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APPLICATION OF THE REGULARIZED DIRECT INTEGRATION TECHNIQUE OF THE OF BOUNDARY ELEMENT METHOD IN DIFFUSION-ADVECTIVE STATIONARY PROBLEMS

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Abstract. *The most usual formulations of the boundary element method for solving the diffusive-advective problems present significant difficulties in the treatment of the transport term, for various reasons. While the classical formulation, which uses the fundamental diffusive-advective solution, is limited in variable velocity fields, the dual reciprocity (DRBEM) formulation presents precision problems, being unable to produce satisfactory results even for only moderate Peclét numbers. This work applies the recent regularized direct interpolation technique with radial basis functions (DIBEM) to model the advective term, thus allowing good accuracy in problems dominated by advection. The DIBEM was superior to the formulation with dual reciprocity in several applications, as in the cases governed by the Poisson and Helmholtz equations, and thus, its extension to diffusive-advective problems is a natural consequence of its development. In order to evaluate performance, this paper solves test problems with known analytical solution and already simulated by the formulations previously mentioned, in order to expose the applicability and adequacy of DIBEM in this context.*

Keywords: *Direct Integration, Advective-Diffusive Problems, Regularization Process, Boundary Element Method*

1 INTRODUCTION

There is a wide range of physical phenomena governed by the advection-diffusion model in the thermofluid area, such as the flow assurance in the oil wells production, gas flows in ducts among several other applications of interest. To the extent of this relevance, the advective-diffusive model presents some challenging aspects regarding its approximation by means of numerical methods, among which we can mention the manipulation of variable velocity fields, compressible flows, nature of the constitutive tensor such as situations where there is a strong dominance of advection.

Among the most widespread numerical techniques, the boundary element method (BEM) stands out as a efficient tool in the treatment of advective-diffusive problems. On the other hand, problems with the instabilities generated by dominant advection still present as critical point in the numerical formulation through BEM. In this line, the dual reciprocity technique, based on radial basis approximation, presents difficulties in the treatment of problems strongly dominated by advection. (Partridge & Brebbia, 1992).

At the state-of-the-art level, the direct integration technique (DIBEM) presents itself as a good alternative tool to the formulation of dual reciprocity, since it is consistently more effective in solving relevant mathematical models, such as the Poisson and Helmholtz equations, in consonance with Loeffler et al.(2017). On the other hand, there is a natural demand for numerical technique (DIBEM) in advective-diffusive problems, in order to confirm an increase in acuity. In the current development, the DIBEM formulation with regularization process is used in simulations with increasing Peclét numbers, in order to determine the sensitivity of the same formulation to applications in problems strongly dominated by advection.

2 MATHEMATICAL MODEL

The advection-diffusion equation to be worked on, is based on the fundamental principle of energy conservation, which refers conceptually to the mechanics of the continuum. The more generalized format of such a principle can be appreciated in detail in such literatures as Reddy (2013) and Schlichting et al. (1955).

$$\frac{\partial}{\partial x_j}\left(\rho c_p u_j T\right) = \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial T}{\partial x_j}\right) \tag{1}$$

The applicability of Eq. (1) is limited to a steady-state analysis where the thermodynamic and thermophysical properties do not vary with temperature and the viscous dissipation can be neglected. In this way, Eq. (2) represents the simplified form of its predecessor.

$$\rho c_p \left[u_j \frac{\partial T}{\partial x_j} + T \frac{\partial u_j}{\partial x_j}\right] = \lambda \frac{\partial^2 T}{\partial x_j^2} \tag{2}$$

The format presented in Eq. (2) shows an expanded writing of the advective term on the left side of Eq. (1), initially in conservative structure, whose first differential term represents the transport of the thermal field by the velocity vector while the second term counts the divergent of the velocity field, correlated to flow compressibility. On the right side, the diffusive term is presented in a compacted form, since the constitutive tensor of the material has an isotropic characteristic. Once modeled in this way, Eq. (2) governs an advective-diffusive problem with the possibility of spatial variation of the velocity field. In the current article, numerically experienced cases are restricted to incompressible flows, and thus, the term that depends on the divergent of velocity field in Eq. (2) cancels out, simplifying the government equation as follows.

