ABSTRACT

PREMKUMAR MUTHEDATH. A Numerical Model to Predict Worker Exposure from a Hand-Held Source. (Under the Direction of Dr. MICHAEL R. FLYNN)

The dispersion of massless tracer particles released from a point source in the wake of a two-dimensional elliptic cylinder is used to model worker exposure from a hand-held source. A discrete vortex flow model is combined with a particle tracking algorithm to calculate time-averaged concentrations in the plane of the source. By space-averaging these concentrations over a computational breathing zone, estimates of breathing zone concentrations are derived. The model predictions are found to be in good agreement with measured values from wind tunnel studies. Such computational models are powerful tools to study local exhaust ventilation.

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This thesis is dedicated to the memory of my grandparents.

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LIST OF SYMBOLS

C, C, C1, C2	:	Concentration field
\overline{C}	:	Time-averaged concentration in ppm
D	:	Major axis of the elliptic cylinder (ft)
De	:	Width of the mannequin in the experiment (ft)
E	:	Expected value
$f(z, t_a)$:	The equation of the Gaussian curve for lateral dispersion
$f_k(z=0;t_a)$:	Weight of the k th particle
ī, <u>j</u>	:	Unit vectors in the x and y directions, respectively
ke	:	Coefficient of turbulent diffusivity (ft2/min)
ñ	:	Unit outward normal at a solid surface
N	;	Number of particles released per time step by the source
Nij	:	Number of particles in the cell ij
N_{ij}^*	:	Total particle weight in cell ij
0	:	Origin of the coordinate system
Р	:	Dynamic Pressure (ft ² /min ²)
Qs	:	Source flow in the experiment (cfm)
S	:	Ratio of the side of the concentration cell and the major
		axis of the elliptical cylinder
<i>t</i> , <i>t</i> ₁ , <i>t</i> ₂	:	Time (min)
ta	:	Dimensionless age of the concentration particle
T_L	:	Lagrangian time scale or attenuation coefficient
\vec{U}	:	Two-dimensional velocity field (fpm)
$\overrightarrow{U}_{\infty}$:	Free stream velocity in the simulation (fpm)
Ue	:	Magnitude of the free stream velocity in the experiment
		(fpm)

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u,v	:	x,y components of the velocity field (fpm)
x,y,z	:	Cartesian coordinates (ft)
δ	:	Initial lateral dispersion of the concentration particle
η_1, η_2	:	Random numbers from a normal distribution (ft)
v	:	Kinematic viscosity (ft2/min)
σ_c	:	Standard deviation of the normal distribution (ft)
σ_z	:	Standard deviation for lateral dispersion
σ_w	:	Standard deviation of the z-velocity fluctuations
X3d	:	Nondimensional concentration at the center of the
		concentration cell
$\omega, \omega_o, \omega_1, \omega_2$:	Vorticity field (min ⁻¹)
Δt	:	Time step size (min)

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INTRODUCTION

Local exhaust ventilation (LEV) is an attractive engineering control to limit employee exposure below acceptable levels. Currently, LEV systems are designed to provide a target capture velocity (ACGIH, 1992). The method has many drawbacks, the most important being the inability to estimate breathing zone concentration at the design stage for the attained capture velocity (Flynn et al., 1988; George et al., 1990). Thus the level of protection offered by an LEV system can be ascertained only through expensive *in situ* field testing. Clearly, the cost associated with field testing various designs would prove prohibitive for design optimization.

To make progress, the mechanism of contaminant transport by ventilation air and its effect on exposure must be understood. Using this information, predictive models can be built that relate design parameters with quantitative estimates of exposure. Wind tunnel studies using a stationary mannequin (George et al., 1990; Kim and Flynn, 1991a; Lackey, 1993) indicate that boundary layer separation leading to reverse flow is an important mechanism determining worker exposure. For a hand-held source, the recirculating wake can capture the contaminant and transport it to the worker's breathing zone, resulting in significantly elevated exposures.

