Application of the Boundary Element Method for stationary scalar orthotropic problems

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Abstract. This work presents an application of the Boundary Element Method in physical problems associated with orthotropic materials. The coordinate transformation resource was applied to use the isotropic model corresponding to the orthotropic model, this enabled a direct application of the Boundary Element Method to find a numerical solution. Solutions obtained with the application of the Finite Element Method were used for comparison. The error was measured through the percentage relative error, having as reference the analytical solution of the analyzed problem, being approached by the Separation of Variables Method.
Keyword. Boundary Element Method, Finite Element Method, Separation of Variables Method, Coordinate Transformation, Orthotropy.

1. Introduction

The material properties cannot be assumed isotropic in many engineering applications. The most common examples occur in non-crystalline substances, such as sedimentary rocks and wood, or in materials obtained through the manufacturing process by lamination or deep drawing **[1]**. Concerning the oil extraction in rocks, many mathematical models use hydraulic diffusivity models based on Darcy's Equation to a simulation of the fluid flow **[2]**. In these problems, a rheological approach in which the constitutive properties are based on the scalar field theory can be used to achieve an effective numerical solution.

Currently, the increasing level of engineering applications has demanded materials with multipurpose characteristics. The best example concerns composite structures, which are made from two or more constituent materials that, when combined, produce a material with improved physical or chemical properties. In many important practical cases, the aim is to achieve a suitable balance between resistance and thermal conductivity. Functionally graded materials **[3]** comprise another class of material, characterized by the gradual variation in composition, resulting in corresponding changes in the properties of the material. Procedures based on, layer processing and melt processing are used to fabricate the functionally graded materials. In this case, the mechanical behavior of the material is anisotropic, beyond non-homogeneous. Some references have investigating heat conduction analysis in functionally graded materials **[4]**. However, despite the non-homogeneity in functional materials,

available mathematical strategies can separate the non-homogeneity and anisotropy, if desired. The most serious problem, in this case, concerns the impossibility of a suitable mathematical treatment that transforms the anisotropic behavior as orthotropic, using a changing in the coordinate system, in applications as seismic prospection. For this, although more complex, many modern usual approaches are general, in which both constitutive phenomena are examined together. These general approaches require mathematical tools for solving domain integrals, which usually employ radial basis functions **[5, 6]**.

Concerning just orthotropic homogeneous scalar diffusion problems, the Boundary Element Method presents many interesting formulations, such as the use of Dual Reciprocity **[7]**, the use of anisotropic fundamental Green's function **[8]**, the natural boundary integral equation **[9]**, and the simple procedure in which the governing equation of anisotropic potential problem is transformed into standard Laplace isotropic equation by the coordinate transformation method **[10]**. Despite being more restrictive, this last technique uses the isotropic fundamental solution, which preserves important Boundary Element Method (BEM) features, particularly related to high accuracy, beyond simple data entry, and approaching non-regular regions in applications to reservoir modeling. Using this approach, it is also possible to use auxiliary numerical tools as the radial basis function to approximate terms related to other physical phenomena, such as impedance or inertia, for example, with higher accuracy, without the use of the time-dependent Green's function.

Indicating that there is a demand for more robust discrete models, in recent years there has been a resurgence of recent specialized literature analyzing orthotropic problems, e.g., using the method of fundamental solutions **[11]**, meshless techniques **[12]**and alternative BEM techniques **[13]**. Thus, in this article, a review of the classic BEM procedure using the standard Laplace fundamental solution is performed, aiming for future more elaborate applications. Two basic problems that have known analytical solutions are solved, ratifying the accuracy and simplicity of this formulation, which allows a more robust development of the BEM model in other classes of anisotropic scalar field problems, especially the transient process in a non-homogeneous medium.

