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A Three Dimensional Finite Element Model for Emergency Response

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A three-dimensional finite element model (FEM) is used with a Lagrangian particle transport (LPT) technique to simulate contaminant transport for emergency response. A three dimensional computational mesh is first generated using USGS Digital Elevation Map (DEM) data. An initial wind velocity is then calculated from the meteorological data using objective analysis technology. The 3-D finite element model is used to construct the massconsistent wind field over irregular terrain. The LPT employs a stochastic/random walk approach to generate the contaminant transport traces. The model runs on PCs and is well suited for use in dealing with emergency response dispersion predictions and assessment. Simulation results utilizing Las Vegas fire stations are presented.

Nomenclature

D Deterministic forcing function n_r Normally distributed random number = t.t Time = U= Mean velocity u, v, wVelocity in x, y, z direction = $u_0, v_0, w_0 =$ Fixed observed velocity value in x, y, z direction = Initial location for particle x_0 Particle location at time t X_t = λ Lagrange multiplier = α_i Gauss precision moduli σ Standard deviation for maximum featured gradients = Ω Physical domain (volume)

Introduction I.

ir pollution is a serious environmental issue that causes serious threats to the health of the public [1, 2]. Serious Aurban smog incidents due to disperse emission sources occurred in London, UK in 1873 (268 deaths); Meuse Valley, Belgium in 1930 (60 deaths); Manchester, UK in 1931 (592 deaths); Donora, Pa USA in 1948 (20 deaths 14,000 ill) and London, UK in 1952 and 1956 (more than 4000 and 1000 deaths, respectively).

Specific substance releases also impacted and endangered populations. In 1945 spills of liquid natural gas (LNG) stored at the Cleveland Illuminating Company, USA, killed 44 people and caused \$12 M damage (largest US industrial accident when adjusted for inflation). The 1979 nuclear incident at the Three Mile Island reactor,

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Harrisburg, Pa, forced the public to reconsider the implications of unexpected accidents. In 1984 the disastrous petrochemical releases in Bohpal, India, killed thousands. The 1986 release of radioactivity during the Chernobyl reactor accident exposed millions to significant radio nuclides.

The ability to accurately and quickly construct wind fields and predict contaminant transport is needed to effectively assess health effects, mitigation, and regulation of emissions and effective siting of instruments.

In this study, a mass-consistent 3-D finite element model is coupled with a random walk technique that can provide near real time contaminant transport simulation.

II. Mass Consistent Finite Element Model

The theoretical basis for the diagnostic mass consistent FEM model is based on the work of Sherman, et al. [3] and Pepper [4]. The main procedure for construction of this model is described as follows:

- A surface wind field is constructed from measured data using inverse squared weighting. A fixed radius is specified and value interpolated from measured tower data to all grid points in the first level above the terrain. Wind data is averaged every 15 minutes.
- 2) The upper level wind fields at all remaining grid points are constructed using inverse weighting from the surface generated values.
- 3) Vertical velocities are calculated at all grid points from the equation of continuity.

$$w = -\int_{0}^{z} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y}\right) dz \tag{1}$$

4) A global check of divergence is determined

$$\mathcal{E} = \int_{\Omega} \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) d\Omega$$
(2)

5) An integral function that minimizes the variance of the difference between the observed and analyzed variables is evaluated. The specific function is:

$$E(u, v, w, \lambda) = \int_{\Omega} \left[\alpha_1^2 (u - u_0)^2 + \alpha_1^2 (v - v_0)^2 + \alpha_2^2 (w - w_0)^2 + \lambda \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} \right) \right] d\Omega$$
(3)

Euler-Lagrange equations for velocity readjustment are solved:

$$u = u_0 + \frac{1}{2\alpha_1^2} \frac{\partial \lambda}{\partial x} \tag{4}$$

$$v = v_0 + \frac{1}{2\alpha_1^2} \frac{\partial \lambda}{\partial y}$$
(5)

$$w = w_0 + \frac{1}{2\alpha_2^2} \frac{\partial \lambda}{\partial z}$$
(6)

