A Hybrid Solution for Advection-Diffusion Problems with Variable Advective Fields and Semi-infinite Domains

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Brian J. Driessen
Jeffrey L. Dohner
Structural Dynamics and Controls
Sandia National Laboratory
Albuquerque, NM 87185-0439

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Abstract

In this paper a hybrid, finite element/boundary element method which can be used to solve for particle diffusion in semi-infinite domains containing geometric obstructions and a variable advective field is presented. In previous work either boundary element or finite element/difference methods were used to solve for particle concentrations in an advective domain. These methods of solution had a number of limitations. Due to limitations in computing spatially dependent Green's functions, the boundary element method of solution was limited to domains containing only constant advective fields, and due to its inherent formulation, finite element/difference methods were limited to only domains of finite spatial extent. Thus, where the finite element solution was limited, the boundary element solution was not, and where the boundary element solution was limited, the finite element solution was not. In this paper it is proposed to split the total domain into two sub-domains where each method of solution is applicable. For each of these sub-domains, the appropriate solution method is used; thereby, producing a general method of solution for the total semi-infinite domain.

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1. Introduction

Numerical methods for advection-diffusion analysis are used to predict the diffusion of particles in domains with complex geometry. Although a number of methods for advection-diffusion analysis presently exist, most focus on applications with domains of finite spatial extent or constant advective fields. Unlike previous work, the work presented in this paper solves the advective-diffusion problem for an infinite space domain with a variable advective field. The work herein builds upon and extends beyond previous work to develop a practical approach to solve the infinite space, advection-diffusion problem.

Although much has been written on the numerical solution of advection-diffusion problems, the semi-infinite space problem with non constant advective fields is still relatively immature. Qiu et al [1] used a Boundary Element Method (BEM) for solving a semi-infinite space advection-diffusion problem with very high Peclet number. In their analysis they used the Green's function associated with a constant advective field; therefore, their analysis was only valid for problems with constant advective fields. Similar in form to advection-diffusion, convection-diffusion problems have been studied extensively in the thermal sciences. Li and Evans [2] used an exponential variable transformation to construct a variational principle which lead to a symmetric banded finite element stiffness matrix. As with Qiu et al, they assumed the convective (advective) field was constant; therefore their solution is limited. Taigbenu and Liggett [3] used the non convective Green's function in an integral approach to model convective domains. This required a domain integration which when discretized leads to fully dense large domain matrices. These matrices are of similar order to that which would result from a finite element approximation. Their method could model convection-diffusion with non constant convective fields; however, it was valid only for domains of finite spatial extent.

Liggett [4] gives a very good discussion of the range of application of the BEM and the extent to which it can be used for advection-diffusion problems. The main points discussed included the fact that the BEM, when it can be applied, is much easier to use than either finite differences or finite elements. The method is inexpensive in terms of human effort (set-up time) and computer run-time. Another main point was that the BEM can handle free surfaces more easily than domain methods; however, it was noted that finite element and finite difference methods can be applied to a larger set of applications.

In conclusion while problems with either bounded domains or constant advective fields have been studied extensively, problems with infinite space domains and variable advective fields have been relatively untouched. In the following sections, we will pursue a method which will allow for the modeling of particle diffusion in semi-infinite space domains with variable advective fields and complex obstacle boundaries. The total domain will be partitioned into two sub domains. That part of the domain with variable advective fields will be modeled using the finite element method, and that part of the domain with nearly constant advective fields will be modeled using the boundary element method.

2. Derivation of Equations of Motion

In this section we will derive the equations of motion for incompressible advection-diffusion. This derivation will be obtained by considering Fick's Law of diffusion and conservation of mass.

Let ϕ be the concentration of a species in a medium. Let $\vec{V}$ be the mass-averaged velocity, α be a diffusivity constant, and ρ be the average density of the medium. The velocity of the species i , $\vec{V}_i$, is the sum of two components--the advection component, $\vec{V}$, and the diffusion component,

$\frac{\rho\alpha}{\rho_i}\nabla\phi$ [8]. This can be stated as

$$\vec{V}_i = \vec{V} - \frac{\rho}{\rho_i}\alpha\nabla\phi \quad (1)$$

where ρ_i is the density of the species. Notice that if the species concentration, ϕ , is uniform, then the species simply moves at the mass averaged velocity $\vec{V}$. On the other hand, if ϕ is not uniform, then the species has a velocity relative to $\vec{V}$ where the relative velocity, $\vec{V}_i - \vec{V}$, is in the "downhill" direction of the concentration field.

