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A finite element–boundary element method for advection–diffusion problems with variable advective fields and infinite domains

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Abstract

In this paper a hybrid, finite element–boundary element method which can be used to solve for particle advection–diffusion in infinite domains with variable advective fields is presented. In previous work either boundary element, finite element, or difference methods were used to solve for particle motion in advective–diffusive domains. These methods have a number of limitations. Due to the complexity of computing spatially dependent Green's functions, the boundary element method is limited to domains containing only constant advective fields, and due to their inherent formulations, finite element and finite difference methods are limited to only domains of finite spatial extent. Thus, finite element and finite difference methods are limited to finite space problems for which the boundary element method is not, and the boundary element method is limited to constant advection field problems for which finite element and finite difference methods are not. In this paper it is proposed to split the total domain into two sub-domains, and for each of these sub-domains, apply the appropriate solution method; thereby, producing a method for the total infinite space, variable advective field domain. © 2001 Elsevier Science Ltd. All rights reserved.

Keywords: Advection–diffusion; Infinite space; Finite elements; Boundary elements

1. Introduction

Numerical methods are used to analyze the advection and diffusion of particles in complex domains. Although a number of numerical methods for advection–diffusion analysis presently exist, most are applicable to problems with domains of infinite spatial extent and constant advective fields or to problems with domains of finite spatial extent and variable advective fields. Few are applicable to problems with domain of both infinite spatial extent and variable advective fields. In this paper, a method will be presented which can be used to solve for a subset of advective-diffusion problems with infinite spatial domains and variable advective fields.

Although much has been written on the numerical solution of advection–diffusion problems, the infinite space problem with non-constant advective fields is still immature. Qiu et al. [1] used a boundary element method (BEM) for solving an infinite space advection–diffusion problem with very high Peclet number. However, 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 field characteristics. 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 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. Their method could model convection–diffusion with non-constant convective

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Nomenclature

ϕ_i	concentration of a species i
$\vec{V}$	mass-averaged velocity of the medium
α	diffusivity of the medium
ρ	average density of the medium
ρ_i	density of species i in the medium
$\vec{V}_i$	particle velocity of the species i
Γ	surface of control volume
$\vec{n}$	normal vector
W	bases function
Ω_{FEM}	interior domain where FEM is applicable
Ω_{BEM}	exterior domain where BEM is applicable
Γ_{in}	surface of obstacles
Γ_{out}	surface shared by Ω_{FEM} and Ω_{BEM}
N_{in}	number of nodes on Γ_{in}
N_{out}	number of nodes on Γ_{out}
$\boldsymbol{\Phi}$	$(\phi_{i_1}, \ldots, \phi_{i_N})^{\mathrm{T}}$
ϕ_{i_j}	jth ϕ_i value at nodes in Ω_{FEM}
$\boldsymbol{\Phi}_{\mathrm{in}}$	vector of ϕ_i values on Γ_{in}
$\boldsymbol{\Phi}_{\mathrm{out}}$	vector of ϕ_i values on Γ_{out}
$\partial\boldsymbol{\Phi}_{\mathrm{in}}/\partial n$	vector of normal derivatives of ϕ_i on Γ_{in}
$\partial\boldsymbol{\Phi}_{\mathrm{out}}/\partial n$	vector of normal derivatives of ϕ_i on Γ_{out}
$\boldsymbol{A}, \boldsymbol{B}, \boldsymbol{C}$	FEM matrices
G	Green's function
$\vec{r}_0$ and $\vec{r}$	points in Ω_{BEM}
$\boldsymbol{M}, \boldsymbol{D}, \boldsymbol{G}$	BEM matrices
ψ	velocity potential
$u\vec{i}$	velocity of wind at infinity

fields; however, it was valid only for domains of finite spatial extent.

Liggett [4] gives a very good discussion of the applicability 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. Moreover, 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, finite element and finite difference methods can be applied to a larger set of applications. Sponge layers, infinite elements and other such boundary conditions (see [5]) could be used to extend the finite element solution to infinite and semi-infinite domains; however, many of these conditions are dependent on the governing equations of motion, and therefore are not applicable to advection–diffusion problems without modifications.

