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

Brian J. Driessen[1] and Jeffrey L. Dohner[2]
[1]*Structural Dynamics and Controls, Sandia National Laboratory, Albuquerque, NM 87185-0439, USA*
bjdries@sandia.gov
[2]*Structural Dynamics and Controls, Sandia National Laboratory, Albuquerque, NM 87185-0439, USA*
jldohne@sandia.gov

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 have been 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 formulation, 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 a 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.

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, but 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 sub set 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. Moreover, since they use a Finite Element Method (FEM), they were limited to finite spatial domains. 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 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. 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 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. 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.

2. Derivation of Equation of Motion

In this section we derive the differential equation of motion for particle advection and diffusion in an incompressible medium. This derivation is obtained by using Fick's Law of diffusion and conservation of mass. In later sections, this equation of motion will be approximated using a FEM and BEM.

Consider the control volume in Figure 1. A fluid medium carries a distribution of diffusive particle species though this volume. Let ϕ_i be the concentration of a species i in the medium, $\vec{V}$ be the mass-averaged velocity of the medium, α be the diffusivity of the medium, ρ be the average density of the medium, and ρ_i be the density of the species i in the medium. From Fick's Law of diffusion, the particle velocity of the species i, $\vec{V}_i$, is the sum of two components--the advection component, $\vec{V}$, and the diffusion component, $-\frac{\rho\alpha}{\rho_i}\nabla\phi_i$ (Edwards [5]). This can be stated analytically as

$$\vec{V}_i = \vec{V} - \frac{\rho}{\rho_i}\alpha\nabla\phi_i \tag{1}$$

Notice that if the species concentration, ϕ_i, is uniform, then the species simply moves at the mass averaged velocity, $\vec{V}$. On the other hand, if ϕ_i 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.

A differential advection-diffusion equation of motion for ϕ_i can be determine by using (eqn 1) and by imposing mass conservation. Assuming no internal particle production, from the conservation of mass,

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

In analytical terms, the accumulation of species i in Ω is

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

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

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

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

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

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

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

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

Notice that if $\vec{V}$ were a variable, (eqn 6) would be a non-linear equation. However, if $\vec{V}$ is a known quantity then (eqn 6) reduces to a linear problem for ϕ_i. Therefore, in this paper, to avoid the complexity of non-linear analysis, the solution for ϕ_i 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 (eqn 6) 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, (eqn 6) cannot be solved for in closed form; therefore, numerical methods must be used. To solve (eqn 6) using a FEM or BEM, it must be placed into a weak formulation. A steady state weak formulation of (eqn 6) for a trial function W is

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

In the following section, a FEM and BEM approximation will be formulated using (eqn 7).

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 a weak form of the equation of motion (eqn 7). 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 Figure 2. In this domain Ω_{FEM} is an interior, finite sub domain with a variable advective field that can be modeled by using FEM, and Ω_{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 Ω_{FEM}, $\Phi = (\phi_{i_1}, \ldots \phi_{i_N})^T$ be a vector containing the values of ϕ_i 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_i on Γ_{in}, Φ_{out} be the vector of nodal values of ϕ_i on Γ_{out}, $\dfrac{\partial\Phi_{in}}{\partial n}$ be the vector of normal derivatives of ϕ_i on Γ_{in}, and $\dfrac{\partial\Phi_{out}}{\partial n}$ be the vector of normal derivatives of ϕ_i on Γ_{out}.

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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 (eqn 7) with a finite element basis function w_j, where j=1,...,N, we obtain

$$\int_{\Omega_{FEM}} (\alpha w_j \nabla^2 \phi_i - w_j \vec{V} \cdot \nabla \phi_i) d\Omega_{FEM} = 0. \tag{8}$$

Applying the first form of Green's theorem to the first term of (eqn 8) gives

$$-\int_{\Omega_{FEM}} (\alpha \nabla \phi_i \cdot \nabla w_j) d\Omega_{FEM} + \int_{\Gamma_{in}} \left(\alpha w_j \frac{\partial \phi_i}{\partial n}\right) d\Gamma_{in}$$

$$+ \int_{\Gamma_{out}} \left(\alpha w_j \frac{\partial \phi_i}{\partial n}\right) d\Gamma_{in} - \int_{\Omega_{FEM}} (w_j \vec{V} \cdot \nabla \phi_i) d\Omega_{FEM} = 0. \tag{9}$$