Substituting into the continuity equation, the resulting Poisson equation is then solved for the multiplier , λ .

$$\frac{\partial^2 \lambda}{\partial x^2} + \frac{\partial^2 \lambda}{\partial y^2} + \left(\frac{\alpha_1}{\alpha_2}\right)^2 \frac{\partial^2 \lambda}{\partial z^2} = -2\alpha_1^2 \left(\frac{\partial u_0}{\partial x} + \frac{\partial v_0}{\partial y} + \frac{\partial w_0}{\partial z}\right)$$
(7)

6) Applying the Galerkin Weighted Residual technique, equation (7) becomes:

$$[K]\{\lambda\} = \{f\}$$
(8)

where

$$K = \int_{\Omega} \left[\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\alpha_1^2}{\alpha_2^2} \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right] d\Omega,$$

and

$$f = 2\alpha_1^2 \int_{\Omega} N_i \left(\frac{\partial u_0}{\partial x} + \frac{\partial v_0}{\partial y} + \frac{\partial w_0}{\partial z} \right) d\Omega$$

- 7) Once λ is calculated, the velocity components are adjusted.
- 8) Return to step 4 until convergence, $\varepsilon \le 10^{-4}$.

III. Lagrangian Particle Transport Technique

Advection and convection are two components in fluid transport processes. Advection transport is due to the mean fluid velocity while diffusion is due to the random (turbulent) fluctuations of the fluid properties. In stochastic approaches to fluid turbulence, the dispersive processes are expressed in terms of certain probabilistic descriptions.

For Lagrangian methods, a large number of moving particles are used to approximate advection and dispersion instead of solving PDEs directly. This technique provides accurate predictions to advection-dominated species transport problems. One of the models that describe such processes is the Random Walk Advective and Dispersive Model (RADM), developed by Runchal [5].

In this study, a stochastic/random walk model is used to predict contaminant transport [6]. The idea for RADM is to solve the transport problem using a large number of particles, each of which is moved according to the equation:

$$x_{t} - x_{0} = \int_{t_{0}}^{t} U(x_{t}, t') dt' + \int_{t_{0}}^{t} D(x_{t}, t') dw_{t'}$$
(9)

where x_0 is the initial condition and U is a mean velocity vector defined over a suitable time interval; D is a deterministic forcing function for the random component of motion.

Equation (9) can be further simplified as:

$$\delta x(w,t) = \delta x_U + \delta x_D \tag{10}$$

and the stochastic integral may be written as:

$$\delta x_D(w,t) = \int_{t_0}^t n_r \sqrt{2k} dt'$$
⁽¹¹⁾

3 American Institute of Aeronautics and Astronautics where $D^2/2$ has been assumed to be equivalent to K and n_r is a normally distributed random number with a mean value of zero and a standard deviation of unity.

Equation (11) can be further simplified to:

$$\delta x_D = n_r \sigma \tag{12}$$

$$\sigma^2 = \int_{t_0}^{t} 2Kdt' \tag{13}$$

Finally the displacement equation (9) can be expressed as:

$$x_{t} - x_{0} = \int_{t_{0}}^{t} U(x_{t'}, t') dt' + n_{r} \left(\int_{t_{0}}^{t} 2K(x_{t'}, t') dt' \right)^{1/2}$$
(14)

For a rigorous application of the random walk method, the net particle displacement must be calculated by integration of equation (14). However, U and K are arbitrary functions of space and time, and it is not always possible to obtain a closed form solution to this equation. For suitably small time steps, it often proves adequate to assume that the mean velocity and the random components can be separately calculated and linearly superimposed.

In the application of RADM, U is calculated using the finite element model at the nodes of the computational domain. The random component of motion due to dispersion is calculated from a general probability distribution or correlation function.