2. Scalar potentials in anisotropic media

It is known from continuous scientific experience that the flux **v** of some physical quantities such as thermal energy, electrical energy, and the fluid flow through granular or porous regions **[14]** obey mathematically the following expression:

$$\mathbf{v} = -\mathbf{K}\nabla u \qquad 01$$

or

$$\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \begin{bmatrix} k_{xx} & k_{xy} & k_{xz} \\ k_{yx} & k_{yy} & k_{yz} \\ k_{zx} & k_{zy} & k_{zz} \end{bmatrix} \begin{pmatrix} \partial u/\partial x' \\ \partial u/\partial y' \\ \partial u/\partial z' \end{pmatrix} \qquad 02$$

In equations (1) and (2), u is representing a scalar potential and Matrix **K** corresponds to a diactic or second-order tensor, representing the constitutive properties of the medium. For the homogeneous case, the formation of **K** depends on the crystalline constitution of the material and, in addition, the physical properties of the single crystals of some substances depend on the crystallographic direction in which the measurements are taken, directions which are here called $X' = X'(x', y', z')$. Properties such as elastic modulus, electrical conductivity, and refractive index can have different values in the [100], [110] and [111] directions (vide **Fig.(1-a)**). According to literature **[15]**, the directionality of the properties (anisotropy) is associated with the difference in atomic or ionic spacing as a function of the crystallographic direction. The magnitude of the anisotropy effects in crystalline materials are functions of the symmetry of the crystalline structure and the degree of anisotropy increases as a function of the reduction of structural symmetry, the triclinic structures developed in **Fig. (1-b)** show marked anisotropy.

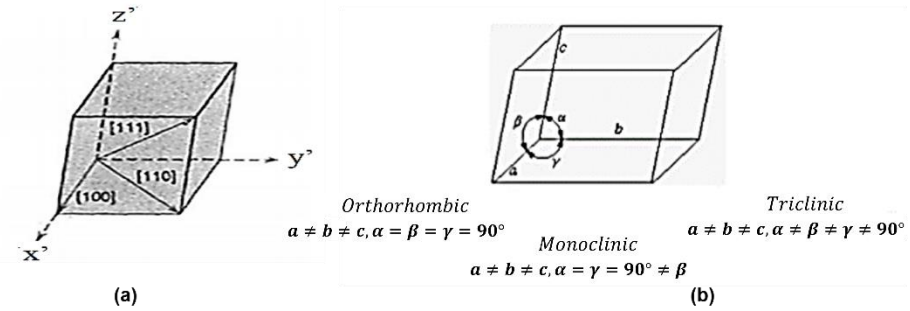

Figure 1: *(a) Unit cell showing your possible preferred directions. Extracted from the book Materials Science and Engineering: An Introduction. (b) Model of an anisotropic structure containing: Orthorhombic, Monoclinic and Triclinic. Extracted from the https://*pt.slideshare.net/guilhermecuzzuol9/estrutura-cristalina-37503063

3. Diagonalization of the anisotropic model

The diagonalization of the dyadic or **K** tensor is possible if it is admitted that it is symmetric. We seek to find a strategic orientation for the coordinate axes, and for a symmetric model diagonalization will always be possible, with only 6 different components existing, considering the components of the diagonal k_{xx}, k_{yy}, k_{zz} and the others where:

$$k_{xy} = k_{yx}; k_{xz} = k_{zx}; k_{yz} = k_{zy} \quad 03$$

The symmetry also implies that the eigenvalues of dyadic **K** are real and given by a well-known determinant procedure, which avoids the trivial solution:

$$det|\mathbf{K} - \lambda\mathbf{I}| = 0 \quad 04$$

Assuming that the eigenvalues are distinct it is possible to determine the three eigenvectors which corresponds to the main coordinates axes, where the dyadic $\bar{\mathbf{K}}$ has a diagonal representation, i.e.:

$$\bar{\mathbf{K}} = \begin{bmatrix} \bar{k}_{11} & 0 & 0 \\ 0 & \bar{k}_{22} & 0 \\ 0 & 0 & \bar{k}_{33} \end{bmatrix} \quad 05$$

4. Governing equation

The presentation of the governing equation is done considering a 2D domain with homogeneous properties. Considering the steady state and sourceless physical assumptions, the application of the continuity equation or another equivalent equation leads the proposed problem to the expression $\nabla_k^2 u(X) = 0$, where:

$$\bar{k}_{11}\frac{\partial^2 u(X)}{\partial x_1^2} + \bar{k}_{22}\frac{\partial^2 u(X)}{\partial x_2^2} = 0 \quad 06$$

Figure 02 presents the two-dimensional domain $\Omega(X)$ arranged in the Cartesian coordinate system indicated by x_1 and x_2, delimited by the boundary conditions Γ_u and Γ_q, representing the boundary conditions.