$$\rho c_p u_j \frac{\partial T}{\partial x_j} = \lambda \frac{\partial^2 T}{\partial x_j^2} \tag{3}$$

Finally, in order to compare the magnitude between the diffusive and advective effects, the previous government equation can be converted to its dimensionless form by using convenient parameters. A clearer and more general physical interpretation of dimensionlessness differential models is a common fact in mathematical-physics. In this way, the dimensionless form of the advection-diffusion governing Eq. (3) follows.

$$u*_j \frac{\partial T*}{\partial x*_j} = \frac{1}{Pe} \frac{\partial^2 T*}{\partial x*_j^2} \tag{4}$$

A close observation of Eq. (4) reveals a concatenation of diffusive and advective effects in a single dimensionless grouping, denoted as Peclét number. In this way dominance of one effect over another can be easily identified with an asymptotic analysis of this parameter. It is possible to emphasize, at last, that this dimensionless number represents the link between the hydrodynamic and thermal problems contemplated in the dimensionless ones of Reynolds and Prandtl, according to the literature in Burmeister (1993).

3 NUMERICAL FORMULATION

In this section the formulation of advective-diffusive problems is exposed via boundary element methods (BEM), using the technique of direct integration with regularization procedure. This technique is based on the Laplace / Poisson fundamental solution presented in Eq. (5), available on Brebbia (1982), since it is a simpler and sufficient solution to approach the problem efficiently.

$$u^*(\xi, X) = -\frac{1}{2\pi} lnr(\xi, X) \tag{5}$$

In order to show a simpler explanation of the algebraism, the equation of government Eq. (3) will be used without coefficients, since they are all constant and for this fact do not require any special treatment by the operators found below. As an initial step, the governing equation is multiplied by Eq. (5), on both sides, thus determining the strong integral formulation of the problem, as follows, which serves as a foundation for all development in BEM .

$$\int_\Omega u_{,ii}(X) u^*(\xi, X) d\Omega(X) = \int_\Omega v_i(X) u_{,i}(X) u^*(\xi, X) d\Omega(X) \tag{6}$$

At this point, it is feasible to divide the numerical treatment in manipulating the diffusive side, located on the left side of Eq. (6), and the right side treatment of the equation, called the advective side (AS), in which the focus of regularized formulation concentrates. The diffusive side (DS) is treated with the complete inversion of the differential operator as seen below, a process widely known and present in the literature as in Brebbia & Dominguez (1994).

$$DS = \quad c(\xi)u(\xi) + \int_{\Gamma} u(X)q^*(\xi,X)d\Gamma - \int_{\Gamma} q(X)u^*(\xi,X)d\Gamma \tag{7}$$

It is possible to note that the structure of Eq. (7) consists of a point function, and two integrals, already located in the boundary as a consequence of the divergence theorem application. In this way the diffusive side, does not represent too much complexity, being in charge of the advective treatment our main focus.

The treatment of the advective term by piecewise integration characterizes the first phase of its mathematical manipulation.After its proper application, and consequent use of the divergence theorem on the largest number of domain integrals as possible, in order to lead them to the boundary, one can arrive at the following format (Wrobel, 2002).

$$\begin{aligned} AS = \int_{\Gamma} v_i(X)n_i(X)u(X)u^*(\xi,X)d\Gamma - \int_{\Omega} v_i(X)u(X)u^*_{,i}(\xi,X)d\Omega \\ - \int_{\Omega} v_{i,i}(X)u(X)u^*(\xi,X)d\Omega \end{aligned} \tag{8}$$

An analysis of the structure of Eq. (8) reveals a boundary integral, already properly treated and two domain integrals, which still require manipulation. However, it is possible to perceive the presence of the divergent of the velocity field as the first term in the kernel of the third integral, and based on the hypothesis of incompressibility previously adopted, it is possible to cancel this integral. In this way, we have only one domain integral that demands manipulation (Massaro, 2001).

$$AS = \int_{\Gamma} v_i(X)n_i(X)u(X)u^*(\xi,X)d\Gamma - \int_{\Omega} v_i(X)u(X)u^*_{,i}(\xi,X)d\Omega \tag{9}$$