Letting

$$\phi_i = \sum_{j=1}^{N} \phi_{i_j} w_j, \tag{10}$$

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

$$\boldsymbol{A}\Phi + \boldsymbol{B}\left(\frac{\partial \Phi_{out}}{\partial n}\right) + \boldsymbol{C}\left(\frac{\partial \Phi_{in}}{\partial n}\right) = 0. \tag{11}$$

(Eqn 11) 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. 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 (eqn 11) 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 (eqn 7) 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 (eqn 7) with the Green's function G, the weak form becomes

$$\int_{\Omega_{BEM}} (\alpha G \nabla^2 \phi_i - G\vec{V} \cdot \nabla \phi_i) d\Omega_{BEM} = 0. \tag{12}$$

Applying the divergence theorem and the second form of Green's theorem to (eqn 12) gives

$$\int_{\Omega_{BEM}} (\alpha \phi_i \nabla^2 G + \phi_i \vec{V} \cdot \nabla G) d\Omega_{BEM} =$$

$$\int_{\Gamma_{out}} (\vec{n} \cdot (-\alpha G \nabla \phi_i + \alpha \phi_i \nabla G + \phi_i G\vec{V})) d\Gamma_{out}. \tag{13}$$

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

$$\alpha \nabla^2 G + \vec{V} \cdot \nabla G = -\delta(\vec{r}_0 - \vec{r}) \tag{14}$$

where $\vec{r}_0$ and $\vec{r}$ are points in Ω_{BEM}, (eqn 13) becomes

$$c_0(\vec{r}_0)\phi(\vec{r}_0) = \int_{\Gamma_{out}} \vec{n} \cdot (\alpha G \nabla \phi_i - \alpha \phi_i \nabla G - \phi_i G\vec{V}) d\Gamma_{out} \tag{15}$$

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 (eqn 14) 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

$$G(\vec{r}, \vec{r}_0) = \frac{1}{4\pi\alpha R} e^{\frac{-u}{2\alpha}(R + (x - x_0))} \tag{16}$$

where

$$R \equiv |\vec{r}_0 - \vec{r}|, \tag{17}$$

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

(Eqn 15) is an integral representation of the equation of motion. Since (eqn 14) 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 advec-

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tive fields. Nevertheless, since it contains only a surface integration, it can easily be used to model infinite space problems.

The surface integral in (eqn 15) can be approximated using the BEM. Using shape functions on Γ_{out} that are compatible with the shape functions in (eqn 8), one can arrive at a matrix equation of the form

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

From (eqn 18), we have

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

3.3. Coupling of the FEM and BEM equations

The coupled $N + N_{out}$ equations, (eqn 11) and (eqn 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

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

Equation (eqn 20) 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 [6] or with a direct sparse solver. For most problems, solving (eqn 20) is not difficult since $N + N_{out}$ is usually small.

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 or almost is 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 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 Figure 3. 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 [7] and therefore, provides a method to verify the FEM-BEM solution.

Figure 2 is an illustration of the mesh used to solve this problem. Due to the difficulty of 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 $\frac{\partial \Phi_{in}}{\partial n}$ 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 Figure 4, 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 a vector in the xy plane shown in Figure 3. In this example, $a=1$, and the vector points to points in Γ_{in}. Figure 4 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.

4.2. Numerical solution for a variable advective field

The second problem is shown in Figure 5. 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

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advective field is almost constant.
An exact solution for the flow of wind around a spherical obstacle exists [8]. If ψ is the mean velocity potential, then for this obstacle

$$\psi = ux + \frac{ub^3 x}{2a^3} \tag{21}$$

where b is the radius of the obstacle, a is 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 Figure 5. The difference between $u\grave{i}$, the velocity at infinity, and the true velocity at any point in Ω_{FEM} or Ω_{BEM} decays as $\frac{b^3}{a^3}$ where the biggest difference between these velocities occurs along the x-axis. For the true velocity to be within 2% of $u\grave{i}$, $a \approx 3b$. In other words, for this problem, the finite element mesh must be about 2 obstacle radii thick or must have a radius 3 times that of the obstacle for the solution to be accurate.