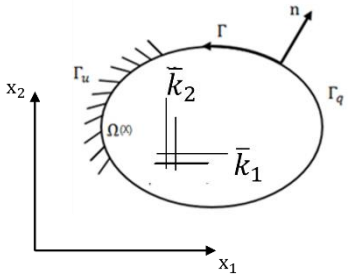

Figure 2: Generic physical model of an orthotropic problem.

5. BEM application

5.1. The fundamental solution in orthotropic problems

The fundamental problem related to **Eq. (06)** involves the presence of a source concentrated at a point ξ in the two-dimensional domain $\Omega(X)$, after changing the coordinate system considering $z_i = x_i/\sqrt{\bar{k}_{ii}}$, the fundamental problem was rewritten according to Laplace's equation, where:

$$\bar{k}_{11}\frac{\partial^2 u^*(X)}{\partial x_1^2} + \bar{k}_{22}\frac{\partial^2 u^*(X)}{\partial x_2^2} = -\Delta(\xi; x_1)\Delta(\xi; x_2);$$
$$\frac{\partial^2 u^*(Z)}{\partial z_1^2} + \frac{\partial^2 u^*(Z)}{\partial z_2^2} = -\Delta(\xi; z_1\sqrt{\bar{k}_{11}})\Delta(\xi; z_2\sqrt{\bar{k}_{22}}) \qquad 07$$

Using the fundamental problem in z_1 and z_2 coordinates, we obtain the fundamental solution, and its derivative as follows:

$$u^*(\xi; Z) = \frac{1}{2\pi\left(\sqrt{\bar{k}_{11}\bar{k}_{22}}\right) ln[(z_1^2 + z_2^2)^{1/2}]};$$
$$q^*(\xi; Z) = -\frac{z_1 n_{z1} + z_2 n_{z2}}{2\pi\left(\sqrt{\bar{k}_{11}\bar{k}_{22}}\right)(z_1^2 + z_2^2)} \qquad 08$$

5.2. Transformation of the government equation using the coordinate system $Z = Z(z_1, z_2)$

To make the problem compatible with the fundamental solution proposed in 5.1, it is necessary to adapt the government equation (vide **Eq. 06**) to its related problem in z_1 and z_2 coordinates. **Fig. (03)** represents this adaptation:

Considering the coordinate transformation function $z_i = x_i/\sqrt{\bar{k}_{ii}}$, its partial derivative is $\partial z_i/\partial x_i = 1/\sqrt{\bar{k}_{ii}}$. This transformation is developed into **Eq. 9**, where we arrive at :

$$\nabla^2 u(Z) = 0;\ \frac{\partial^2 u(Z)}{\partial z_1^2} + \frac{\partial^2 u(Z)}{\partial z_2^2} = 0;\ \frac{\partial u(Z)}{\partial z_i} = \sqrt{\bar{k}_{ii}}\frac{\partial u(X)}{\partial x_i} \qquad 09$$

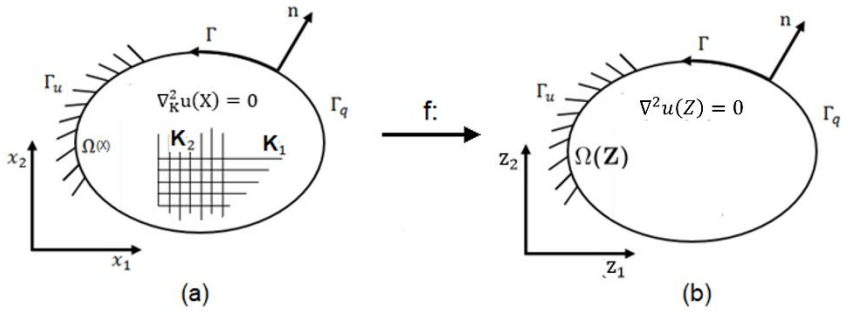

Figure 3: (a) Real problem in the Cartesian domain and (b) Equivalent problem in the coordinate system $Z = Z(z_1, z_2)$

