A numerical study on the effect of the material’s anisotropy in diffusion convection reaction problems

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Abstract. A boundary element method (BEM) is utilized to find numerical solutions to boundary value problems of homogeneous media governed by an anisotropic-diffusion convection-reaction (DCR) equation. Some problems are considered. A FORTRAN script is developed for the computation of the solutions. The numerical solutions verify the validity of the analysis used to derive the boundary element method with accurate and consistent solutions. The computation shows that the BEM procedure elapses very efficient time in producing the solutions. In addition, results obtained for the considered examples show the effect of the anisotropy of the media on the solutions.

1. Introduction

A number of publications on DCR equation for isotropic media, towards finding its numerical solution have been done using various techniques. Among them may be found in [1, 2, 3, 4, 5, 6]. The diffusion-convection-reaction equation with anisotropic diffusion, namely

$$\beta_{ij} \frac{\partial^2 c(x)}{\partial x_i \partial x_j} - \nu_i \frac{\partial c(x)}{\partial x_i} - k c(x) = 0$$ (1)

will be reconsidered, $i, j = 1, 2$, $x = (x_1, x_2)$, $\beta_{ij}$ is the anisotropic diffusion or conduction coefficient, $\nu_i$ is the velocity, $k$ is the reaction coefficient and $c$ is the dependent variable. Within the domain in question $[\beta_{ij}]$ is a real symmetrical matrix satisfying $\beta_{11} \beta_{22} - \beta_{12}^2 > 0$. For the repeated indices in equation (1) summation convention applies.

Equation (1) is usually used for modeling heat transfer and mass transport problems which involve anisotropic diffusion, convection and reaction processes in homogeneous media. Similar works of anisotropic materials but for different kinds of applications have been done previously (see for example [7, 8, 9, 10, 11]).

Numerical solutions $c$ and its derivatives $\partial c / \partial x_1, \partial c / \partial x_2$ to (1) in the domain $\Omega$, subjected to the boundary condition that either $c$ or

$$P = \beta_{ij} (\partial c / \partial x_i) n_j$$ (2)

is known on the boundary $\partial \Omega$, are sought. The investigation of this paper is strictly mathematical. The purpose is mainly to develop a boundary element method for finding the numerical solutions.
2. The boundary integral equation

Multiplying both sides of (1) by function $A(x, \chi(x))$ and then integrating it over domain gives

$$\int_{\Omega} \beta_{ij} \frac{\partial^2 c}{\partial x_i \partial x_j} \Lambda \, d\Omega - \int_{\Omega} \nu_i \frac{\partial c}{\partial x_i} \Lambda \, d\Omega - \int_{\Omega} k c \Lambda \, d\Omega = 0 \quad (3)$$

Using Gauss divergence theorem twice in (3) we obtain

$$\kappa(\chi) c(\chi) = \int_{\partial\Omega} \{P(x) \Lambda(x, \chi) - [P_r(x) \Lambda(x, \chi) + \Theta(x, \chi)] c(x)\} \, ds(x) \quad (4)$$

where $P_r(x) = \nu_i n_i(x)$ and $\chi = (\chi_1, \chi_2)$, $\kappa = 0$ if $(\chi_1, \chi_2) \notin \Omega \cup \partial\Omega$, $\kappa = 1$ if $(\chi_1, \chi_2)$ lies inside the domain $\Omega$, $\kappa = \frac{1}{2}$ if $(\chi_1, \chi_2)$ is on the boundary $\partial\Omega$ given that $\partial\Omega$ has a continuously turning tangent at $(\chi_1, \chi_2)$. In (4) the fundamental solution $\Lambda(x, \chi)$ for equation (1) satisfies

$$\beta_{ij} \frac{\partial^2 \Lambda(x, \chi)}{\partial x_i \partial x_j} + \nu_i \frac{\partial \Lambda(x, \chi)}{\partial x_i} - k \Lambda(x, \chi) = -\delta(x - \chi)$$

and $\Theta(x, \chi)$ satisfies

$$\Theta(x, \chi) = \beta_{ij} \frac{\partial \Lambda(x, \chi)}{\partial x_j} n_i$$

where $\delta$ is the Dirac delta function. For 2-D problems the function $\Lambda$ is given as (see Azis [12])

$$\Lambda(x, \chi) = \frac{\tilde{\tau}}{2\pi B} \exp \left(-\frac{\tilde{\nu} \tilde{R}}{2B}\right) K_0 \left(\mu \tilde{R}\right)$$