In a normal sequence, the treatment of the second integral of Eq. (9) by BEM, can be done using an approximation through radial basis functions. In the case of the DIBEM technique, the entire kernel of the domain integral is approximate. However, before, a new procedure of regularization of the latter term of Eq. (9) is proposed, based on simple algebra. A same regularizing term analogous to the target integral is summed and subtracted in Eq. (9) in order to maintain intact the algebraic validity, as given below.

$$\begin{aligned} AS = \int_{\Gamma} v_i(X)n_i(X)u(X)u^*(\xi,X)d\Gamma - \int_{\Omega} v_i(X)u^*_{,i}(\xi,X)u(X)d\Omega \\ + \int_{\Omega} v_i(X)u^*_{,i}(\xi,X)u(\xi)d\Omega - \int_{\Omega} v_i(X)u^*_{,i}(\xi,X)u(\xi)d\Omega \end{aligned} \tag{10}$$

The grouping of the second and third integrals results in a three part structure, as follows. The first integral is already located in the boundary and does not demand major treatments. The second integral can be called a regularized term (RT), whose treatment is based essentially on radial basis approximation. The third integral, despite being in the domain, has simple treatment as shown in the sequence.

$$AS = \int_{\Gamma} v_i(X) n_i(X) u(X) u^*(\xi, X) d\Gamma - \int_{\Omega} v_i(X) u_{,i}^*(\xi, X) \left[u(X) - u(\xi)\right] d\Omega \\ - \int_{\Omega} v_i(X) u_{,i}^*(\xi, X) u(\xi) d\Omega \qquad (11)$$

First, the treatment of the regularized term consists in the approximation of the kernel of the integral by a sum of radial basis functions, weighted by coefficients to be determined. The effectiveness of the direct integration technique as an approximation tool has already been extensively investigated in the work of Souza (2013). This technique is proving to be accurate and efficient, and even superior to dual reciprocity in some applications, as in the researches of Loeffler et al. (2015). For a clearer view, the regularized term to be approximated is brought down in isolation.

$$RT = \int_{\Omega} v_i(X) u_{,i}^*(\xi, X) \left[u(X) - u(\xi)\right] d\Omega \qquad (12)$$

As predicted by the direct integration technique, the entire kernel of the integral of Eq. (12) will be approximated, using radial basis functions of, as follows. A detailed background on these functions can be found in the literature (Buhmann, 2003).

$$v_i(X) u_{,i}^*(\xi, X) \left[u(X) - u(\xi)\right] \cong \quad \alpha_j^{\xi} F_j(X_j, X) \qquad (13)$$

Once the radial basis function chosen as a tool for interpolations is known, its primitive is also known. Thus, by using the divergence theorem it is possible to rewrite the integral of Eq. (12) , as function of the primitive of the radial function chosen, and already in the boundary, as follows.

$$RT \cong \int_{\Omega} \alpha_j^{\xi} F_j(X_j, X) d\Omega = \alpha_j^{\xi} \int_{\Omega} \psi_{,ii}{}^{j} d\Omega = \alpha_j^{\xi} \int_{\Omega} \left(\psi_{,i}\right)_{,i}{}^{j} d\Omega = \alpha_j^{\xi} \int_{\Gamma} (\psi_{,i} n_i)^j d\Gamma \qquad (14)$$

In order to synthesize the notation, a new variable η is introduced to condense the kernel of the last integral developed in the equation Eq. (14).

$$\eta_j = \psi_{,i}{}^{j} n_i \qquad (15)$$

In this way the regularized term, written in function of η can be synthesized as follows. Such integrals are calculated numerically, usually by classical gaussian quadrature, which is one of the most accurate alternative available for this type of numerical integration.

$$RT \cong \alpha_j^{\xi} \int_{\Gamma} \eta_j d\Gamma \qquad (16)$$

$$N_j = \int_{\Gamma} \eta_j d\Gamma \qquad (17)$$

Given this, all integral quantification is stored in a new variable N, so that the expression of the regularized term can be expressed more compactly as in Eq. (18).

$$RT \cong \quad \alpha_j^\xi N_j \tag{18}$$

For the finalization of the treated integral formulation of the problem, the excedent domain term (DT), represented as the third integral in Eq. (11), must be manipulated.

$$DT = \int_\Omega v_i(X) u,_i^*(\xi, X) u(\xi) d\Omega \tag{19}$$

The integral of Eq. (19) can be properly dismembered by integrating by parts, and then exposed to the divergence theorem, being properly driven to the boundary, as follows, thereby closing the integral formulation of the advective-diffusive problem via direct integration technique with regularization.