5.3. BEM application in the domain $\Omega(Z)$

As presented in topic 5.1 of this section, the fundamental problem proposed by **Eq. (07)**, together with its fundamental solution **Eq. (08)** and transformation showed in **Eq. (09)** can be associated with the inverse integral form over the isotropic domain $\Omega(Z)$ **[10]** as follows:

$$\frac{1}{\sqrt{\bar{k}_{11}\bar{k}_{22}}}c(\xi)u(\xi) + \int_{\Gamma(Z)} u(Z)\, q^*(\xi; Z)d\Gamma(Z) - \int_{\Gamma(Z)} q(Z)\, u^*(\xi; Z)d\Gamma(Z) = 0 \qquad 10$$

Since the values of $c(\xi)$ correspond to:

$$c(\xi) = \begin{cases} \dfrac{\alpha}{2\pi}, & in\ the\ boundary \\ 1, & in\ the\ internal\ point \end{cases} \qquad 11$$

and α represents the geometric corner angle.

After applying the discretization process on the $\Omega(Z)$ domain, using **Eq. (10)**, the matrix system is obtained as follows:

$$\begin{bmatrix} H_{11} & \cdots & H_{1n} \\ \vdots & \ddots & \vdots \\ H_{n1} & \cdots & H_{nn} \end{bmatrix} \begin{pmatrix} u_1 \\ \vdots \\ u_n \end{pmatrix} = \begin{bmatrix} G_{11} & \cdots & G_{1n} \\ \vdots & \ddots & \vdots \\ G_{n1} & \cdots & G_{nn} \end{bmatrix} \begin{pmatrix} q_1 \\ \vdots \\ q_n \end{pmatrix} \qquad 12$$

As the matrix system of **Eq. (12)** allows solving the government equation for the coordinates $Z = Z(z_1, z_2)$, the values of $u(Z)$ and $q(Z)$ obtained must be transferred to the system of original coordinates. The values of $u(Z)$ are equal to $u(X)$ and to obtain the values of the derivative $q(X)$, the transformation according to **Eq. (09)** must be applied, returning to the Cartesian system, in addition to also repositioning its values to the corresponding ordered pairs.

6. Simulation

Normally, orthotropic problems have a much higher level of numerical difficulty than isotropic ones. This is the case of the example chosen here for numerical simulation. Despite the apparent simplicity of the geometrical configuration and boundary conditions, the number of boundary elements needed to solve it with a high degree of accuracy is meaningfully greater than in an equivalent isotropic case.

This can be confirmed by the number of terms required by the series that characterizes the analytical solution available for this example, whose expression is presented later on.

Concerning the discretization process, 84 internal points were used for all meshes, which were subdivided into 40, 80, 160, 320 and 640 boundary elements. The percent error was analyzed (vide **Eq. 13**), where "n" corresponds to the number of points calculated, M_{analit} represents the highest analytical value found and $|analit - num|_i$ defines the difference in module between each analytical **[16]** and numerical value evaluated. The interpolation used for this method will be done using linear polynomials.

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$$p_e\% = \frac{100}{n|M_{analit}|}\sum_{i=1}^{n}|analit - num|_i \qquad 13$$

6.1. Simulation

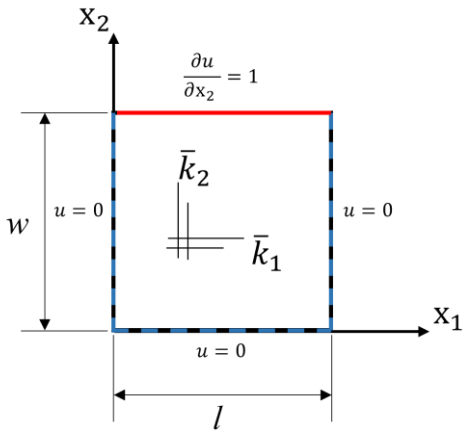

Figure 4: Square geometry region and its boundary conditions for the example.

In this problem, the points analyzed for the potential values are located internally and all the boundary with $x_2 = w$, whereas for the potential derivative, the analyzed points will be on the boundary where $x_2 < w$. The analytical solution $u_{(x_1,x_2)}$ for this problem is expressed as follows:

$$u_{(x_1,x_2)} = \sum_{\substack{n=1 \\ (impar)}}^{\infty} \frac{4L}{(n\pi)^2}\sqrt{\frac{\bar{k}_{22}}{\bar{k}_{11}}}sen\left(\frac{n\pi x_1}{L}\right)\left[senh\left(\frac{n\pi x_2}{L}\sqrt{\frac{\bar{k}_{11}}{\bar{k}_{22}}}\right)\Big/cosh\left(\frac{n\pi W}{L}\sqrt{\frac{\bar{k}_{11}}{\bar{k}_{22}}}\right)\right] \qquad (14)$$