In conclusion, while problems with either finite domains with variable advective fields or infinite domains with 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 present a method which allows for the modeling of particle motion in infinite space domains with variable advective fields produced by complex obstacle boundaries. In this presentation, it is assumed that the total domain can be partitioned into two sub domains: one sub domain is infinite and contains a constant advective field and the other sub domain is finite and contains a variable advective field. A general rule of thumb for this partitioning is presented. The sub domain with the variable advective fields is modeled using the FEM, and the sub domain with constant advective fields is modeled using the BEM. There are other methods in the literature, such as infinite elements, which may be applicable to this problem; however, at present, their formulations are relatively immature for advection–diffusion types of problems.

2. Equation of motion

The partial differential equation for steady state particle advection and diffusion in an incompressible medium is well known and is given by

$$-\vec{V} \cdot \nabla\phi_i + \alpha\nabla^2\phi_i = 0, \tag{1}$$

where $\vec{V}$ is the mass-averaged velocity of the medium, α the diffusivity constant of the medium, and ϕ_i is the species concentration. Notice that if $\vec{V}$ were a variable, (1) would be a non-linear equation. However, if $\vec{V}$ is a known quantity then (1) reduces to a linear problem for ϕ_i. Therefore, in this paper, to avoid the complexity of non-linear analysis, the solution ϕ_i for will be decomposed into two steps. In the first step, the mean wind velocity, $\vec{V}$, is calculated assuming potential flow (this does not require any knowledge of ϕ_i), and in the second step, the solution $\vec{V}$ is substituted into (1) and ϕ_i is calculated. Since calculation of the first step is usually straight forward, the rest of this paper will be focused toward the calculation of the second step.

In general (1) cannot be solved for in closed form; therefore, numerical methods must be used. To solve (1) using a FEM or BEM, it must be placed into a weak formulation. A steady state weak formulation of (1) for a trial function W is

$$\int_\Omega W\left(\alpha\nabla^2\phi_i - \vec{V} \cdot \nabla\phi_i\right) \mathrm{d}\Omega = 0. \tag{2}$$

In the following section, a FEM and BEM approximation will be formulated using (2).

3. Discretization of the equation of motion

In this section the equation of motion will be discretized using a FEM and BEM. In many problems, obstacles reside in a bounded, finite domain of limited extent, and at distances removed from these obstacles, the mean velocity, $\vec{V}$, is practically constant. As will be shown, a BEM can be used to model particle motion at locations removed from these obstacles, and a FEM can be used to model particle motion at locations in the vicinity of these obstacles. In the following subsections, a FEM and BEM are used to produce approximations to the weak form of the equation of motion (Eq. (2)). These approximations are valid for limited sub domains. To model the total domain, the two approximations are then coupled at their domain interfaces.

3.1. A FEM approximation of the equation of motion

Consider the simple domain shown in Fig. 1. In this domain $\Omega_{\rm FEM}$ is an interior, finite sub domain with a variable advective field that can be modeled by using FEM, and $\Omega_{\rm BEM}$ is an exterior, infinite sub domain with a constant advective field that can be modeled by using BEM. Let N denote the number of nodes in $\Omega_{\rm FEM}, \Phi = (\phi_{i_1}, \dots, \phi_{i_N})^{\rm T}$ be a vector containing the values of ϕ_i at node locations, $\Gamma_{\rm in}$ denote the surface of the obstacles in $\Omega_{\rm FEM}$, and $\Gamma_{\rm out}$ denote the exterior surface that bounds $\Omega_{\rm FEM}$. Let $N_{\rm in}$ be the number of nodes on the inner surface, $\Gamma_{\rm in}$, and $N_{\rm out}$ be the number of nodes on the outer surface, $\Gamma_{\rm out}$. Let $\Phi_{\rm in}$ be the vector of nodal values of ϕ_i on, $\Gamma_{\rm in}$, $\Phi_{\rm out}$ be the vector of nodal values of ϕ_i on $\Gamma_{\rm out}$, $\partial\Phi_{\rm in}/\partial n$ be the vector of normal derivatives of ϕ_i on $\Gamma_{\rm in}$, and $\partial\Phi_{\rm out}/\partial n$ be the vector of normal derivatives of ϕ_i on $\Gamma_{\rm out}$.