The governing equations for fluid motion and contaminant transport are well known, however closed-form analytical solutions to them are rare. To model the transport of contaminant in the near wake, computational techniques must be employed. Important issues in numerical modeling are the computational time and memory required. For example, at present, simulation of the three-dimensional flow field around a worker for exposure estimation is not an economical proposition, therefore simplifications are required.

A conceptual model based on mass transport by vortex shedding indicates that reasonable estimates of exposure can be made from a two-dimensional approach (George et al., 1990). Based on this finding, a two-dimensional numerical model was developed to estimate exposure (Flynn and Miller, 1991). Approximating the worker as an elliptic cylinder, the Navier-Stokes equations were solved using the discrete vortex method to obtain the shedding frequency and size of the eddies. Average near-wake concentrations were then computed based on contaminant transport by vortex shedding. The model was extended by including a particle tracking algorithm to predict time-averaged concentrations in the plane of the point source (Chen, 1992).

In this thesis, these ideas are extended to predict time-averaged breathing zone concentrations of a worker in a uniform stream from a hand-held source. Exposure is determined from the space-time average of concentrations in a computational breathing zone. The main feature of the model is the ability to predict the effect of free stream velocity on worker exposure. The results are compared with experimental observations from wind tunnel tracer gas studies employing a mannequin.

THEORY

The problem of estimating concentrations in the near wake of a worker in a uniform stream is studied here using a two-dimensional model (Figure 1). The worker is represented by the elliptic cylinder and a passive point source of contaminant is located downstream. A Cartesian coordinate system is used with the origin at the center of the ellipse. The governing equations are discussed below.

Concentration Field:

The transport of a passive contaminant released in the flow field is governed by the advective-dispersive equation:

$$\frac{\partial C}{\partial t} + \vec{U} \cdot \nabla C = \nabla \cdot [k_e \cdot \nabla C]$$
^[1]

where C = C(x,y; t) is the contaminant concentration at spatial location x, y at time t, k_e is the turbulent diffusion coefficient and $\vec{U} = \vec{U}(x, y; t)$ is the two-dimensional velocity field.

Velocity Field:

The air velocity field $\hat{U}(x, y; t)$ is governed by the incompressible continuity equation:

$$\nabla \cdot \vec{U} = 0$$
 [2]

and the Navier-Stokes equations:

$$\frac{\partial \vec{U}}{\partial t} + \vec{U} \cdot \nabla \vec{U} = v \nabla^2 \vec{U} - \nabla P$$
[3]

where ν is the kinematic viscosity and P is the dynamic pressure. In vorticity-transport form, equation [3] is:

$$\frac{\partial \omega}{\partial t} + \hat{U} \cdot \nabla \omega = \nu \nabla^2 \omega$$
[4]

where $\omega = \omega(x, y; t)$ is the vorticity field given by

$$\omega = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} - \frac{\partial \mathbf{u}}{\partial \mathbf{y}}$$
[5]

where u and v are the velocity components in the x and y directions, respectively.

To have unique solutions, boundary and initial conditions must be specified. On solid boundaries, we must have

$$\vec{U} = (\nabla C) \cdot \vec{n} = 0$$
 [6]

where \vec{n} is the outward unit normal, and at infinity

$$\vec{U} = \vec{U}_{\infty}; C = 0$$
 [7]

where $\overrightarrow{U}_{\infty}$ is the free stream velocity. Initial conditions required are

$$\vec{U}(x, y; t = 0) = \vec{U}_{\infty}; C(t = t_o) = 0$$
[8]

where to is the instant the source is turned on.

In these equations, the operator ∇ is defined as

$$\nabla = \frac{\partial(\mathbf{x})}{\partial \mathbf{x}}\vec{i} + \frac{\partial(\mathbf{x})}{\partial \mathbf{y}}\vec{j}$$
[9]

where \vec{i} and \vec{j} are unit vectors in the x and y directions, respectively.