$$DT = u(\xi) \int_\Gamma v_i(X) n_i(X) u^*(\xi, X) d\Gamma \tag{20}$$

The final treated integral formulation of the problem is shown below, in order to provide an overview of the algebraic steps performed up to the current point. It is important to point out that the only approximation inserted in the formulation to date has been the approximation of the term regularized by radial basis functions.

$$\begin{aligned} c(\xi)u(\xi) + \int_\Gamma u(X) q^*(\xi, X) d\Gamma - \int_\Gamma q(X) u^*(\xi, X) d\Gamma = \\ \int_\Gamma v_i(X) n_i(X) u(X) u^*(\xi, X) d\Gamma + \quad \alpha_j^\xi N_j + u(\xi) \int_\Gamma v_i(X) n_i(X) u^*(\xi, X) d\Gamma \end{aligned} \tag{21}$$

The application of the discretization procedure to Eq. (21) consists conceptually in transferring the problem from its continuous nature to the discrete analysis. Such procedure, in the case in the current formulation is relatively long, culminating in a final linear system as product of the discretization with the following structure.

$$\{[H'] - [G'] + [Z] + [S]\} [u] = [G] [q] \tag{22}$$

Such a system has a striking similarity and is compatible with the classical system of the diffusive problem, differing by the appearance of other matrices, due to the effects of the advection that incorporate the matrix of coefficients that multiplies the vector u of potentials to be determined. Matrix structures associated with the matrix formulation of Eq. (22) are correlated to the integrals present in the final integral formula of Eq. (21).

The final system previously illustrated by Eq. (22) could be represented in simplified form as an altered system with classical BEM formatting, such as in the sequence. It is important to emphasize that since the numerical matrices generated by the boundary elements are dense, a conscious choice of the solution technique of linear systems is relevant in order to generate a computational effort within the compatible, optimizing resources, even if this is not the focus of this article.

$$\left[\overline{H}\right]\{u\} = [G]\{q\} \tag{23}$$

In order to validate the consistency of the formulation and to test its breadth some numerical experiments are performed in the following section. It is worth emphasizing that the formulation structure is valid for incompressible flows, that is, boundary value problems whose divergent of the hydrodynamic field remains zero.

4 NUMERICAL EXPERIMENTS

The current section presents the execution of two numerical tests in order to determine the robustness of the regularized integral formulation proposed by direct integration technique (DIBEM). The central focus is to evaluate the stability of the formulation against the dominance of advection on the diffusive effect. For this, after the convergence of a suitable numerical mesh, we test the integral arrangement parameterized in relation to the dimensionless Peclét (Pe), in order to infer about the performance of the formulation.

Regarding the methodology used for the tests, a set of at least four numerical meshes towards the greater refinement is tested for both cases. Once the convergence is verified via graph and tabular, the dominance analysis of the advection is simulated. The numerical errors are determined based on the analytical solution of each case, having the highest analytical value as a percentage proportionality parameter.

4.1 Case I - One-Dimensional Problem

The first case to be tested consists of a one-dimensional flow over a square domain of unit dimensions, thermally isolated at two edges, with homogeneous potencial condition imposed at the left edge and prescribed flux at the right edge, as shown in Fig. 1 below. The upstream flow of the left edge has a constant velocity field.

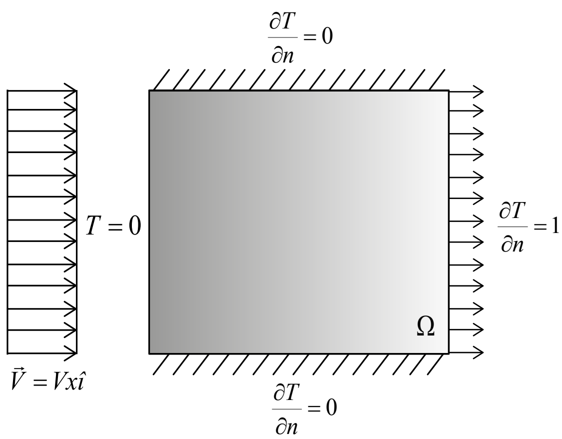

Figure 1: Boundary Value Problem - Case I

Initially, a one-dimensional case is tested in order to follow a growing logic of complexity of the numerical experiments performed with respect to the proposed formulation. Firstly a mesh test is performed considering meshes with different amounts of boundary points, however with a number of internal points fixed at 324 points. Convergence is verified graphically and tabularly, when very close results of mean error between consecutive simulations are observed. It is important to note that the mesh test simulations were done for Peclét number equal to unity. The Fig. 2 synthesizes the mesh test, where the convergence already exists in the mesh of 320 boundary elements.