A relation between Φ, $\partial\Phi_{\rm out}/\partial n$, and $\partial\Phi_{\rm in}/\partial n$ can be obtained by a Galerkin approach. Replacing W in (2) with a finite element basis function w_j, where $j = 1, \dots, N$, we obtain

$$\int_{\Omega_{\rm FEM}} \left(\alpha w_j \nabla^2 \phi_i - w_j \vec{V} \cdot \nabla\phi_i\right) {\rm d}\Omega_{\rm FEM} = 0. \qquad (3)$$

Applying the first form of Green's theorem to the first term of (3) gives

$$-\int_{\Omega_{\rm FEM}} (\alpha\nabla\phi_i \cdot \nabla w_j)\,{\rm d}\Omega_{\rm FEM} + \int_{\Gamma_{\rm in}} \left(\alpha w_j \frac{\partial\phi_i}{\partial n}\right) {\rm d}\Gamma_{\rm in} + \int_{\Gamma_{\rm out}} \left(\alpha w_j \frac{\partial\phi_i}{\partial n}\right) {\rm d}\Gamma_{\rm in} - \int_{\Omega_{\rm FEM}} \left(w_j \vec{V} \cdot \nabla\phi_i\right) {\rm d}\Omega_{\rm FEM} = 0. \qquad (4)$$

Letting

$$\phi_i = \sum_{j=1}^{N} \phi_{i_j} w_j, \qquad (5)$$

taking the summation outside the integrals and performing the resulting integrations for each j, one arrives at a matrix equation of the form

$$\boldsymbol{A}\Phi + \boldsymbol{B}\left(\frac{\partial\Phi_{\rm out}}{\partial n}\right) + \boldsymbol{C}\left(\frac{\partial\Phi_{\rm in}}{\partial n}\right) = 0. \qquad (6)$$

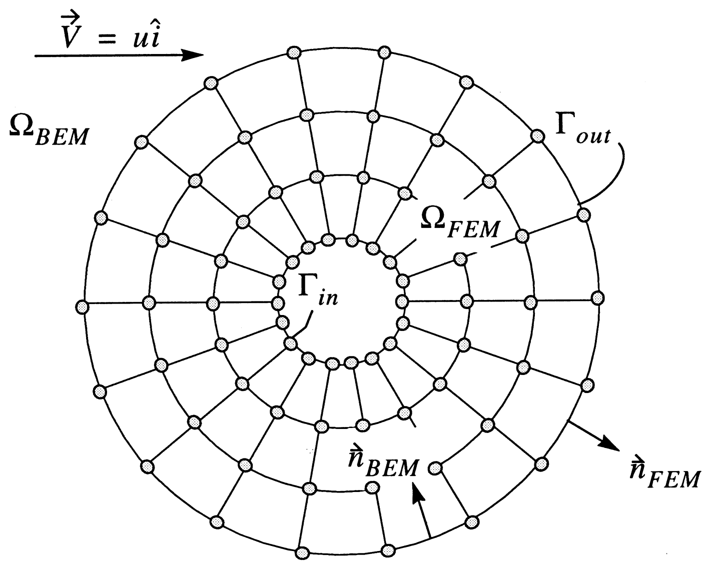

Fig. 1. A schematic of a hybrid FEM–BEM domain.

Eq. (6) is a FEM formulation for modeling steady state advection and diffusion in the bounded domain, Ω_{FEM}. This formulation is not limited to a constant $\vec{V}$ field since $\boldsymbol{A}$ is a function of $\vec{V}$, but is limited to finite space domains and small Peclet numbers. (Extension of the Galerkin method to advection-dominated problems has been considered in previous work, such as [6,7].) Since high wind velocities are not of concern in this paper, the limitation due to the Peclet number is not of relevance; however, the limitation due to the infinite spatial domain is of relevance and is overcome by coupling this solution to a BEM formulation. In the next subsections, this formulation and its coupling to Eq. (6) will be discussed.

3.2. A BEM approximation of the equation of motion

The steady state equation of motion can also be expressed in integral equation form, and from this form, a BEM can be used to produce a discrete approximation. The integral representation is derived from (2) and the Green's function, G. For constant advective fields, this Green's function can be easily computed; however, for variable advection, calculation of the Green's function becomes complex. Therefore, the BEM is seldom used to model particle motion in non-constant advective domains. In this paper, the BEM is used to model particle motion in only the constant advection portion of the total domain.