NUMERICAL METHODS

The discrete vortex method (DVM) is used to obtain the velocity field. In this technique, operator splitting (Bui and Oppenheim, 1987; Marchuk, 1990) is used to write equation [4] as

$$\frac{\partial \omega_1}{\partial t} = v \nabla^2 \omega_1 \tag{10}$$

and

$$\frac{\partial \omega_2}{\partial t} + \vec{U} \cdot \nabla \omega_2 = 0$$
[11]

In any given time interval $t_1 \le t \le t_2$, we first solve equation [10] with the initial condition

$$\omega_1 (t_1) = \omega_0$$
[12]

and then equation [11] with the initial condition

$$\omega_2(t_1) = \omega_1(t_2)$$
 [13]

Equations [10] - [13] are solved using a Lagrangian approach, i.e., the vorticity field $\omega(x,y;t)$ is approximated by a finite collection of vortex blobs and sheets. The time evolution of the flow is dictated by the motion of these vortex elements. The velocity field is determined by the sum of the potential and rotational components (Batchelor, 1967). Details of the method are described elsewhere (Chorin, 1973, 1978; Tiemroth, 1986; Sethian et al., 1990). In this work, the algorithm developed by Flynn and Miller (1991) is used with slight modifications - the boundary integral equation method is used to compute

the potential flow and a multipole expansion algorithm (Greengard and Rokhlin, 1987) is used to calculate the rotational component. The latter is used to speed up the computations.

A similar technique is used for the solution of equation [1] for the concentration field. The method is reviewed here briefly, details are given elsewhere (Chen, 1992). Under the assumption of constant diffusivity k_e , operator splitting of equation [1] in a given time interval $t_1 \le t \le t_2$ results in

$$\frac{\partial C_1}{\partial t} = k_e \nabla^2 C_1 \tag{14}$$

with the initial condition

 $C_1(t_y) = C_o$ [15]

and

$$\frac{\partial C_2}{\partial t} + \vec{U} \cdot \nabla C_2 = 0 \qquad [16]$$

with the initial condition

$$C_2(t_1) = C_1(t_2)$$
 [17]

The solutions of equations [14] - [17] are approximated by a finite collection of massless concentration particles whose x, y locations at time step n+1 are given by

$$x_{n+1} = x_n + \Delta t u_n + \eta_1$$
 [18]

and

,

$$y_{n+1} = y_n + \Delta t v_n + \eta_2$$
 [19]

where Δt is the time step size, u is the x-velocity component and v is the y-velocity component at particle location x_n , y_n . Here, η_1 and η_2 are random variables drawn from a Gaussian distribution of zero mean, and variance, σ_e^2 , equal to $2k_e\Delta t$. If we assume 10% free stream turbulence intensity, k_e can be calculated using the equation (Chen, 1992)

$$k_e = 0.00112 U_{\infty}$$
 [20]

where U_{∞} is the magnitude of the free stream velocity in feet per minute (fpm) and k_e has units of ft²/ minute.

Concentration particles are generated by the point source at the rate of N per time step. To account for three-dimensional effects associated with the point source, each concentration particle is modeled as a puff described by a Gaussian curve centered in the x-y plane and extending in the z direction (Turfus, 1988). The equation of this curve is

$$f(z; t_a) = \sqrt{\frac{1}{\left(2\pi \sigma_z^2(t_a)\right)}} \exp\left(-\frac{z^2}{2\sigma_z^2(t_a)}\right)$$
[21]

where $\sigma_{Z}^{2}(t_{a})$, the variance of the distribution in the z direction at a dimensionless particle age t_{a} , given by

$$\sigma_Z^2(t_a) = \delta^2 + 2\sigma_W^2 T_L^2 \left(1 - \exp\left(\frac{-t_a}{T_L}\right) + \frac{t_a}{T_L} \right)$$
[22]

In equation [22], δ^2 is the variance at $t_a = 0$, σ^2_w is the z-velocity variance, and T_L is the Lagrangian integral time scale based on the streamwise velocity correlation. The contribution of each puff to the x-y plane, known as the particle weight, is obtained by letting z = 0 in equation [21].