Mesh	Average Error (%)
40 BE	0,216
80 BE	0,102
160 BE	0,053
320 BE	0,036
640 BE	0,032

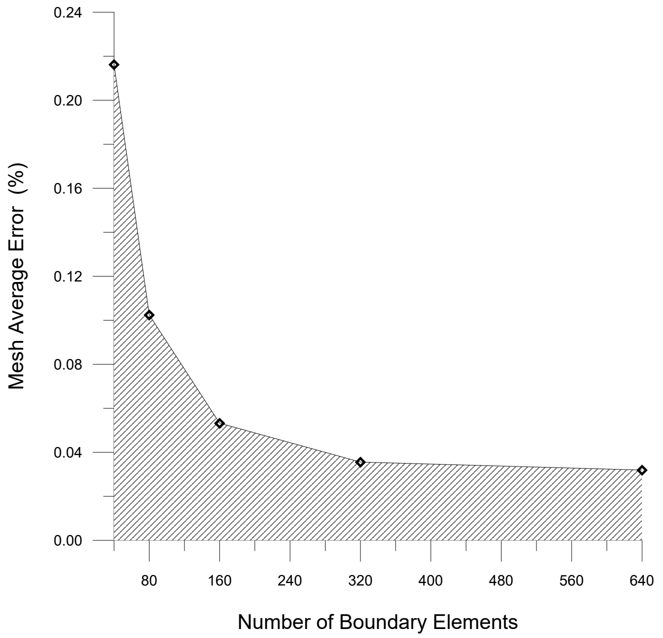

Figure 2: Convergence Analysis Caso I - Pe=1

Once the mesh in which convergence has been established is known, an analysis of the influence of Peclét's dimensionless on the proposed formulation is executed. In this case, Peclét numbers ranging from 1 to 50 were tested at convenient intervals as shown in the graph of Fig. 3, as follows.

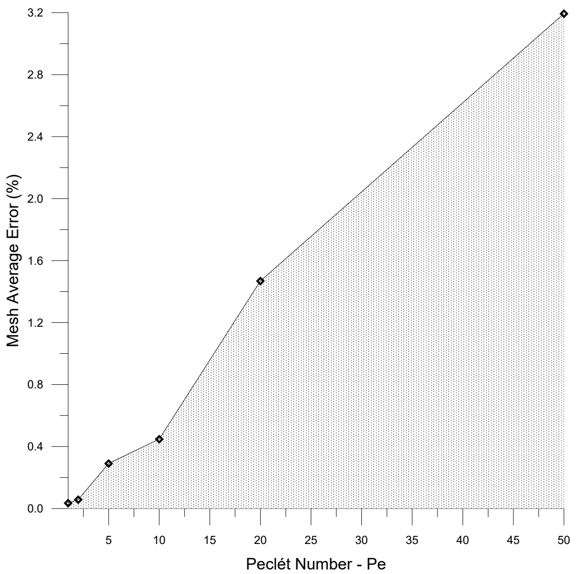

Figure 3: Parametric Analysis of Peclet Number - Case I

The graph above synthesizes a good performance of the DIBEM technique for all configurations with increasing advective effect tested. For the highest dimensionless value, the formulation maintains an average error with magnitude close to 3%, which is an very good result compared to formulating the dual reciprocity for the same conditions, as can be confirmed in Massaro (2001).

4.2 Case II - Two-Dimensional Problem

The second case, with the highest level of complexity, is a two-dimensional problem with a variable potential field imposed as a boundary condition on all edges of the square domain. In this case the flow velocity field also has constant components, as summarized below in Fig. 4.