Replacing the basis function W in (2) with the Green's function G, the weak form becomes

$$\int_{\Omega_{\mathrm{BEM}}} \left(\alpha G \nabla^2 \phi_i - G\vec{V}\cdot\nabla\phi_i\right) \mathrm{d}\Omega_{\mathrm{BEM}} = 0. \tag{7}$$

Applying the divergence theorem and the second form of Green's theorem to (7) gives

$$\int_{\Omega_{\mathrm{BEM}}} \left(\alpha\phi_i\nabla^2 G + \phi_i\vec{V}\cdot\nabla G\right) \mathrm{d}\Omega_{\mathrm{BEM}} = \int_{\Gamma_{\mathrm{out}}} \left(\vec{n}\cdot\left(-\alpha G\nabla\phi_i + \alpha\phi_i\nabla G + \phi_i G\vec{V}\right)\right) \mathrm{d}\Gamma_{\mathrm{out}}. \tag{8}$$

Since, by definition of the Green's function, G, satisfies

$$\alpha\nabla^2 G + \vec{V}\cdot\nabla G = -\delta\left(\vec{r}_0 - \vec{r}\right), \tag{9}$$

where $\vec{r}_0$ and $\vec{r}$ are points in Ω_{BEM}, (8) becomes

$$c_0(\vec{r}_0)\phi(\vec{r}_0) = \int_{\Gamma_{\mathrm{out}}} \vec{n}\cdot\left(\alpha G\nabla\phi_i - \alpha\phi_i\nabla G - \phi_i G\vec{V}\right) \mathrm{d}\Gamma_{\mathrm{out}}, \tag{10}$$

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

When $\vec{V}$ is not a constant or is not a very simple function of spatial location, the closed form solution to (9) is difficult to calculate; however, when $\vec{V}$ is constant, the closed form solution for G is well known (see [8]) and is given by

$$G\left(\vec{r}, \vec{r}_0\right) = \frac{1}{4\pi\alpha R}\mathrm{e}^{(-u/2\alpha)(R+(x-x_0))}, \tag{11}$$

where

$$R \equiv \left|\vec{r}_0 - \vec{r}\right|, \tag{12}$$

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

Eq. (10) is an integral representation of the equation of motion. Since (9) is difficult to solve for when $\vec{V}$ is not a constant, this equation of motion is seldom (if ever) used to model problems with non-constant advective fields. Nevertheless, since it contains only a surface integration, it can easily be used to model infinite space problems.

The surface integral in (10) can be approximated using the BEM. Using shape functions on Γ_{out} that are compatible with the shape functions in (3), one can arrive at a matrix equation of the form

$$c_0\Phi_{\mathrm{out}} = \boldsymbol{M}\Phi_{\mathrm{out}} + \boldsymbol{G}\left(\frac{\partial\Phi_{\mathrm{out}}}{\partial n}\right). \tag{13}$$

From (13), we have

$$\Phi_{\mathrm{out}} = \boldsymbol{D}\Phi = (c_0\boldsymbol{I} - \boldsymbol{M})^{-1}\boldsymbol{G}\left(\frac{\partial\Phi_{\mathrm{out}}}{\partial n}\right). \tag{14}$$

The singularity in the derivative of Eq. (11) is included in the geometric coefficients, c_0, in Eq. (10) as is commonly done in boundary element analysis. The values of these coefficients, c_0, can be determined by the surface's solid angle at the observation point at $\vec{r}_0$ as mentioned above. The diagonal components of the matrices $\boldsymbol{M}$ and $\boldsymbol{G}$ in Eq. (13) still contain a singularity in the integrand; however, this is an integrable singularity. This integration is performed by switching to polar coordinates and completing the integration in the radial direction in closed form. The integration in the angular direction can then be computed numerically using a Gauss quadrature. In Eq. (14), the inversion of the matrix $(c_0\boldsymbol{I} - \boldsymbol{M})^{-1}\boldsymbol{G}$ can be performed by producing an LU factorization of $c_0\boldsymbol{I} - \boldsymbol{M}$ and then using back/forward substitution on each column of the matrix $\boldsymbol{G}$.