2.1 Differential Equation of Motion

From conservation of mass of species i in a control volume, Ω , a differential advection-diffusion equation for an incompressible medium can be derived. Assuming no internal particle production,

$$\begin{array}{l} \text{accumulation of species} \\ i \text{ in } \Omega \end{array} = \begin{array}{l} \text{net flux of species } i \text{ through} \\ \text{the surface of } \Omega. \end{array} \quad (2)$$

The accumulation of species i in Ω is

$$\int_{\Omega} \frac{\partial \rho_i}{\partial t} d\Omega \quad (3)$$

where $\rho_i = \phi\rho$. Letting Γ be the surface of Ω and $\hat{n}$ the outward unit normal vector, then the net flux through Γ is given by

$$-\int_{\Gamma} \hat{n} \cdot \rho_i \vec{V}_i d\Gamma = -\int_{\Omega} \nabla \cdot (\rho_i \vec{V}_i) d\Omega \quad (4)$$

Combining (4) and (1), and noting that $\nabla \cdot \vec{V} = 0$ for an incompressible medium,

$$-\int_{\Gamma} \hat{n} \cdot \rho_i \vec{V}_i d\Gamma = -\int_{\Omega} (\vec{V} \cdot \nabla \rho_i - \rho\alpha \nabla^2 \phi) d\Omega \quad (5)$$

Combining (2), (3), and (5) gives

$$\frac{\partial \phi}{\partial t} = -\vec{V} \cdot \nabla \phi + \alpha \nabla^2 \phi \quad (6)$$

which is the governing partial differential equation for incompressible advection-diffusion.

The steady state weak formulation of (6) for basis function W is

$$\int_{\Omega} W(\alpha \nabla^2 \phi - \vec{V} \cdot \nabla \phi) d\Omega = 0. \quad (7)$$

Using this weak formulation, the Finite Element Method (FEM) and the Boundary Element Method (BEM) can be used to produce discrete approximations to the equation of motion.

2.2. Integral Equation of Motion

The steady state equation of motion can also be expressed in integral form. Replacing the basis function W in (7) with the Green's function G , the weak form becomes

$$\int_{\Omega} (\alpha G \nabla^2 \phi - G \vec{V} \cdot \nabla \phi) d\Omega = 0. \quad (8)$$

Applying the divergence theorem and Green's second identity to (8) gives

$$\int_{\Omega} (\alpha \phi \nabla^2 G + \phi \vec{V} \cdot \nabla G) d\Omega = \int_{\Gamma} (\vec{n} \cdot (-\alpha G \nabla \phi + \alpha \phi \nabla G + \phi G \vec{V})) d\Gamma. \quad (9)$$

Now, letting G satisfy

$$\alpha \nabla^2 G + \vec{V} \cdot \nabla G = -\delta(\vec{r}_0 - \vec{r}) \quad (10)$$

where $\vec{r}_0$ and $\vec{r}$ are points in Ω , (9) becomes

$$c_0(\vec{r}_0)\phi(\vec{r}_0) = \int_{\Gamma} \vec{n} \cdot (\alpha G \nabla \phi - \alpha \phi \nabla G - \phi G \vec{V}) d\Gamma \quad (11)$$

where c_0 is determined by the surface solid angle at $\vec{r}_0$.

When $\vec{V}$ is not a constant or is a very simple function of spatial location, the Green's function is difficult to calculate; however, when $\vec{V}$ is constant, the closed form solution for G is well known (see Qiu et al [1]) and is given by

$$G(\vec{r}, \vec{r}_0) = \frac{1}{4\pi\alpha R} e^{\frac{-u}{2\alpha}(R + (x - x_0))} \quad (12)$$

where

$$R \equiv |\vec{r}_0 - \vec{r}|, \quad (13)$$

$\vec{V} = u\vec{i}$, and u is a constant.

