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To cite this article: Moh. Ivan Azis *et al* 2018 *J. Phys.: Conf. Ser.* **979** 012075

IOP Conf. Series: Journal of Physics: Conf. Series **979** (2018) 012075 doi:10.1088/1742-6596/979/1/012075

On some examples of pollutant transport problems solved numerically using the boundary element method

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Abstract. A boundary element method (BEM) is obtained for solving a boundary value problem of homogeneous anisotropic media governed by diffusion-convection equation. The application of the BEM is shown for two particular pollutant transport problems of Tello river and Unhas lake in Makassar Indonesia. For the two particular problems a variety of the coefficients of diffusion and the velocity components are taken. The results show that the solutions vary as the parameters change. And this suggests that one has to be careful in measuring or determining the values of the parameters.

1. Introduction

The boundary element method (BEM) has been used extensively for solving numerically a wide range of problems. This includes deformation problems of elastic materials, heat conduction problems, infiltration problems, pollutant transport problems and many others. And the use of the BEM has also been applied not only to homogeneous but also to inhomogeneous materials, and not only to isotropic but also to anisotropic materials. For example, [1] used the BEM for solving infiltration problems of isotropic homogeneous media, [2] derived a fundamental solution, [3] considered diffusion-convection problems for anisotropic homogeneous materials, [4] solved elasticity problems for isotropic inhomogeneous materials and [5] studied elasticity problems, [6] worked on elliptic boundary value problems, [7] solved heat conduction problems, [8] worked on elasticity problems and [9] considered transient heat conduction problems for anisotropic inhomogeneous materials.

In this paper, some more examples of pollutant transport problems will be solved using the BEM, in addition to those considered by [3]. In the following sections the analysis used in [3] for deriving a boundary integral equation will be shown again.

2. The boundary value problems

The dimensionless governing equation of pollutant transport problems for anisotropic media with constant coefficients may be written as

$$\lambda_{ij}\frac{\partial^2 p(\mathbf{x})}{\partial x_i \partial x_j} - v_i \frac{\partial p(\mathbf{x})}{\partial x_i} = 0 \qquad (1)$$

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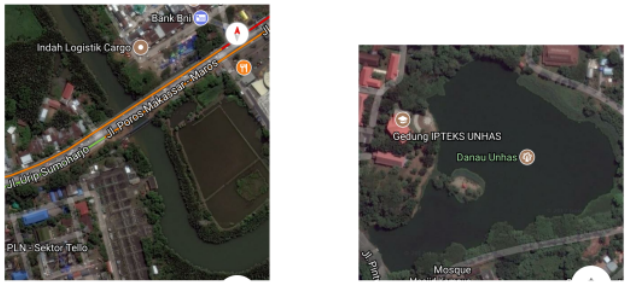

Figure 1. Circumstances of Tello River (left) and Unhas Lake (right).

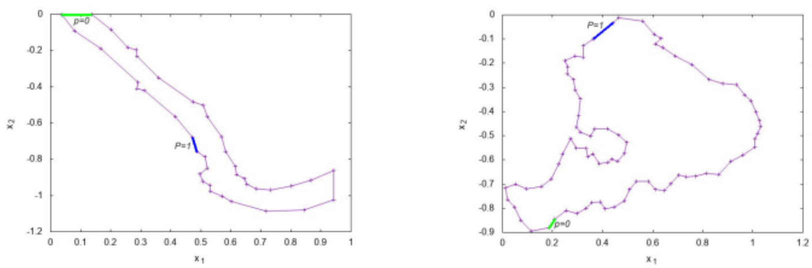

Figure 2. Discretization of the boundary Γ of Tello River (left) and Unhas Lake (right)

where $\lambda_{ij} = \kappa_{ij}/k$, $p = C/C'$, $x_i = X_i/l$, $v_i = (l/k)\,V_i$, κ_{ij} is the components of dispersion/diffusion coefficients ($\mathrm{L}^2\mathrm{T}^{-1}$), C is dissolved concentration of the pollutant (ML^{-3}), X_i is the component of the point coordinates $\mathbf{X}$ (L), V_i is the component of the seepage velocity (LT^{-1}), k is a reference dispersion coefficient, C' is a reference concentration of pollutant and l is a reference length. See [10] for the governing equation of pollutant transport problems.