3.3. Coupling of the FEM and BEM equations

The coupled $N + N_{\mathrm{out}}$ Eqs. (6) and (14), can be solved simultaneously to yield the variables Φ and $\partial\Phi_{\mathrm{out}}/\partial n$. In particular with $(\partial\Phi_{\mathrm{in}}/\partial n)$ known, the coupled matrix equation to be solved is

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{B} \\ \boldsymbol{D} & -(c_0\boldsymbol{I}-\boldsymbol{M})^{-1}\boldsymbol{G} \end{bmatrix} \begin{bmatrix} \Phi \\ \left(\frac{\partial \Phi_{\text{out}}}{\partial n}\right) \end{bmatrix} = \begin{bmatrix} -\boldsymbol{C}\left(\frac{\partial \Phi_{\text{in}}}{\partial n}\right) \\ 0 \end{bmatrix}. \quad (15)$$

Eq. (15) is mostly sparse with O(N) non-zero entries except for the relatively small dense sub-matrix in the lower right associated with the BEM. It can be solved with an iterative method such as the generalized minimum residual method [9] or with a direct sparse solver. In the problems in this paper, these methods were used.

4. Numerical results

Fluid flow about obstacles produces non-constant advective fields; however, in many problems, when no obstacles are present, the advective field is almost constant. As described in Section 3, advection–diffusion in finite space domains with non-constant advective fields can be modeled using FEM while the advection–diffusion in infinite domains with constant advective fields can be modeled using BEM. Therefore, near obstacles a FEM is used to model particle motion and away from obstacles a BEM method is used. In this section results using this hybrid finite element–boundary element method (FEM–BEM) of solution are presented. When an exact solution exists, it will be presented with these results for the purpose of quantifying numerical error.

Three problems will be presented 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. In the second problem, the point source is replaced with a source of spherical geometry, and in the third problem, the FEM–BEM is used to model particle motion around a set of realistic complex obstacles.

4.1. Numerical solution for a constant advective field

The first problem is shown in Fig. 2. A constant flux of particles flow from a point source in an infinite domain. Within the domain a constant wind is blowing. Therefore, the advective field is constant. The solution to this problem is well known [8] and therefore, provides a method to verify the FEM–BEM solution.

Fig. 1 is an illustration of the mesh used to solve this problem. Due to the concentration singularity resulting from applying a Dirac Delta function to model the point source in the FEM domain, the center portion of the mesh has been removed and the forcing term $\partial\Phi_{\text{in}}/\partial n$ was calculated from the exact solution and applied on Γ_{in}. The value of ϕ_i could then be predicted at points in Ω_{FEM} and Ω_{BEM}.

In this problem the FEM domain is the region bounded by an inner sphere of radius 1.0 and an outer sphere of radius 3.0. The wind velocity u was 2.0 and the diffusivity constant α was 1.0. The strength of the source was 1.0. Thus the exact analytical solution from [8] is: $\phi_{(i)\text{exact}} = (1/R)\mathrm{e}^{(-u/2)(R-x)}$. The mesh qualitatively appeared as in Fig. 1. The number of layers of elements (in the radial direction) was 7, so that there are 8 layers of nodes, with 250 nodes on each layer. All elements are standard isoparametric brick Hex8 elements, thus making the surface elements standard isoparametric Quad4 elements.

In Fig. 3 the closed form and the numerical solution are compared. In this figure the value of ϕ_i is plotted for $a = 1$ and various values of θ, where θ is the angle and a is the magnitude of the vector in the xy plane shown in Fig. 2. In this example $a = 1$, and the vector points to points in Γ_{in}. Fig. 3 is a polar plot with radial distance equal to ϕ_i for various θ values. The maximum error shown in this plot between the FEM–BEM solution and the exact solution is 2%. Overall the FEM–BEM solution agreed very well with the exact solution.

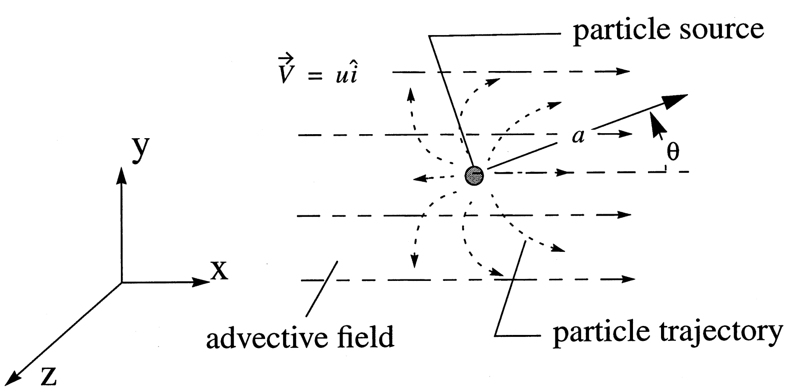

Fig. 2. Problem 1 geometry: particles diffuse from a point source in a domain with a constant advective field.