The mesh used to model this problem is also illustrated in Figure 2. The boundary conditions for a uniform particle flux were applied on Γ_{in}, and the resulting coupled equations (eqn 20) were used to solve for Φ and $\frac{\partial\Phi_{out}}{\partial n}$. A polar plot of ϕ_i versus θ on the circle $a = 1$ is given in Figure 6 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 Figure 7. 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. Then the domain was divided into sub-domains with almost constant and variable advective fields. The BEM method was applied to the constant advective field sub-domain and the FEM was applied to the variable advective field sub-domain. The two solutions were then coupled and a total advective-diffusion solution was solved for. A resultant particle concentration plot is shown in Figure 8.

5. Conclusion

In this paper, a hybrid finite element - boundary element method (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 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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Appendix A--Figures

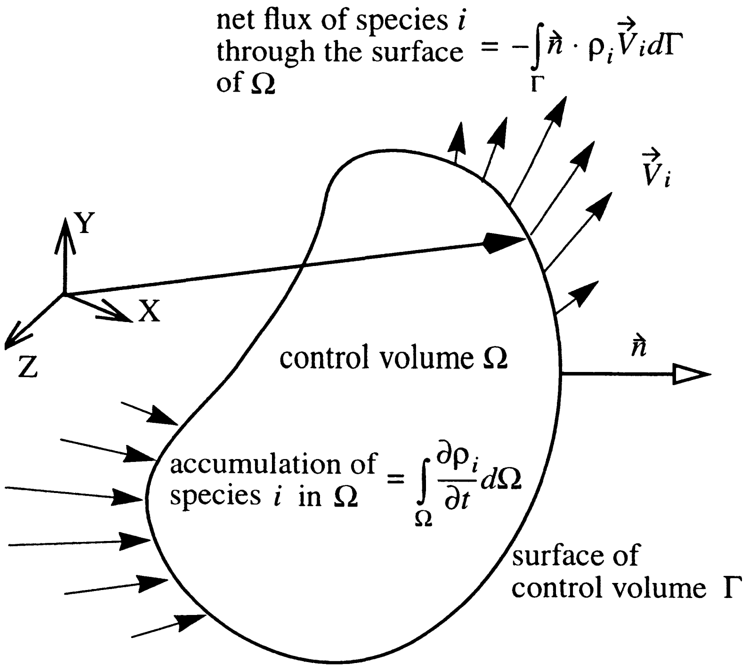

Figure 1. Mass conservation of species i through the control volume

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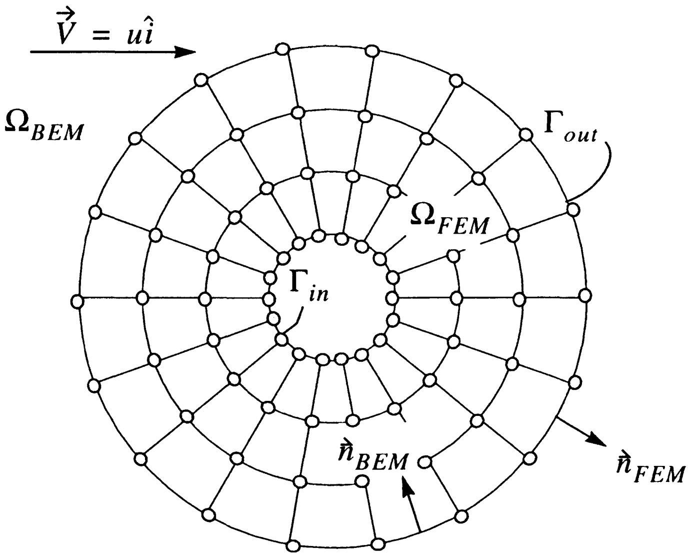

Figure 2. A schematic of a hybrid FEM/BEM domain

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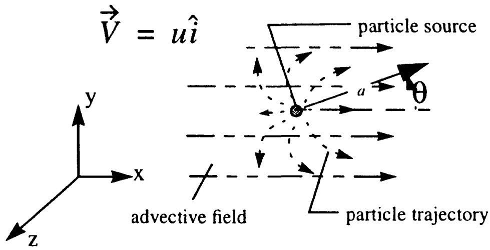

Figure 3. Problem 1 geometry: Particles diffuse from a point source in a domain with a constant advective field