Referred to the Cartesian frame Ox_1x_2 we will consider the boundary value problems governed by (1) where $\mathbf{x} = (x_1, x_2)$, λ_{ij} and v_i are constant coefficients, $i, j = 1, 2$. The coefficient $[\lambda_{ij}]$ is a real positive definite symmetrical matrix. Also, in (1) the summation convention for repeated indices apply, so that (1) can be written explicitly as

$$\lambda_{11}\frac{\partial^2 p}{\partial x_1^2} + 2\lambda_{12}\frac{\partial^2 p}{\partial x_1 \partial x_2} + \lambda_{22}\frac{\partial^2 p}{\partial x_2^2} - v_1\frac{\partial p}{\partial x_1} - v_2\frac{\partial p}{\partial x_2} = 0$$

A solution p to (1) is sought which is valid in a region Ω in R^2 with boundary Γ which consists of a finite number of piecewise smooth curves. On Γ_1 the dependent variable $p\,(\mathbf{x})$ is specified, and $P = \lambda_{ij}\,(\partial p/\partial x_i)\,n_j = l/(kC')\kappa_{ij}\,(\partial C/\partial X_i)\,n_j$ is specified on Γ_2 where $\Gamma = \Gamma_1 \cup \Gamma_2$ and $\mathbf{n} = (n_1, n_2)$ denotes the outward pointing normal to Γ. The method of solution will be to obtain a boundary integral equation from which numerical values of the dependent variable p and P may be obtained for all points in Ω.

3. The boundary integral equation

Multiplying both sides of (1) by function p^* and then integrating it over the domain Ω yields

$$\int_\Omega \left(\lambda_{ij}\frac{\partial^2 p}{\partial x_i \partial x_j} - v_i\frac{\partial p}{\partial x_i}\right) p^*\, d\Omega = 0 \qquad (2)$$

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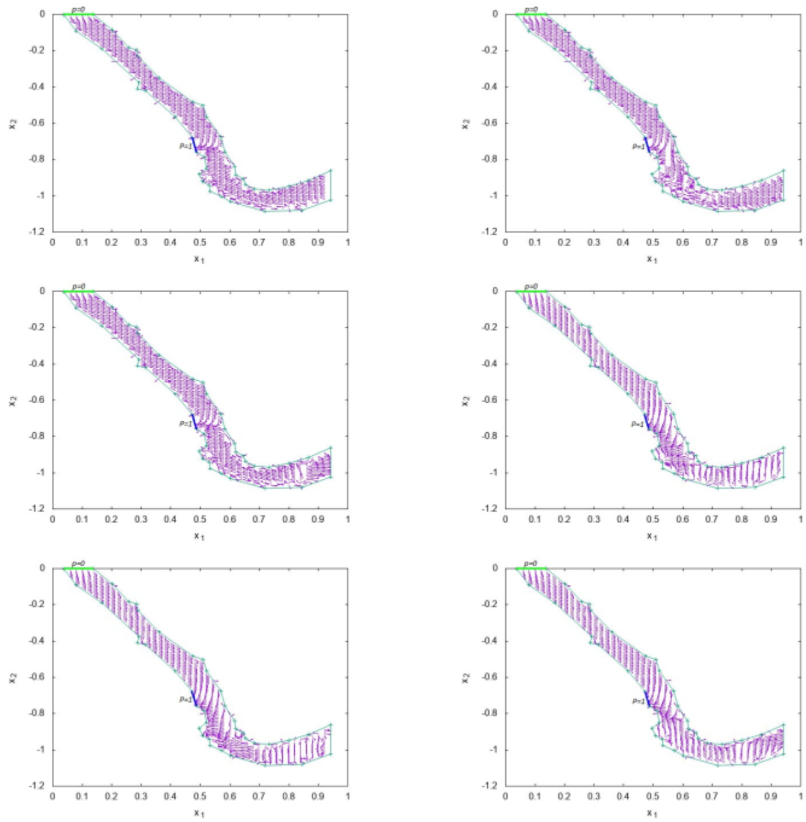

Figure 3. Vectors of $(\partial p/\partial x_1, \partial p/\partial x_2)$ for the Tello River. **Upper, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = 1$. **Upper, right:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = -1$. **Middle, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 1, v_2 = 1.5$. **Middle, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = 1$. **Lower, left:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = -1$. **Lower, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 1, v_2 = 1.5$.