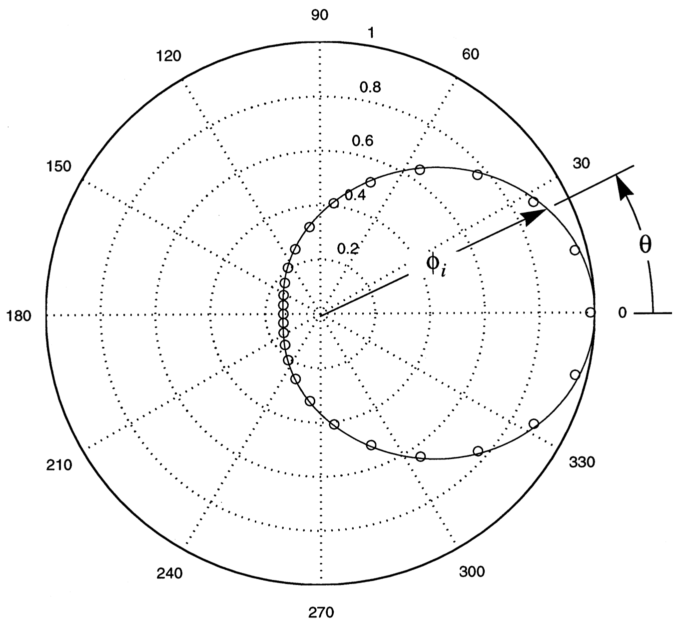

Fig. 3. Problem 1 results: a comparison of the FEM–BEM solution to the exact solution, (○) FEM/BEM solution, (–) exact solution.

4.2. Numerical solution for a variable advective field

The second problem is shown in Fig. 4. In this problem particles flow from a spherical source. The source not only emits particles but also alters the flow of wind in the domain. Therefore, the advective field is not constant but varies near the source; however, far from the source, the wind flow and therefore the advective field *is* almost constant.

In this problem the FEM domain is the region bounded by an inner sphere of radius 1.0 and an outer radius of 3.3. The wind velocity u was 2.0 and the diffusivity constant α was 1.0. The mesh qualitatively appeared as in Fig. 1. The number of layers of elements (in the radial direction) was 12 so that there are 13 layers of nodes, with 250 nodes on each layer. All elements are standard isoparametric brick Hex8 elements, thus making the surface elements standard isoparametric Quad4 elements.

An exact solution for the flow of wind around a spherical obstacle exists [10]. If ψ is the mean velocity potential, then for this obstacle

$$\psi = ux + \frac{ub^3x}{2a^3}, \tag{16}$$

where b is the radius of the obstacle, a the distance from the center of the obstacle, $\vec{V} = \nabla\psi$, and $x = a \cdot \cos\theta$ as θ and a are defined in Fig. 4. The difference between $u\vec{i}$,

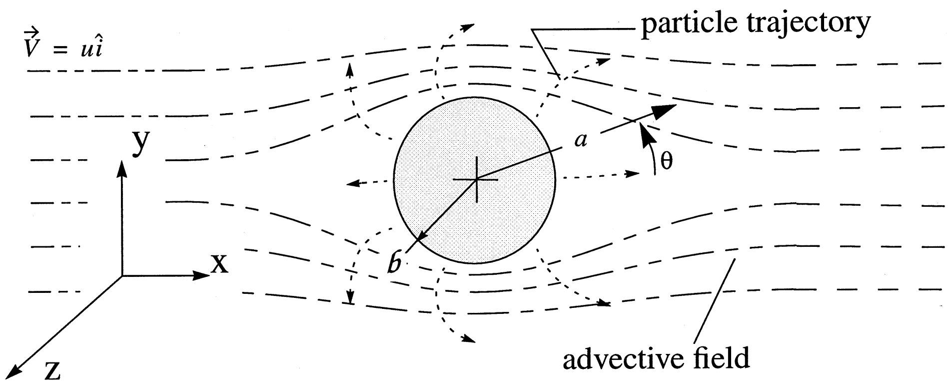

Fig. 4. Problem 2 geometry: particles diffuse from a spherical source in a domain with a non-constant advective field, (○) 2750 DOF mesh, (+) 3250 DOF mesh.