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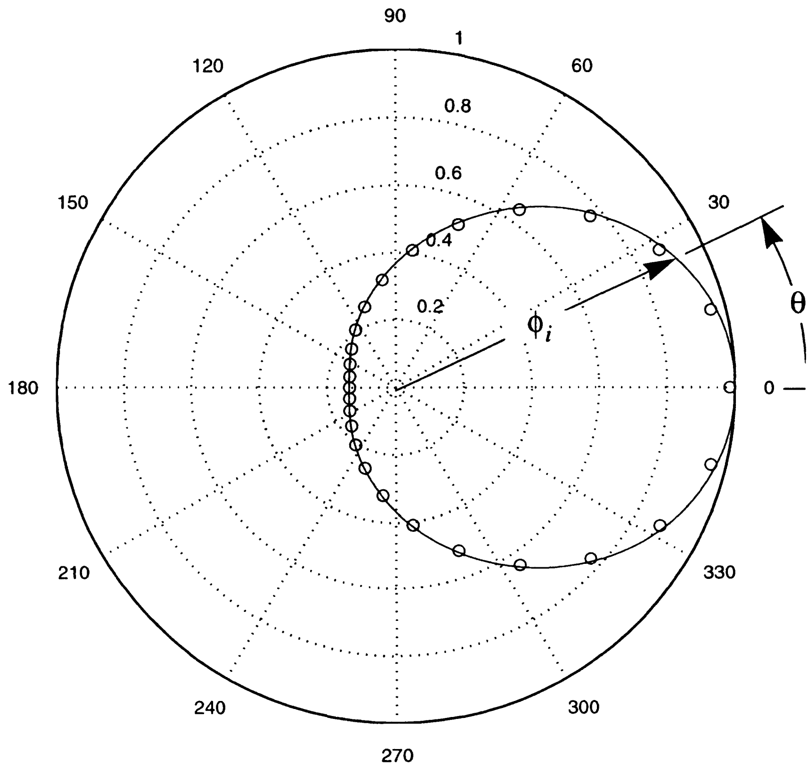

Figure 4. Problem 1 results: A comparison of the FEM/BEM solution to the exact solution, o - FEM/BEM solution, -- exact solution

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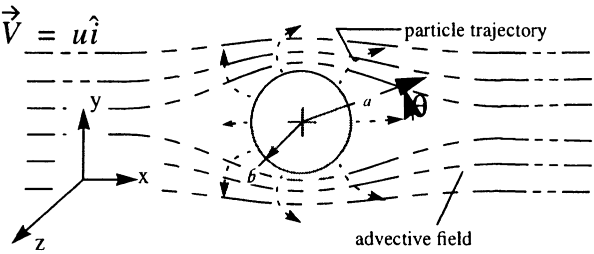

Figure 5. Problem 2 geometry: Particles diffuse from a spherical source in a domain with a non constant advective field

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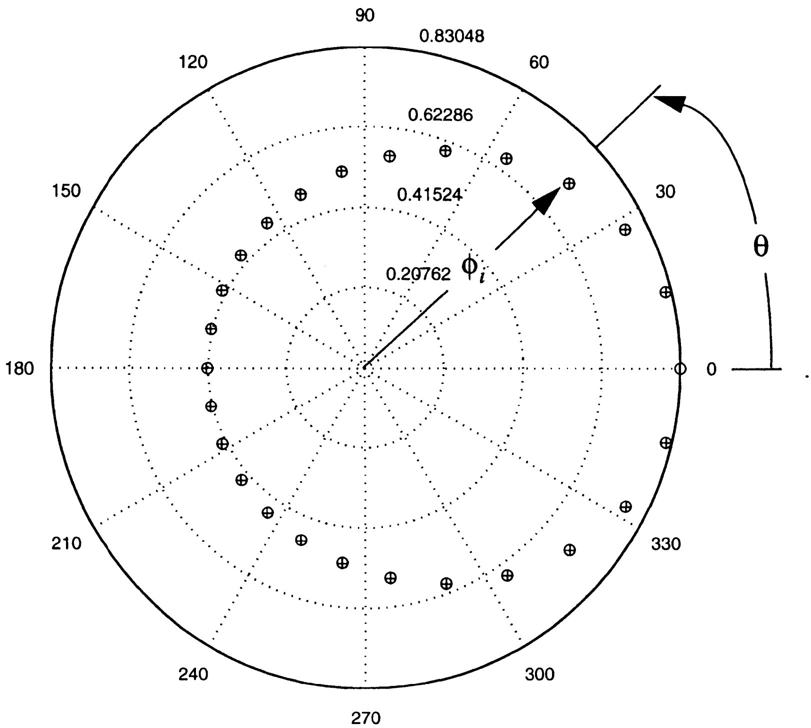

