=1,2)$ | | | $1.65200E-17$ | $1.43E-4$ | $1.29E-3$ | $3.58E-3$ | $1.43E-2$ |
| Number of iterations | | | 14 | 13 | 12 | 13 | 13 |

Table 3: The numerical results obtained using 60 CBEs and input data with 0%, 1%, 3%, 5% and 10% noise, for Example 3.

It should also be mentioned here that other examples have been investigated for the case when the method assumes the existence of two sources, but in reality there is only one. Two contrasting types of results have been obtained, depending on the example being considered. The first type is the one presented in this example, namely two sources are found at virtually the same location, the sum of their strengths being equal to the value of the source strength we wish to identify. The second type, present in other examples, also found two sources, one of them being the real source, while the other source was identified at a random location inside the solution domain but with a very small strength, e.g. a value of $\mathbf{O}(10^{-10})$. Therefore, we may say that the method deals very well with this situation. The only inconvenience is that more computational time is required than in the case when the number of sources is known correctly, as the matrix $\mathbf{I}$ and the vector $\underline{\phi}$ from eqns. (11) and (23) have higher dimensions and therefore their storage occupies more memory in the computer and their use in mathematical operations requires more computational time.

## 7. CONCLUSIONS

In this study we have presented a numerical technique for solving the inverse source problem for the steady-state convection-diffusion equation with constant or variable coefficients. The BEM and the DRBEM are applied in the constant and variable coefficients case, respectively, and the resulting nonlinear system of algebraic eqns. is solved using an iterative procedure based on the SQP method.

The BEM proved to be very suitable for situations when the number of sources is correctly or over estimated. In the over estimated case the numerical solutions were of two distinct types, both suggesting very clearly the real number of sources and at the same time approximating accurately their location and strength. Although it has been seen that the method deals very effectively with over estimated number of sources, it is advisable to use the method with a number of sources that is relevant for each case considered and not artificially increase the number of sources that are sought, as this increases the computational time needed by the method. We also mention that when the number of sources is under estimated then the method finds the numerical solution that, among all the solutions with the corresponding under estimated number of sources, best fits the real situation. However, from a practical point of view, this solution is irrelevant. In this case, the value of the objective function has been found to be a very effective and reliable indicator of how relevant is the numerical solution. More specifically, when an irrelevant solution is obtained the objective function takes values which are at least one order of magnitude higher than those taken when a relevant solution is obtained. Thus, if the number of sources is unknown, then the method should be employed for different estimates of the number of sources and then the numerical solution with the smallest corresponding value for the objective function should be considered.

Future work should investigate the use of the DRBEM in cases when the number of sources is over or under estimated. Also the development of similar numerical techniques to deal with inverse problems for the transient convection-diffusion equation should be considered.

**Acknowledgements**
Alexandru Rap would like to acknowledge the financial support received from the ORS and the School of the Environment, University of Leeds, UK.

## REFERENCES

1. M. Abramowitz and I.A. Stegun, *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables*, Dover Publications, New York, 1972.

2. S. Alapati and Z. J. Kabala, Recovering the release history of a groundwater contamination using a non-linear least-squares method, *Hydrological Processes* (2000) **14**, 1003–1016.

3. M.M. Aral, J. Guan and M.L. Maslia, Identification of contaminant source location and release history in aquifers, *J. Hydrologic Eng.* (2001) **6**(3), 225–234.

4. J. Atmadja and A.C. Bagtzoglou, Pollution source identification in heterogeneous porous media, *Water Resour. Res.* (2001) **37**(8), 2113–2125.

5. A.C. Bagtzoglou and J. Atmadja, Marching-jury backward beam equation and quasi-reversibility methods for hydrologic inversion: Application to contaminant plume spatial distribution recovery, *Water Resour. Res.* (2003) **39**(2), 10-1–10-14.