Concentration calculations are initiated after the initial transient phase. According to Turfus (1988), a sufficient indication of stationarity is the constancy between time steps, of the expected value of the sum $\Sigma f(z = 0; t_a)$, in the region of interest. Under such conditions, the computational domain is divided into square cells of side S(D) where D is the length of the major axis of the ellipse and S is a fraction. A count is then made of the number of particles in each cell. If N_{ij}^* is the mean aggregate particle weight in cell ij, the nondimensional mean concentration χ_{3d} at the cell center can be approximated as (Turfus, 1988)

$$\chi_{3d} \cong \frac{N_{ij}^* U_{\infty} \Delta t}{S^2 DN}$$
[23]

where

$$N_{ij}^{*} = E\left\{\sum_{k=1}^{N_{ij}} f_{k}(z=0; t_{a})\right\}$$
[24]

In equation [24], E represents the expected value and N_{ij} is the number of concentration particles in cell *ij*.

In the numerical simulations, for each cell, the sum $\sum_{k=1}^{N_{ij}} f_k(z=0; t_a)$ is computed at individual time steps and averaged over time to estimate N_{ij}^* . This value is used in equation [23] to obtain the time-averaged nondimensional mean concentration at the cell-center locations. To compare with measured values, the dimensional time-averaged mean concentration \overline{C} , in ppm, at cell locations is calculated using the result

$$\overline{C} = \left(\frac{\chi_{3d}Q_s}{U_e D_e^2}\right) \times 10^6$$
[25]

where U_e is the magnitude of the free stream velocity, D_e is the mannequin width, and Q_s is the source flow used in the experiment. Following Chen (1992), we choose N=10, $\delta^2 = 0.0001$, $\sigma_w = 0.10$, and S = 0.25.

The numerical method outlined here is strictly for the prediction of time-averaged concentrations in the plane of the point source. However, if worker exposure is governed primarily by two-dimensional flow patterns in the near wake, these methods can be employed, after adequate adjustment for lateral dispersion, to predict exposure. The amount of lateral dispersion required is determined by choosing a value of T_L that results in agreement with one measured value.

RESULTS

A worker's exposure in a uniform air stream from a hand-held source is simulated using the configuration shown in Figure 1. The worker is modeled by the elliptic cylinder, 2.0 ft wide and 1.0 ft deep. This configuration represents the plan view of the horizontal plane approximately at the level of the worker's chest. The free stream velocity is parallel to the positive y direction and a point source of contaminant generating massless concentration particles is located at x = 0 ft, y = 1.0 ft. To ensure uniform flow conditions upstream and at distances far from the ellipse, a domain of 200 ft x 200 ft is chosen to simulate the flow field. This is termed the flow domain here. Concentration particles are tracked in the region -7.50 ft $\le x \le 7.50$ ft, $-0.25 \le y \le 18.0$ ft. This is termed the concentration domain. These domains are shown in Figure 1. The time-averaged concentration field is determined in the region -2.25 ft $\le x \le 2.25$ ft, -0.25 ft $\le y \le 2.75$ ft. Known as the sub-domain, it consists of square cells of side 0.50 ft; see Figure 2.

Simulations are performed at free stream velocities of 33.33 fpm, 50 fpm, and 83.33 fpm. These velocities, source location, and the dimensions of the concentration region are chosen to maintain dynamic and geometric similarity with the experimental conditions of Kim and Flynn (1991b). The boundaries EH and FG of the concentration domain shown in Figure 1 represent the walls of the wind tunnel in the experiment. Particles crossing these boundaries are reflected back into the concentration domain. Particles crossing the boundary HG (located at y = 18.0 ft) are removed from calculations as they have negligible effect on the predicted breathing zone concentrations.