Partial derivatives with respect to x_1 and x_2 are respectively:

$$\frac{\partial u_{(x_1,x_2)}}{\partial x_1} = \sum_{\substack{n=1 \\ (impar)}}^{\infty} \frac{4}{n\pi}\sqrt{\frac{\bar{k}_{22}}{\bar{k}_{11}}}cos\left(\frac{n\pi x_1}{L}\right)\left[senh\left(\frac{n\pi x_2}{L}\sqrt{\frac{\bar{k}_{11}}{\bar{k}_{22}}}\right)\Big/cosh\left(\frac{n\pi W}{L}\sqrt{\frac{\bar{k}_{11}}{\bar{k}_{22}}}\right)\right]; \quad \frac{\partial u_{(x_1,x_2)}}{\partial x_2} = \sum_{\substack{n=1 \\ (impar)}}^{\infty} \frac{4}{n\pi}sen\left(\frac{n\pi x_1}{L}\right)\left[cosh\left(\frac{n\pi x_2}{L}\sqrt{\frac{\bar{k}_{11}}{\bar{k}_{22}}}\right)\Big/cosh\left(\frac{n\pi W}{L}\sqrt{\frac{\bar{k}_{11}}{\bar{k}_{22}}}\right)\right]. \qquad (15)$$

In this example, dimensions w and l are taken unitary. Therefore, the potential distribution obtained through **Eq. (14)** over the domain of **Fig. (04)** is shown in **Fig. (5)**:

The numerical simulation applied to the proposed model showed good results and this can be seen in **Fig. (6)** and **Fig. (7)**. The potential values were evaluated in **Fig. (6)** considering $\bar{k}_1 = 2$ and $\bar{k}_2 = 0{,}5$. The error of 0.6577% for the mesh with less refinement in **Fig. (6a)**, being even better when the values between $\bar{k}_{11}$ and $\bar{k}_{22}$ are exchanged (see **Fig. (6b)**) resulting in an error of approximately 0.0600%.

The influence of the effects of orthotropy on the numerical results is highlighted, and this influence persists in the calculation of the derivatives (**Fig. (7a)** and **Fig. (7b)**) even if the alteration in the results is smaller when compared to the potential values. The calculated values for the derivative and flux were also considered satisfactory for the problem.

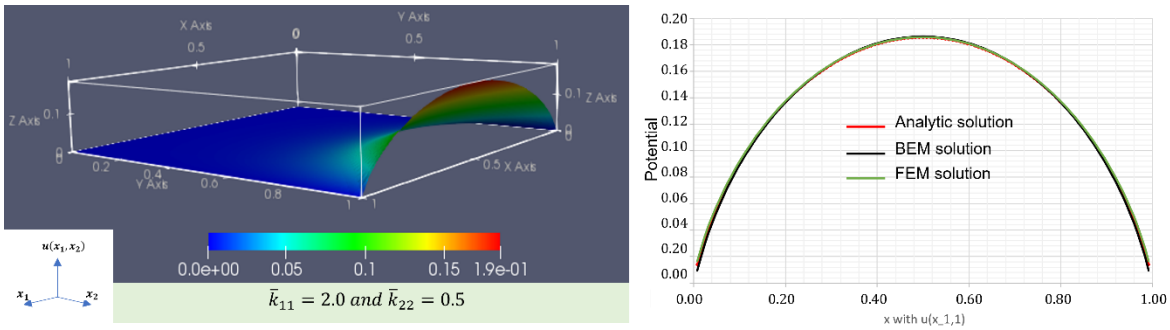

Figure 5:Analytical and numerical solution of the Fourier series with n = 226 in isotropic medium, where $\bar{k}_{11} = 2.0$ *and* $\bar{k}_{22} = 0.5$.