Using Gauss divergence theorem in (2) we obtain

$$\int_\Gamma \left(\lambda_{ij} \frac{\partial p}{\partial x_i} n_j - p v_i n_i \right) p^* \, d\Gamma - \int_\Omega \left(\lambda_{ij} \frac{\partial p}{\partial x_i} \frac{\partial p^*}{\partial x_j} - p \, v_i \, \frac{\partial p^*}{\partial x_i} \right) d\Omega = 0 \tag{3}$$

Use of Gauss divergence theorem once again for the first integrand function $\lambda_{ij} \frac{\partial p}{\partial x_i} \frac{\partial p^*}{\partial x_j}$ in the domain integral in (3) results in

$$\int_\Gamma \left(\lambda_{ij} \frac{\partial p}{\partial x_i} n_j - p v_i n_i \right) p^* \, d\Gamma - \int_\Gamma p \lambda_{ij} \frac{\partial p^*}{\partial x_i} n_j d\Gamma + \int_\Omega \left(p \lambda_{ij} \frac{\partial^2 p^*}{\partial x_i \partial x_j} + p \, v_i \, \frac{\partial p^*}{\partial x_i} \right) d\Omega = 0 \tag{4}$$

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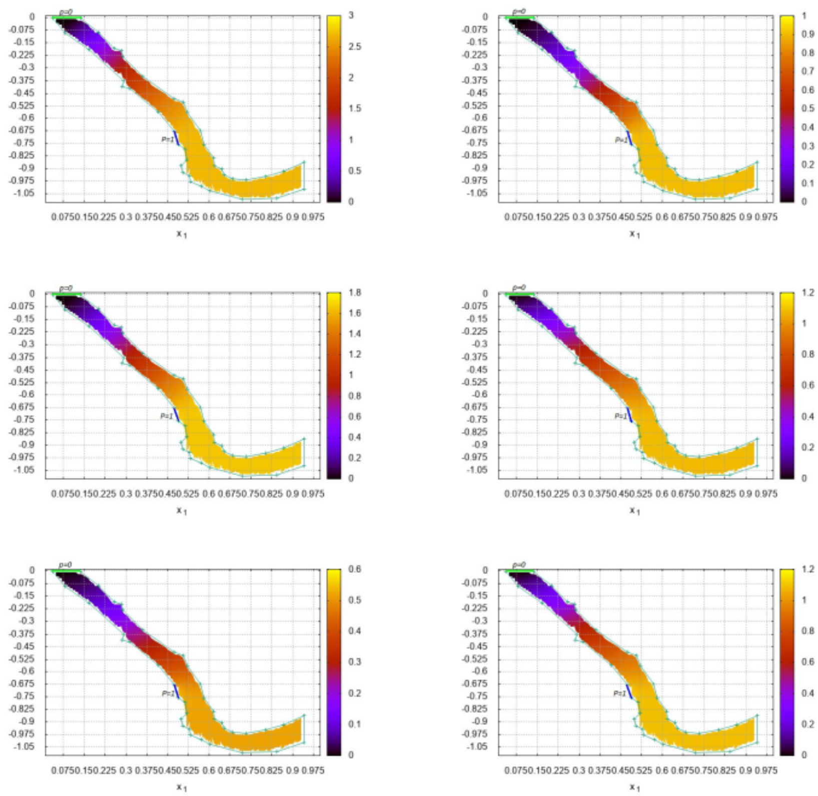

Figure 4. Values of p for the Tello River. **Upper, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = 1$. **Upper, right:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = -1$. **Middle, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 1, v_2 = 1.5$. **Middle, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = 1$. **Lower, left:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = -1$. **Lower, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 1, v_2 = 1.5$.