3. Discretization of the Equations of Motion

Because the Green's function is difficult to calculate for variable advective fields, the boundary-integral approach is not feasible when obstacles are present. However, in many problems, obstacles reside in a bounded domain of limited extent and at distances removed from these obstacles, the mean velocity, $\vec{V}$, is essentially constant. Therefore, a BEM can be used to model particle diffusion at locations removed from the obstacles, whereas a finite element method can be used to model particle diffusion at locations in the vicinity of obstacles.

3.1 Discretization of the Differential Equations of Motion

In Figure 1 Ω_{FEM} is a sub domain that is modeled by using FEM and Ω_{BEM} is an exterior sub domain modeled by using BEM. Let N denote the number of nodes in Ω_{FEM} , $\Phi = (\phi_1, \dots, \phi_N)^T$ be a vector containing the values of particle concentration at node locations, Γ_{in} denote the surface of the obstacles in Ω_{FEM} , and Γ_{out} denote the exterior surface that bounds Ω_{FEM} . Let N_{in} be the number of nodes on the inner surface, Γ_{in} , and N_{out} be the number of nodes on the outer surface Γ_{out} . Let Φ_{in} be the vector of nodal values of ϕ on Γ_{in} , Φ_{out} be the vector of nodal values of ϕ on Γ_{out} , $\frac{\partial \Phi_{in}}{\partial n}$ be the vector of normal derivatives of ϕ on Γ_{in} , and $\frac{\partial \Phi_{out}}{\partial n}$ be the vector of normal derivatives of ϕ on Γ_{out} .

A relation between Φ , $\frac{\partial \Phi_{out}}{\partial n}$, and $\frac{\partial \Phi_{in}}{\partial n}$ can be obtained by a Galerkin approach. Replacing W

in (7) with a finite element basis function w_i , where $i=1,\dots,N$, we obtain

$$\int_{\Omega_{FEM}} (\alpha w_i \nabla^2 \phi - w_i \vec{V} \cdot \nabla \phi) d\Omega = 0. \quad (14)$$

Applying the first form of Green's theorem to the first term of (14) gives

$$- \int_{\Omega_{FEM}} (\alpha \nabla \phi \cdot \nabla w_i) d\Omega + \int_{\Gamma_{in}} \left(\alpha w_i \frac{\partial \phi}{\partial n} \right) d\Gamma + \int_{\Gamma_{out}} \left(\alpha w_i \frac{\partial \phi}{\partial n} \right) d\Gamma - \int_{\Omega_{FEM}} (w_i \vec{V} \cdot \nabla \phi) d\Omega = 0. \quad (15)$$

Letting

$$\phi = \sum_{i=1}^N \phi_i w_i, \quad (16)$$

taking the summation outside the integrals and performing the resulting integrations for each i ,

one arrives at a matrix equation of the form

$$A\Phi + B\left(\frac{\partial \Phi_{out}}{\partial n}\right) + C\left(\frac{\partial \Phi_{in}}{\partial n}\right) = 0 \quad (17)$$

This is a FEM formulation for the advection-diffusion in Ω_{FEM} . The solution to (17) is not limited to a constant $\vec{V}$ field since A is a function of $\vec{V}$.

3.2. Discretization of the Integral Equation of Motion

In this section we will approximate the surface integral (11) using the BEM. Using shape functions on Γ_{out} that are compatible with the shape functions in (16), one can arrive at a matrix equation of the form

$$c_0 \Phi_{out} = M\Phi_{out} + G\left(\frac{\partial \Phi_{out}}{\partial n}\right). \quad (18)$$

From (18), we have

$$\Phi_{out} = D\Phi = (c_0 I - M)^{-1} G\left(\frac{\partial \Phi_{out}}{\partial n}\right). \quad (19)$$

3.3. Coupling of the FEM and BEM Discrete Representations

Finally, the coupled $N + N_{out}$ equations, (17) and (19), can be solved simultaneously to yield the

variables Φ and $\frac{\partial \Phi_{out}}{\partial n}$. In particular with $\left(\frac{\partial \Phi_{in}}{\partial n}\right)$ known, the coupled matrix equation to be solved is

$$\begin{bmatrix} A & B \\ D & -(c_0 I - M)^{-1} G \end{bmatrix} \begin{bmatrix} \Phi \\ \left(\frac{\partial \Phi_{out}}{\partial n}\right) \end{bmatrix} = \begin{bmatrix} -C \left(\frac{\partial \Phi_{in}}{\partial n}\right) \\ 0 \end{bmatrix}. \quad (20)$$

Equation (20) is mostly sparse with $O(N)$ non zero entries except for the relatively small dense submatrix in the lower right associated with the BEM. It can be solved with an iterative method such as the generalized minimum residual method [11].