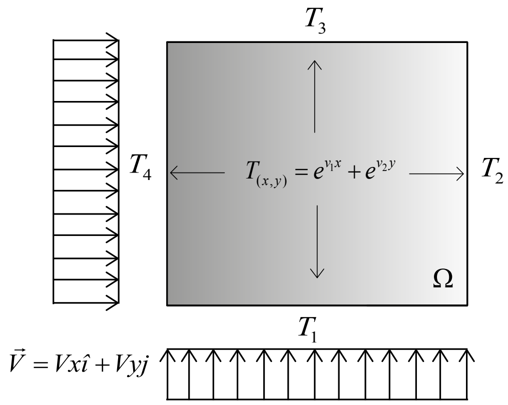

Figure 4: Boundary Value Problem - Case II

This problem presents some numerical peculiarities. The first of these is the imposition of the calculation of the flux around the boundary, since the potentials are prescribed. This fact introduces an initial obstacle, since all the numerical methods, among them, the boundary element method, present a smaller precision in the calculations of flux, in detriment to the numerical determination of potentials. A second characteristic is related to the nature of the imposed function, which, because it is exponential, grows very rapidly depending on the intensity of the velocity field, generating inaccuracies, especially with high numbers of Peclét. Due to these facts, case II is presented as a more rigorous test for the formulation evaluated in the current article.

Similar to case I, the mesh test is performed for meshes with increasing number of boundary points, but with a number of internal points fixed at 625, differing from the previous case with bias to maintain the stability of the method tested by a reasonable balance between internal and boundary points. The mesh test is also performed here for a dimensionless case of Peclét equal to unity. The results are summarized in tabular and graphical form in Fig.5, and the convergence is already found in the mesh of 160 boundary elements.

Although the convergence was already verified from the mesh with 160 boundary elements, as mentioned previously, the mesh with 320 boundary elements was selected for the performance of the parametric tests in relation to the dimensionless of Peclét, to maintain a pattern in relation to case I. In this line, it is pertinent to observe that for case II, two analyzes are generated in parallel: the first one regarding the errors committed in the calculated boundary fluxes

Mesh	Average Error (%)
40 BE	2,457
80 BE	1,264
160 BE	0,791
320 BE	0,767

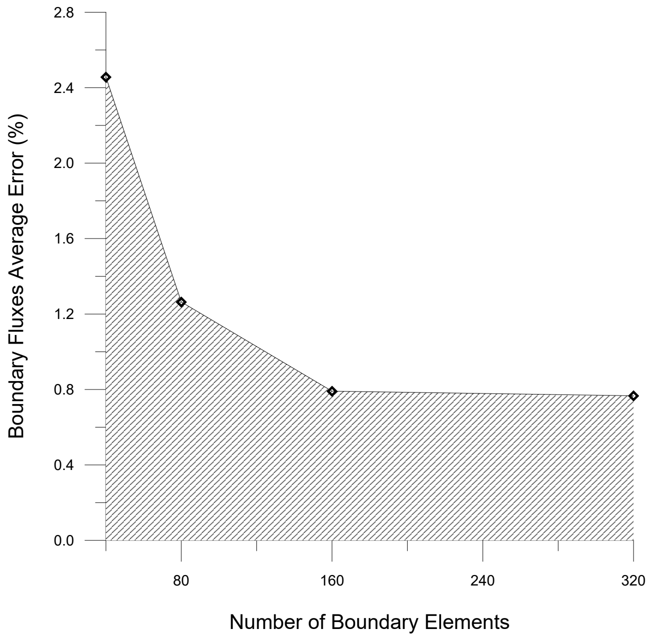

Figure 5: Convergence Analysis Caso II - Pe=1

and a second connected to the determination of the potentials in the internal points. The results are summarized in the graph of Fig. 6 which follows.