or

$$\int_\Omega \left(\lambda_{ij} \frac{\partial^2 p^*}{\partial x_i \partial x_j} + v_i \frac{\partial p^*}{\partial x_i} \right) p \, d\Omega = - \int_\Gamma [P p^* - (P_v p^* + P^*) p] \, d\Gamma \tag{5}$$

where

$$P_v(\mathbf{x}) = v_i \, n_i(\mathbf{x}) \qquad \text{and} \qquad P^*(\mathbf{x}, \boldsymbol{\xi}) = \lambda_{ij} \frac{\partial p^*(\mathbf{x}, \boldsymbol{\xi})}{\partial x_i} n_j(\mathbf{x})$$

If the function p^* is taken such that

$$\lambda_{ij} \frac{\partial^2 p^*}{\partial x_i \partial x_j} + v_i \frac{\partial p^*}{\partial x_i} = -\delta(\mathbf{x} - \boldsymbol{\xi}) \tag{6}$$

where δ is the Dirac delta function and $\boldsymbol{\xi} = (\xi_1, \xi_2)$, then (5) may be written as

$$\int_\Omega p(\mathbf{x}) \, \delta(\mathbf{x} - \boldsymbol{\xi}) \, d\Omega = \int_\Gamma \{ P(\mathbf{x}) \, p^*(\mathbf{x}, \boldsymbol{\xi}) - [P_v(\mathbf{x}) \, p^*(\mathbf{x}, \boldsymbol{\xi}) + P^*(\mathbf{x}, \boldsymbol{\xi})] \, p(\mathbf{x}) \} \, d\Gamma \tag{7}$$

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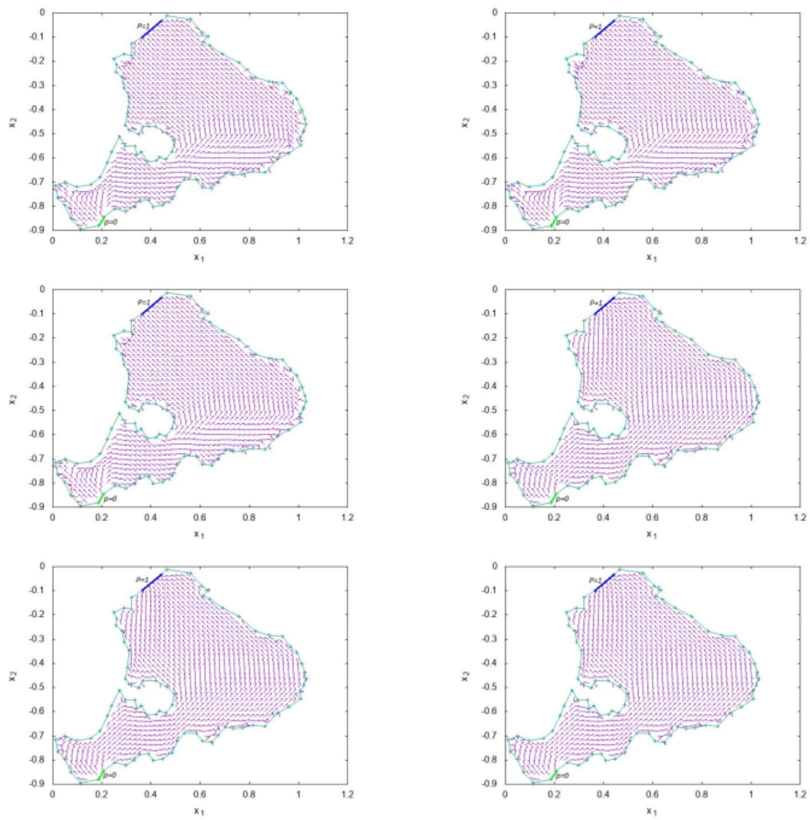

Figure 5. Vectors of $(\partial p/\partial x_1, \partial p/\partial x_2)$ for the Unhas Lake. **Upper, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = 1$. **Upper, right:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = -1$. **Middle, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 1, v_2 = 1.5$. **Middle, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = 1$. **Lower, left:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = -1$. **Lower, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 1, v_2 = 1.5$.