4. Numerical Results

Fluid flow about obstacles produces non constant advective fields; however, when no obstacles are present, the advective field is constant. As described in Section 3, advection-diffusion near obstacles can be modeled using FEM while the advection-diffusion away from these obstacles can be modeled using BEM. In this section results from the Section 3 hybrid FEM/BEM method are presented. When an exact solution exists, it will be presented with these results for the purpose of quantifying numerical error.

Two problems will be solved in this section. In the first problem, a point source diffuses particles into an infinite domain in the presence of constant wind. A closed form solution exists for this problem; therefore, a comparison between the exact and numerical solutions can be made. This problem is illustrated in Figure 2.

In the second problem, the point source is replaced with a source of spherical geometry. The source is assumed to have a zero mean normal velocity condition on its boundary. The advective field around this source is non constant due to this boundary condition. This problem is illustrated in Figure 4. The finite element and boundary element mesh for both of these problems is shown in Figure 1.

4.1. Numerical Solution for a Constant Advective Field

In the first problem, the coupled equations (20) were solved assuming a constant advective field.

The forcing term $\frac{\partial \Phi_{in}}{\partial n}$ on Γ_{in} was calculated from the gradient of (12). As shown in Figure 3, the closed form solution and the numerical solution agreed very well. The worst case deviation from (12) was 2% for ϕ values on Γ_{in} .

4.2. Numerical Solution for a Variable Advective Velocity

In the second problem, the source was assumed to be impervious to mean fluid motion across its boundary. This source was an obstacle to mean fluid flow. If ψ is the mean velocity potential, then for this obstacle

$$\psi = ux + \frac{ua^3x}{2r^3} + A_0 \quad (21)$$

where A_0 is an arbitrary constant, a is the radius of the spherical obstacle, r is the distance from the center of the obstacle, $\vec{V} = \nabla \psi$ inside Ω_{FEM} , and x is measured from the center of the spherical obstacle. In Ω_{BEM} $\vec{V}$ is approximated by $u\vec{i}$ and $\frac{\partial \Phi_{in}}{\partial n}$ was constant with a value of 1.

The resulting coupled equations (20) were solved for Φ and $\frac{\partial \Phi_{out}}{\partial n}$. A polar plot of ϕ on the cir-

cle: $x^2 + y^2 = 1$, $z=0$ is given in Figure 5.

It can be seen from (21) that the difference between $u\hat{i}$ and the true velocity decays as $\frac{a^3}{r^3}$, and the

biggest difference occurs along the x-axis with $V_x = u - u\left(\frac{a^3}{r^3}\right)$. It can be shown then that the

required value of r for V_x to be within 2% of u is $r \approx 3a$. In other words, the finite element mesh must be about 2 obstacle radii thick or must have a radius 3 times that of the obstacle. Such a thickness cannot be immediately assumed to imply that the error in the solution will also be 2%, and this is a subject for future investigation.

5. Conclusion

A hybrid finite element/boundary element method (FEM/BEM) was proposed for the solution of advection-diffusion problems in which the advective field was non constant and the spatial domain unbounded. By placing finite element meshes around obstacles where the advective field varies, one can handle a set of advection-diffusion problems with variable advective fields. Away from the obstacles, external to the domain containing the finite element mesh and where the advective field is nearly constant, a BEM was used. The coupled FEM and BEM equations can be solved simultaneously to yield an efficient solution.

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Figure 1. Schematic of hybrid FEM/BEM mesh used to model Problem 1 and Problem 2

Figure 2. Problem 1: particles diffuse from a point source in a domain with a constant advective field

Figure 3. Problem1 results: a comparison of the FEM/BEM Solution to the Exact Solution

Figure 4. Problem 2: particles diffuse from a spherical source in a domain with a non constant advective field

Figure 5. Problem 2 results: polar plot of concentration values for advection-diffusion emanating from a spherical source in a variable advective field.