In reality, the time-weighted average breathing zone concentration is a space-time average of the concentration field in the worker's vicinity. This feature is taken into account here by defining a computational breathing zone. It is a region in the wake of the cylinder in which a concentration particle has a reasonable chance of reaching the body surface. An estimate of the dimensions of this zone is made from the size of the eddies seen in the simulation. A typical shed eddy is shown in Figure 3. It is approximately 2.0 ft long in the direction of the flow. Since eddies are shed from both ends of the cylinder, the numerical breathing zone is defined as the region -1.25 ft $\le x \le 1.25$ ft, -0.25 ft $\le y \le 2.75$ ft. These dimensions are in reasonable agreement with those reported in the literature (Bloor, 1964; Kim and Flynn, 1991a). The region is shown in Figure 1. In the numerical simulations, the time-averaged concentrations at the cell centers are spatially averaged over the computational breathing zone to estimate worker exposure.

The value of T_L is determined by trial and error. For a free stream velocity of 50 fpm (150 fpm in the experiment), a T_L value of 10 resulted in a breathing zone concentration of 13.2 ppm. This is within one standard deviation of the measured average of Kim and Flynn (1991b); see Table 1. The utility of this model in predicting the effect of free stream velocity on breathing zone concentrations was tested next. Predicted breathing zone concentrations for experimental free stream velocities of 100 fpm and 250 fpm are provided in Table 1. Good agreement with experimental results (Kim and Flynn, 1991b) is noted.

The values of the key parameters for the DVM calculations are given in Table 2. They were obtained from numerical experiments with guide lines from the literature (Sethian and Ghoniem, 1988; Sethian et al., 1990; Chorin, 1980; Flynn and Miller, 1991) as starting points, to provide reasonable Strouhal numbers for the range of Reynold's numbers examined. Numerical probes positioned at x = 1.0 ft, y = 4.0 ft and x = -1.0 ft, y = 4.0 ft recorded the fluctuations of the y-velocity component. A typical trace is shown in Figure 4. For a given free stream velocity, the average time interval between consecutive peaks was used to compute the Strouhal number. These are provided in Table 2. They compare very well with published results (Roshko, 1954; Kim and Flynn, 1991a). A convergence study of the solution with refinement of these parameters would require substantial computer resources and is beyond the scope of this work.

A typical time-averaged velocity profile is shown in Figure 5. Such profiles are used to evaluate the accuracy of the DVM solution for high Reynold's number flows (Sethian and Ghoniem, 1988). Although the profile is symmetric about the minor axis of the ellipse, it does not contain the expected pair of standing eddies downstream.

In all simulations, particle generation is started 15 time steps after the start of the simulation. This ensured that sufficient number of vortex elements (approximately 800) are present to affect contaminant transport. Concentration averaging is initiated after 200 steps or 185 steps after turning on the source. Plots of the total particle weight in the

concentration domain and the sub-domain -2.25 ft $\le x \le 2.25$ ft, -0.25 ft $\le y \le 2.75$ ft are shown in Figure 6. They indicate that stationarity is attained within 200 time steps in the computational breathing zone and within 300 time steps in the concentration domain. Concentrations were averaged over 600 time steps to obtain time-weighted means over 6 - 8 vortex shedding events. The simulations were carried out for a total of 800 time steps and took about 5 - 6 hours of CPU time on a Convex C240 mid-range supercomputer.

DISCUSSION

The ability of the model to predict changes in breathing zone concentrations with free stream velocity indicate that exposure is primarily determined by two-dimensional vortex shedding. As the Strouhal number is a constant in the Reynold's number regime considered here, increased free stream velocity results in more rapid shedding of vortices. The residence time of the contaminant in the numerical breathing zone is therefore, lower for higher velocities, leading to lower exposure.

The Lagrangian time scale T_L is used to account for lateral dispersion due to a point source (Turfus, 1988). However, in this work, T_L is used to attenuate the concentrations in the plane of the point source to obtain breathing zone concentrations. Therefore, it is not a Lagrangian time scale, but rather an attenuation coefficient that relates the average concentration in the computational breathing zone to worker exposure. The value of T_L is dependent on the size of the computational breathing zone - the larger this region, the smaller the value of T_L and vice versa. However, smaller averaging zones have shorter transient periods (Figure 6) and therefore, require reduced simulation times.