As one of the Dirac delta function's properties, the following equation holds

$$\int_\Omega p(\mathbf{x})\, \delta(\mathbf{x} - \boldsymbol{\xi})\, d\Omega = \eta(\boldsymbol{\xi})\, p(\boldsymbol{\xi}) \tag{8}$$

with $\eta = \frac{1}{2}$ if $\boldsymbol{\xi}$ lies on the boundary Γ, $\eta = 1$ if $\boldsymbol{\xi}$ is inside of the domain Ω, $\eta = 0$ if $\boldsymbol{\xi}$ is outside of the domain Ω. By substituting (8) into (7) we obtain a boundary integral equation

$$\eta(\boldsymbol{\xi})\, p(\boldsymbol{\xi}) = \int_\Gamma [P(\mathbf{x})\, p^*(\mathbf{x}, \boldsymbol{\xi}) - (P_v(\mathbf{x})\, p^*(\mathbf{x}, \boldsymbol{\xi}) + P^*(\mathbf{x}, \boldsymbol{\xi}))\, p(\mathbf{x})]\, d\Gamma \tag{9}$$

The so called fundamental solution p^* which satisfies (6) may be written (see Azis [2])

$$p^*(\mathbf{x}, \boldsymbol{\xi}) = \frac{K}{2\pi} \exp\left(-\frac{\dot{\mathbf{v}}.\dot{\mathbf{R}}}{2D}\right) K_0\left(\frac{\dot{v}\dot{R}}{2D}\right) \tag{10}$$

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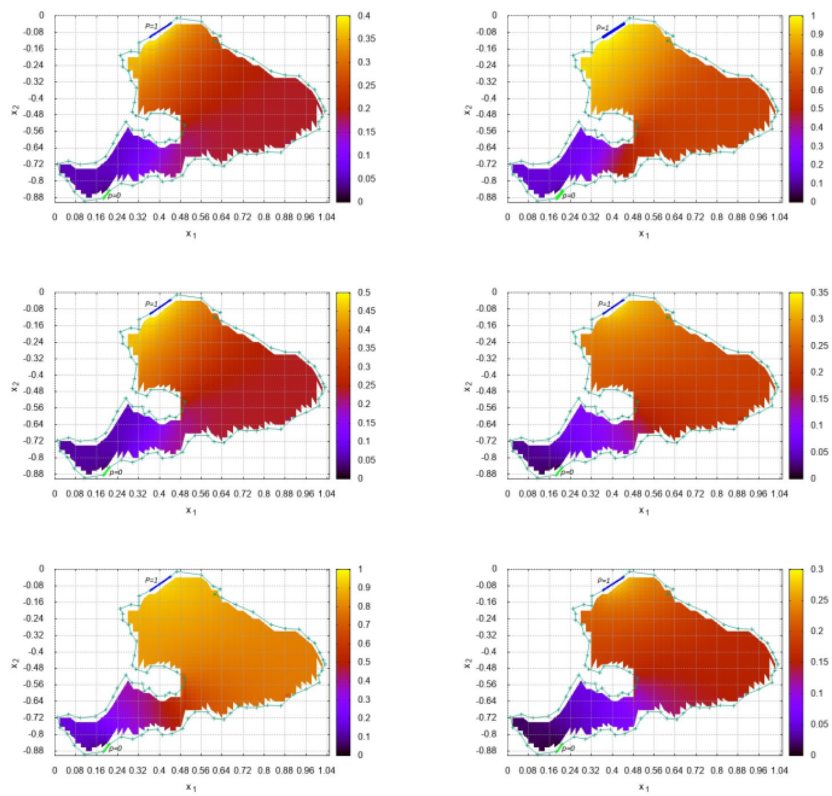

Figure 6. Values of p for the Unhas Lake. **Upper, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = 1$. **Upper, right:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 0, v_2 = -1$. **Middle, left:** $\lambda_{11} = 1, \lambda_{12} = 1, \lambda_{22} = 2, v_1 = 1, v_2 = 1.5$. **Middle, right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = 1$. **Lower, left:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 0, v_2 = -1$. **Lower right:** $\lambda_{11} = 1, \lambda_{12} = 0, \lambda_{22} = 1, v_1 = 1, v_2 = 1.5$.