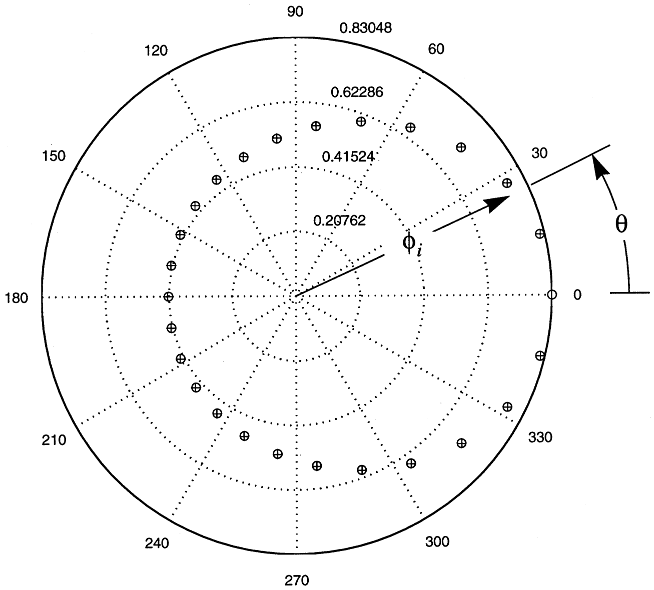

Fig. 5. Problem 2 results: a plot of particle concentration at locations in the xy plane for a 2750 and 3250 DOF mesh.

the velocity at infinity, and the true velocity at any point in Ω_{FEM} or Ω_{BEM} decays as b^3/a^3 where the biggest difference between these velocities occurs along the x-axis. For the true velocity to be within 2% of $u\,\underline{i}$, $a \approx 3b$. In other words, for this problem, the finite element mesh must be about two obstacle radii thick or must have a radius three times that of the obstacle for the solution to be accurate.

The mesh used to model this problem is also illustrated in Fig. 1. The boundary conditions for a uniform particle flux were applied on Γ_{in}, and the resulting coupled equation (15) were used to solve for Φ and $\partial\Phi_{\mathrm{out}}/\partial n$. A polar plot of ϕ_i versus θ on the circle $a = 1$ is given in Fig. 5 for two different mesh densities. As seen in this figure, for these mesh densities, the solution has converged.

4.3. Numerical solution for realistic obstacles

A more realistic problem is illustrated in Fig. 6. A set of buildings block the flow of wind in an infinite space domain. In proximity to these buildings is a particle source distribution. This distribution emits particles into the domain which both diffuse through the wind and are carried by the wind around and over the buildings. The buildings are assumed to be impervious to both the diffusion of the particles and to the flow of the wind.

Using the FEM–BEM solution developed in this paper, this complex problem was solved. First the flow field around the buildings was numerically determined using standard potential theory. Specifically, we used the same FEM–BEM approach presented in this paper with $u = 0$. The wind potential is the solution of this partial differential equation with a different set of boundary conditions. We then calculated the gradient of the potential to determine the velocity field around the obstacles.

To solve the advective-diffusion problem, the domain was divided into sub-domains with almost constant and variable advective fields. Using results from Section 4.2, the radius of the outer surface of the FEM domain was determined by defining a sphere that enclosed all obstacles, and by specifying the radius of this outer surface to be at least three times the radius of the enclosing sphere. This three radii approximation is a general rule of thumb for estimating the location of sub-domain boundaries. The BEM method was applied to the constant advective field sub-domain and the FEM method was applied to the variable advective field sub-domain. The two methods were then coupled and a total advective-diffusion solution was solved for. A resultant particle concentration plot is shown in Fig. 7. In this figure the wind velocity, u, was 2.0 and the diffusivity constant α was 1.0.

5. Conclusions

In this paper, a hybrid FEM–BEM of solution was presented for a set of advection–diffusion problems. For many problems, the advective field is variable close to obstacles in the domain, but at distances removed from those obstacles, the field is almost constant. By placing finite element meshes around