Figure 6. Problem 2 results: A plot of particle concentration at locations in the xy plane for a 2750 and 3250 DOF mesh, o - 2750 DOF mesh, + - 3250 DOF mesh

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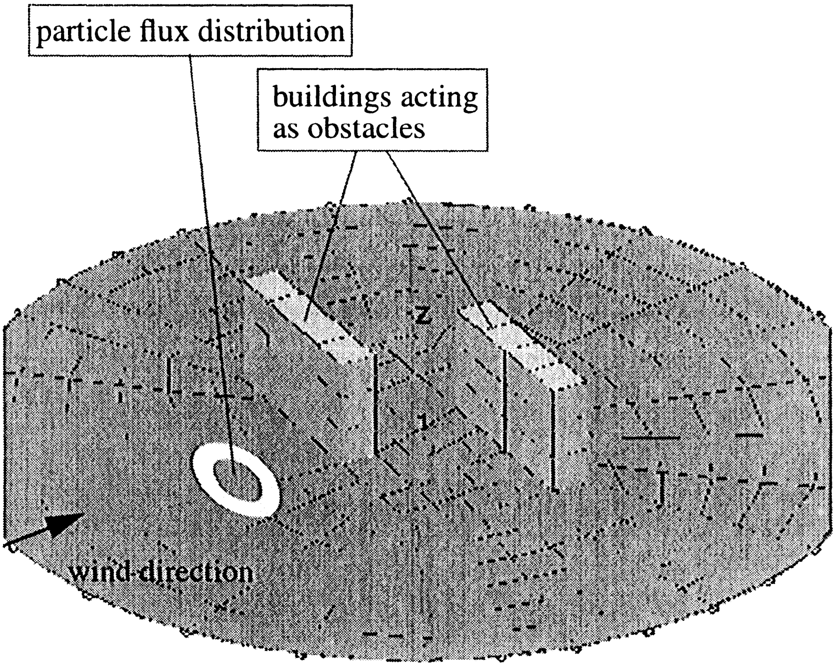

Figure 7. Problem 3 geometry: Two buildings surrounded by an infinite half space

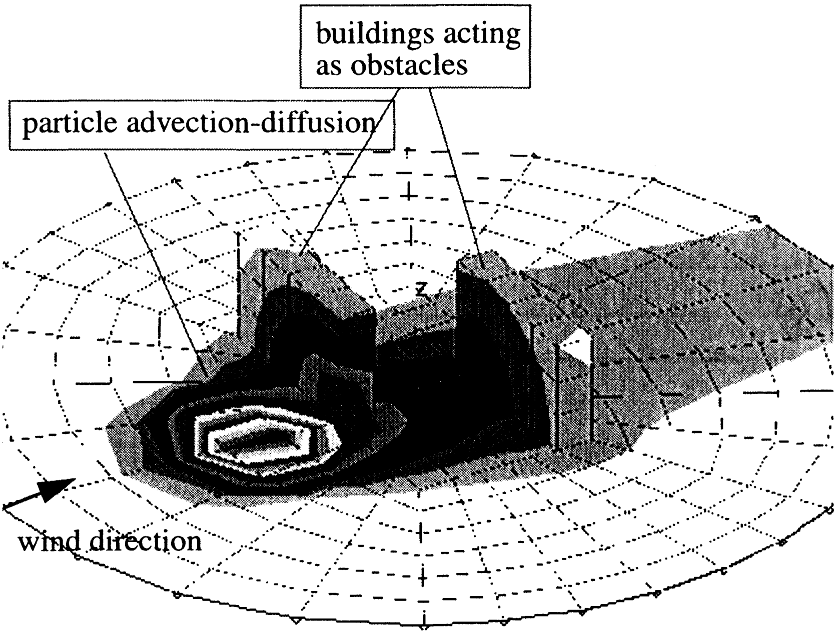

Figure 8. Problem 3 results: Particles diffuse in a variable advective field around buildings.