where

$$D = [\lambda_{11} + \lambda_{12}(\rho + \overline{\rho}) + \lambda_{22}\rho\overline{\rho}]/2 \qquad K = \ddot{\rho}/D \qquad \dot{\mathbf{R}} = \dot{\mathbf{x}} - \dot{\boldsymbol{\xi}} \qquad \dot{\mathbf{x}} = (x_1 + \dot{\rho}x_2, \ddot{\rho}x_2)$$

$$\dot{\boldsymbol{\xi}} = (\xi_1 + \dot{\rho}\xi_2, \ddot{\rho}\xi_2) \qquad \dot{\mathbf{v}} = (v_1 + \dot{\rho}v_2, \ddot{\rho}v_2)$$

$$\dot{R} = \sqrt{(x_1 + \dot{\rho}x_2 - \xi_1 - \dot{\rho}\xi_2)^2 + (\ddot{\rho}x_2 - \ddot{\rho}\xi_2)^2} \qquad \dot{v} = \sqrt{(v_1 + \dot{\rho}v_2)^2 + (\ddot{\rho}v_2)^2}$$

where $\dot{\rho}$ and $\ddot{\rho}$ are respectively the real and the positive imaginary parts of the complex root ρ of the quadratic equation

$$\lambda_{11} + 2\lambda_{12}\rho + \lambda_{22}\rho^2 = 0$$

and the bar notation $(^{-})$ denotes complex conjugate and K_0 is the modified Bessel function.

Now equation (9) may be used to calculate the solutions p and P for all points $\mathbf{x}$ on the boundary Γ. Once the boundary solutions are found then we can calculate solutions p and its derivatives $\partial p/\partial x_1$, $\partial p/\partial x_2$ in the domain Ω.

4. Numerical results

An example of problem with analytical solution had been shown in Haddade et. al [3]. The example showed the feasibility and the accuracy of the BEM in solving diffusion-convection problems. In this section two more problems will be solved numerically by using the boundary integral equation (9). The two problems will consider simulation adopting the circumstances of the Tello River around which an electricity generating industry (in the map written in Indonesian language as PLN - Sektor Tello), assumed as a source of pollutant, stands and Unhas Lake (in the map written as Danau Unhas) (see figure 1) around which a source of pollutant is assumed to be existing. Both sites mentioned are located in Makassar city of Indonesia.

The standard BEM is used to find the numerical solutions of p and the derivatives $\partial p/\partial x_1$ and $\partial p/\partial x_2$ in the domain Ω. The boundary Γ is divided into a number of sides and each side is divided into a number of elements of equal length. See figure 2. The constant element is used for which it is assumed that the values of p and P are constant along an element. The integrals over each element are evaluated numerically using Bode's quadrature with error of order $O(h^{11})$.

One side of the boundary Γ is where the pollutant flux is located, that is $P = 1$. Another side is where the boundary condition is set to be $p = 0$. All other sides are assumed to be parts of the boundary of no flux that is $P = 0$. See figure 2.

For each problem we consider the cases of isotropic ($\lambda_{11} = \lambda_{22} = 1, \lambda_{12} = \lambda_{21} = 0$) and anisotropic ($\lambda_{11} = 1, \lambda_{22} = 2, \lambda_{12} = \lambda_{21} = 1$) media. And for each case we take a variation of the values of the velocity (v_1, v_2), that is $(v_1, v_2) = (0, 1)$, $(v_1, v_2) = (0, -1)$ and $(v_1, v_2) = (1, 1.5)$. The results are shown in figures 3 – 6. The results show that the change of the parameters λ_{ij} and v_i to some extent effects the values of p and its derivatives. Therefore as a recommendation, for implementation it is very important to measure carefully the values the parameters, and also of course the values of the boundary data.

Acknowledgment

This work was financially supported by the LP2M (Lembaga Penelitian dan Pengabdian pada Masyarakat) of Hasanuddin University Makassar and The Higher Education Ministry of Indonesia.

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