To accurately portray contaminant transport by vortex shedding, eddy size, shedding frequency, and eddy shape must be correctly determined. In the simulations performed, the eddies are seen to occupy the entire length of the ellipse before being shed; see Figure 3. This is in contrast to the expected shape in which an eddy occupies only one-half of the length of the cylinder and is considerably more elongated in the direction of the flow. This problem results in the absence of the two recirculating bubbles in the time-averaged profile shown in Figure 5.

These problems may be due to numerical errors associated with poor resolution and the approximate elliptic coordinate transformations used in the sheet convection calculations. Sethian and Ghoniem (1988) report a strong dependence of the size and shape of the shed eddies on flow resolution. Despite these problems, the model is able to capture the effect of free stream velocity on exposure quite well. This indicates that as long as the eddies are shed at the right frequency and are large enough to capture the contaminant, eddy shape will not be a critical factor. However, in cases where the source location is far enough to escape capture by the flattened eddies, predictions would underestimate exposure.

The major limitation of this technique is the assumption of two-dimensionality. In industrial environments, worker activity, presence of objects, contaminant generation with momentum, and turbulence can introduce substantial three-dimensional effects that cannot be captured here. Nevertheless, the model can be used to study the effects of worker position relative to air flow, source position and generation rate, and cross drafts on worker exposure. In this regard, it is an advancement in the study of local exhaust ventilation.

CONCLUSIONS

The widespread use of local exhaust ventilation to protect the worker requires that its protective efficiency be gauged accurately. At present, such assessment is made through field testing - a reliable but expensive option. To develop reliable and cost-effective ventilation systems where a known level of worker protection is assured, alternate strategies are required.

The effectiveness of a local exhaust hood in reducing worker exposure depends critically, among other things, on the flow patterns in conditions of actual use. The nonlinearity of the governing equations of fluid flow indicate that substantial changes in flow patterns can result from relatively minor changes in boundary conditions. Therefore, reliance on empirical models to assess exposure and design LEV systems is not a desirable proposition.

Computational models like the one used in this study can account for a variety of factors including changes in boundary conditions. Moreover, they are based on fundamental principles of conservation of mass and momentum. At present, the major obstacle in using these techniques is the enormous computer resource required to model real-life scenarios. Improvements in computer power and numerical algorithms will make these problems more tractable in the future. In the interim, two-dimensional models like the one used here can be used to identify important design variables that affect exposure.

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Free Stream Velocity (fpm) in the Experiment	Measured Average Breathing Zone Concentration (ppm)	Predicted Average Breathing Zone Concentration (ppm)	
100	19.5 (17.0, 22.0)**	17.19	
150	12.0 (9.78, 14.22)	13.21	
250	7.20 (8.31, 6.08)	9.04	

Table 1: Comparison of Predicted and Experimental Breathing Zone Concentrations

- * : From Kim and Flynn (1991b)
- **: Denotes one standard deviation

Table 2: Paramet	er Values	Used in	the DVM	Simulations
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Free Stream Velocity (fpm)	Time step size (minutes)	Numerical boundary layer thickness (ft)	Maximum sheet strength as fraction of the free stream velocity	Average Strouhal Number
33.33	0.0025	0.00600	0.10	0.19
50.0	0.002	0.00489	0.50	0.21
83.33	0.0015	0.00379	0.50	0.20





Figure 1: Computational Domain for the Simulation of Worker Exposure



PQRS: Sub-domain

- Contaminant Source
- · : Cell Center



y location (ft)

x location (ft)

Figure 3: Velocity Field Around the Elliptic Cylinder at 1.25 min. (Free stream velocity = 33.33 fpm)

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Figure 4: Time Variation of y-Velocity Component at x = 1.0 ft, y = 4.0 ft. (Free stream velocity = 83.33 fpm, time step size = 0.0015 min.)



x location (ft)

Figure 5: Time-Averaged Velocity Profile Around the Elliptic Cylinder (Free stream velocity = 33.33 fpm, time step size = 0.0025 min, averaging period = 800 time steps)

y location (ft)



Figure 6: Variation of Total Particle Weight with Time (Free stream velocity = 50 fpm, time step size = 0.002 min.)