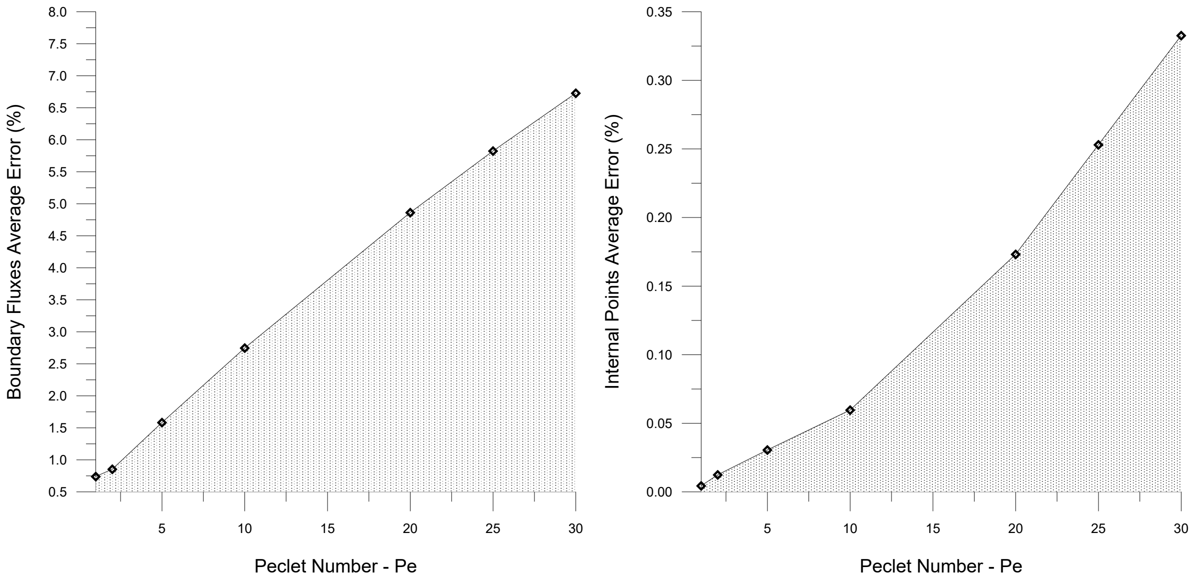

Figure 6: Parametric Analysis of Peclet Number - Case II

It is possible to see, as already expected, that the errors presented in the left chart inherent to the fluxes are substantially larger due to the lower precision with which they are calculated. However the errors are reasonably low compared to the dual reciprocity technique (DRBEM), characterizing a good performance of the formulation. It is important to point out that for the generations of these results, in particular for this case, the lower and left edges were excluded because they presented instabilities that also appear in double reciprocity, and therefore, do not translate the real performance of the DIBEM formulation as well as of dual reciprocity technique (DRBEM).

In the right graph that counts the average errors for the internal points located in the domain it is possible to perceive very low average errors even for medium values in Pe, in the order of 30. This performance of the DIBEM technique with regularization is substantially more robust than the formulation of dual reciprocity, showing that its extension to advective-diffusive problems must be explored.

5 CONCLUSION

Extensive applications of the boundary element method for solving diffusive-advective problems had been restricted due to meaningful limitations of the actual available boundary element models. The classic BEM formulation that uses a correlate diffusive-advective problem as fundamental solution is capable of solving with great accuracy just problems in which the velocity field is constant. Thus the approach is not adequate to more general cases as the compressible fluid flow, for example. Another drawback concerning this formulation is the difficulty to apply it to time dependent problems, as the fundamental solution for this case is quite cumbersome.

On the other hand, the dual reciprocity procedure, despite to overcome the restriction of the previous formulation which could only be applied if the velocity field was constant, presents serious problems concerning the accuracy and numerical instability problems, being recommended only for fluid flow with low Peclét numbers. Thus there was a hiatus to be filled with the development of a flexible formulation capable of simulating diffusive-advective problems with median Peclet numbers. On fact, the limitations on problems with dominance of advection still remain as a major obstacle to the formulations that employs radial basis functions as auxiliary tool to simplify the BEM mathematical model.

The new formulation named to direct interpolation BEM has been shown sufficient robustness for solving problems governed by the Poisson and Helmholtz equations so that its extension to the diffusive-advective cases approached in this article was a natural step in its development in the context of scalar field problems. The numerical experiments presented here in two problems corroborate a substantial superiority of the DIBEM formulation in these cases of convective problems relatively to the DRBEM, analogously to what has already been demonstrated in the literature.

The parametric analyzes performed according to the number of Peclet indicated a satisfactory numerical stability by the DIBEM discrete model, which remains with good accuracy even for medium values of Peclet numbers. This fact stimulates the explorations of the DIBEM formulation to new problems belonging to the diffusive-advective theory.

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