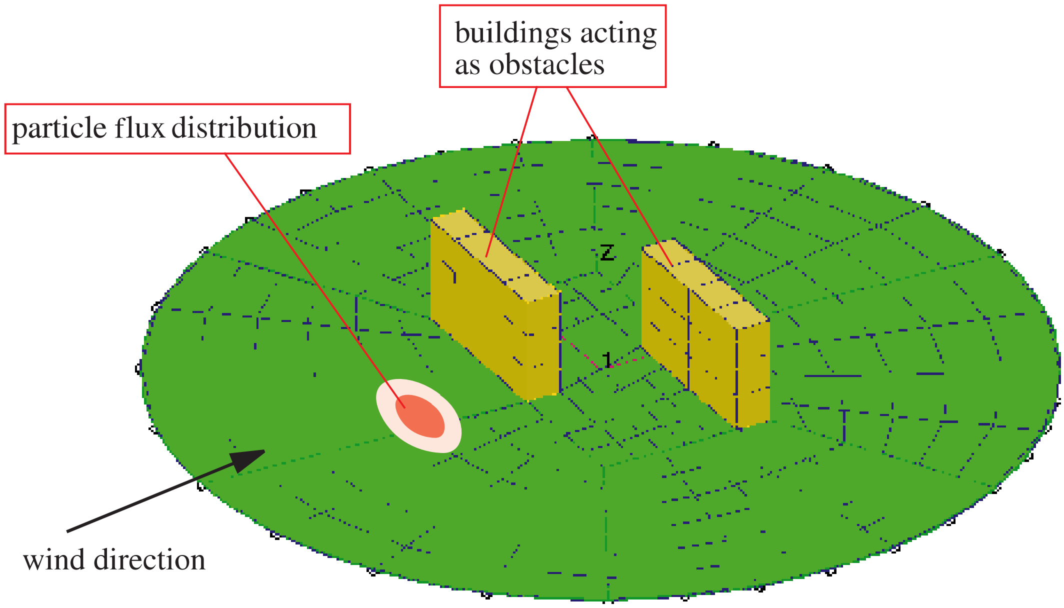

Fig. 6. Problem 3 geometry: two buildings surrounded by an infinite half space.

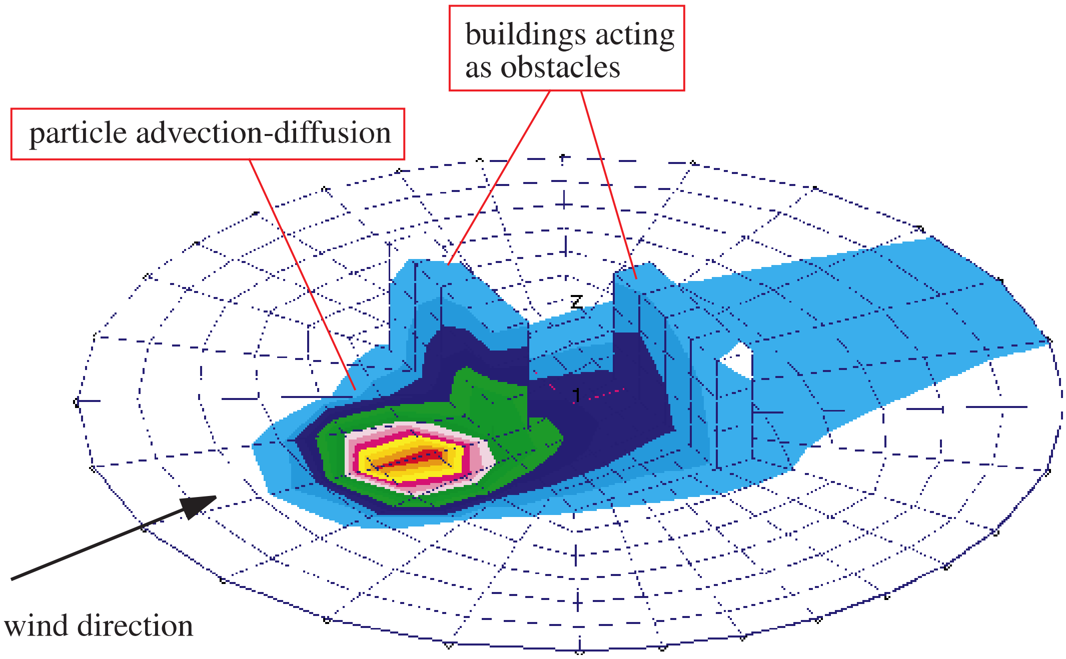

Fig. 7. Problem 3 results: particles diffuse in a variable advective field around buildings.

obstacles where the advective field varies and by using the BEM at locations removed from these obstacles, one can solve a set of advective-diffusion problems which are seldom addressed in the present literature.

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