where $\mu = \sqrt{\left(\tilde{\nu}/2B\right)^2 + (k/B)}$, $B = [\beta_{11} + 2\beta_{12} \tilde{\tau} + \beta_{22} (\tilde{\tau}^2 + \tilde{\tau}^2)]/2$, $\tilde{R} = \tilde{x} - \tilde{R}$, $\tilde{x} = (x_1 + \tilde{\tau} x_2, \tilde{\tau} x_2)$, $\tilde{\chi} = (\chi_1 + \tilde{\tau} \chi_2, \tilde{\tau} \chi_2)$, $\tilde{\nu} = (\nu_1 + \tilde{\nu}_2, \tilde{\nu}_2)$, $\tilde{\nu} = \sqrt{(\nu_1 + \tilde{\nu}_2)^2 + (\tilde{\nu}_2)^2}$, and $\tilde{\tau}$ and $\tilde{\tau}$ are respectively the real and the positive imaginary parts of the complex root $\tau$ of the quadratic equation $\beta_{11} + 2\beta_{12} \tau + \beta_{22} \tau^2 = 0$ and $K_0$ is the modified Bessel function.

3. Numerical results

Some boundary value problems governed by equation (1) will be considered. The boundary integral equation (4) is used to find the solution. The integrals in equation (4) are evaluated numerically using the Gaussian quadrature rule (see Abramowitz and Stegun [13]).

3.1. Example 1: A problem with analytical solution

Consider the boundary value problem governed by (1) with coefficients

$$[\beta_{ij}] = \begin{bmatrix} 1 & 1 \\ 1 & 2 \end{bmatrix} \quad \nu_i = (1, 1.5) \quad k = 1$$

The analytical solution to (1) is

$$c = \exp(0.5x_1 - 0.675391x_2)$$

and the domain $\Omega$ is chosen to be a unit square with corner points $A = (0, 0)$, $B = (1, 0)$, $C = (1, 1)$, and $D = (0, 1)$. The boundary conditions are that $P$ is given on $AB$, $BC$, $CD$ and $c$ is given on $AD$.

Table 1 shows a comparison between the boundary element method (BEM) solution and the analytical solution. The results show that the BEM solution converges to the analytical solution as the number of segments of the same length increases from 80, 160 to 320. The results are as expected.
Table 1. BEM and analytical solutions for Example 1

| (x₁, x₂) | c     | ∂c/∂x₁ | ∂c/∂x₂ | c     | ∂c/∂x₁ | ∂c/∂x₂ |
|----------|-------|---------|---------|-------|---------|---------|
|          | BEM 80 segments | BEM 160 segments |          | BEM 320 segments | Analytical |          |
| (0.5,0.1) | 1.1980 | 0.5975 | -0.8084 | 1.1992 | 0.5984 | -0.8093 |
| (0.5,0.3) | 1.0469 | 0.5210 | -0.7056 | 1.0478 | 0.5228 | -0.7070 |
| (0.5,0.5) | 0.9149 | 0.4549 | -0.6164 | 0.9155 | 0.4566 | -0.6177 |
| (0.5,0.7) | 0.7995 | 0.3973 | -0.5387 | 0.8000 | 0.3989 | -0.5397 |
| (0.5,0.9) | 0.6987 | 0.3478 | -0.4711 | 0.6990 | 0.3485 | -0.4716 |
| (0.1,0.5) | 0.7500 | 0.3731 | -0.5062 | 0.7500 | 0.3742 | -0.5064 |
| (0.3,0.5) | 0.8283 | 0.4110 | -0.5579 | 0.8287 | 0.4129 | -0.5590 |
| (0.7,0.5) | 1.0106 | 0.5029 | -0.6811 | 1.0116 | 0.5048 | -0.6826 |
| (0.9,0.5) | 1.1164 | 0.5559 | -0.7523 | 1.1178 | 0.5580 | -0.7542 |

3.2. Example 2: Comparison between isotropic and anisotropic solutions

Now consider a problem with three cases, two of them are anisotropic cases with β₁₁ = 1, β₁₂ = 0, β₂₂ = 2 and β₁₁ = 1, β₁₂ = 1, β₂₂ = 2, and the other one is isotropic case with β₁₁ = 1, β₁₂ = 0, β₂₂ = 1. For all cases we take ν₁ = (1, 1.25), k = 0.1 and use 640 segments of equal length, and the domain and boundary conditions are as depicted in Figure 1.

![Geometry of Example 2](image)

*Figure 1. Geometry of Example 2*

Figures 2–4 show a certain difference between the solutions of anisotropic and isotropic cases.
4. Conclusion
A BEM for the DCR boundary value problems has been derived. The method are generally easy to implement to obtain numerical values for particular problems. The numerical solutions obtained using the BEM indicate that it produces accurate solutions. The results for Example 1 of Section 3 show the convergence of the solution. And the results for Example 2 show a consistency of the flow and the scattering solutions. They also show that the anisotropy of the medium under consideration gives an effect on the solutions. Therefore for application, the anisotropy of the medium should be considered to be taken into account.
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