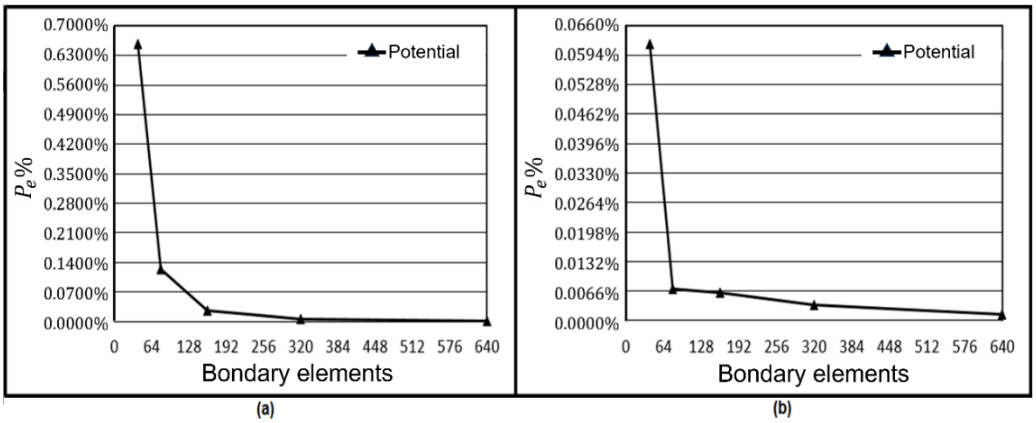

Figure 6: Percent relative error for the potential where in (a) $\bar{k}_{11} = 2$ and $\bar{k}_{22} = 0.5$ and in (b) $\bar{k}_{11} = 0.5$. and $\bar{k}_{22} = 2$.

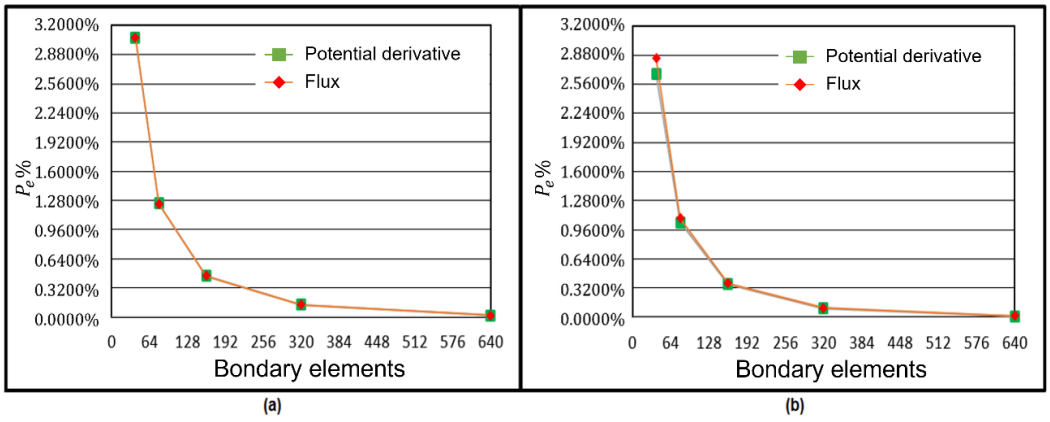

Figure 7: Percent relative error for the flux/derivative potential where in (a) $\bar{k}_{11} = 2$ and $\bar{k}_{22} = 0.5$ and in (b) $\bar{k}_{11} = 0.5$. and $\bar{k}_{22} = 2$.

7. Conclusions

The transformation of the orthotropic model to a correlated isotropic model allows the application of the BEM model in its standard formulation, which is simpler and produces more accurate results. Simulations confirm the satisfactory results achieved for the example discussed, despite a large number of boundary elements being necessary to reach relative errors smaller that 1%. Isotropic problems which are also given by the Laplace equation are solved with a reduced number of boundary elements with higher degree of accuracy.

To get an idea of the numerical difficulties, the Finite Element Method **[17]** also was applied for comparison, using a structured mesh, comprising 4096 triangular elements and 2113 nodal points, of which 128 points will be on the boundary. The MEF results for potential errors were 0.0859% for $\bar{k}_{11} = 2$ and $\bar{k}_{22} = 0.5$ and 0.2283% for $\bar{k}_{11} = 0.5$ and $\bar{k}_{22} = 2$. The BEM performance was better from 320 boundary elements, as shown in **Fig. (6a)** and **Fig. (6b).**

Considering new advances for the subject addressed in this work, it is intended to expand the research approaching heterogeneous orthotropic media.

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