6. A.C. Bagtzoglou, A.F.B. Tompson and D.E. Dougherty, Probabilistic simulations for reliable solute source identification in heterogeneous porous media, (ed. J. Ganoulis), Springer-Verlag, Berlin Heidelberg, 1991, **G29**, pp.189–201.

7. W.W. Bell, *Special Functions for Scientists and Engineers*, Van Nostrand, London, 1968.

8. C.A. Brebbia, J.F.C. Telles and L.C. Wrobel, *Boundary Element Techniques*, Springer-Verlag, Berlin, 1984.

9. S.M. Gorelick, B. Evans and I. Remson, Identifying sources of groundwater pollution: An optimization approach, *Water Resour. Res.* (1983) **19**(3), 779–790.

10. C. Kauffmann and W. Kinzelbach, Parameter estimation in contaminant transport modelling, *Contaminant Transport in Groundwater*, (eds. H.E. Kobus and W. Kinzelbach), Balkema Publishers, Rotterdam, 1989, pp.355–362.

11. C. LeNiliot and F. Lefèvre, A method for multiple steady line heat sources identification in a diffusive system: application to an experimental 2D problem, *Int. J. Heat Mass Transfer* (2001) **44**, 1425–1438.

12. C. LeNiliot and F. Lefèvre, A parameter estimation approach to solve the inverse problem of point heat sources identification, *Int. J. Heat Mass Transfer* (2004) **47**, 827–841.

13. A.M. Michalak and P.K. Kitanidis, A method for enforcing parameter nonnegativity in Bayesian inverse problems with an application to contaminant source identification, *Water Resour. Res.* (2003) **39**(2), 7-1–7-13.

14. D. Nardini and C.A. Brebbia, A New Approach to Free Vibration Analysis using Boundary Elements, *Boundary Element Methods in Engineering*, Computational Mechanics Publications, Southampton, 1982, pp.312-326.

15. R.M. Neupauer, B. Borchers and J.L. Wilson, Comparison of inverse methods for reconstructing the release history of a groundwater contamination source, *Water Resour. Res.* (2000) **36**(9), 2469–2475.

16. R.M. Neupauer and J.L. Wilson, Adjoint-derived location and travel time probabilities for a multidimensional groundwater system, *Water Resour. Res.* (2001) **37**(6), 1657–1668.

17. P.W. Partridge, C.A. Brebbia and L.C. Wrobel, *The Dual Reciprocity Boundary Element Method*, Computational Mechanics Publications, Southampton, 1992.

18. P.W. Partridge, *Transport Analysis using Boundary Elements*, Computational Mechanics Publications, Southampton, 1993.

19. A. Rap, L. Elliott, D.B. Ingham, D. Lesnic and X. Wen, The Cauchy problem for the steady-state convection-diffusion equation using BEM, *Advances in Boundary Element Techniques IV*, (eds. R. Gallego and M.H. Aliabadi), Queen Mary University of London, 2003, pp.281-286.

20. A. Rap, L. Elliott, D.B. Ingham, D. Lesnic and X. Wen, DRBEM for Cauchy convection-diffusion problems with variable coefficients, *Eng. Anal. Boundary Elements* (2004) **28**, 1321–1333.

21. K.M. Singh and M. Tanaka, On exponential variable transformation based boundary element formulation for advection-diffusion problems, *Eng. Anal. Boundary Elements* (2000) **24**, 225–235.

22. T.H. Skaggs and Z.J. Kabala, Recovering the release history of a groundwater contaminant, *Water Resour. Res.* (1994) **30**(1), 71–79.

23. M.F. Snodgrass and P.K. Kitanidis, A geostatistical approach to contaminant source identification, *Water Resour. Res.* (1997) **33**(4), 537–546.

24. A.D. Woodbury and T.J. Ulrych, Minimum relative entropy inversion: Theory and application to recovering the release history of a groundwater contaminant, *Water Resour. Res.* (1996) **32**(9), 2671–2681.