The calculation to advance the particle in time proceeds in steps as described as follows:

$$x_i(t + \Delta t) = x_i(t) + U_i \Delta t \tag{15}$$

The velocity components are the fictitious total velocities determined for the beginning of the time interval and initial particle positions. Every particle is advanced each time step using equation (15). Thus the particle traces out in time a trajectory for the pollutant material.

IV. Model Application

We apply the mass consistent diagnostic FEM model coupled with the RADM LPT technique to simulate contaminant transport traces. Meteorological towers at fire stations provide wind data that is used to initialize the diagnostic model.

A. Mesh Generation

The map shown in Fig. 1 displays the locations of the Las Vegas Fire Stations, as denoted by the red dots.

A three-dimensional, terrain-following mesh is constructed from DEM data. The mesh consists of 6 layers: surface layer; 50-meter layer; 100-meter layer; 300-meter layer; 500-meter layer; and 1500-meter layer respectively. The 3D computational mesh is shown in Figure 2.

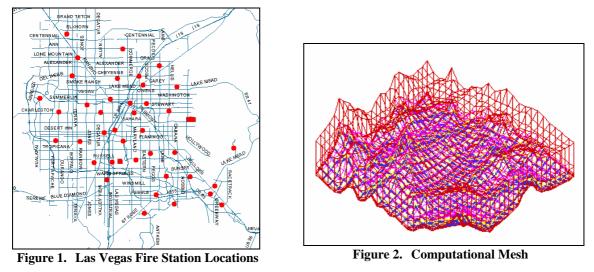


Figure 3 shows the location of 15 fictitious meteorological towers at 15 fire station locations. A plan view of the meteorological tower locations is shown in Figure 4; Figure 5 shows the topography contours.

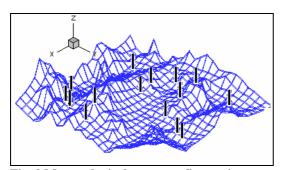


Fig. 3 Meteorological towers at fire stations

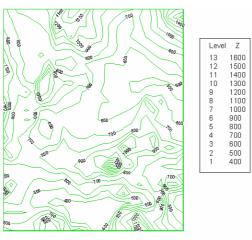


Figure 5. Topographic contours

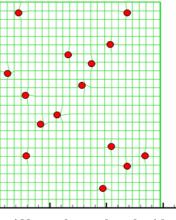


Fig. 4 Non-orthogonal mesh with towers as grid points

B. Velocity Calculation

Figure 6 shows hypothetical tower wind velocity vectors at each of the fire station locations.

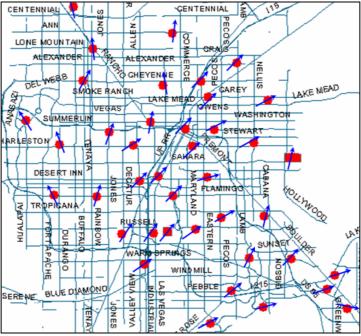


Figure 6. Fictitious wind velocity at fire station

Velocity vectors for the 50m level are shown in Figure 7., following the diagnostic calculation. In Figure 8, a vertical slice is displayed to show the wind velocities at each layer.

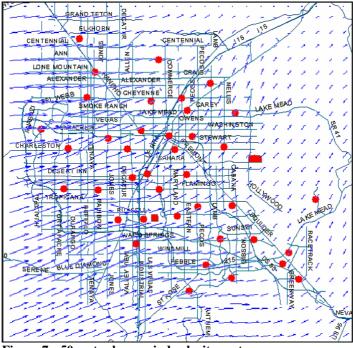


Figure 7. 50 meter layer wind velocity vector

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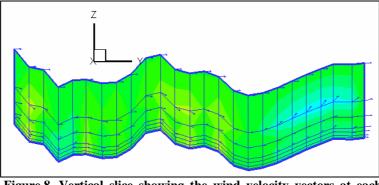


Figure 8. Vertical slice showing the wind velocity vectors at each layer

C. LPT Contaminant Transport Trace

Figure 9 shows the wind velocity vector at the 50 meter height layer in 3D perspective.

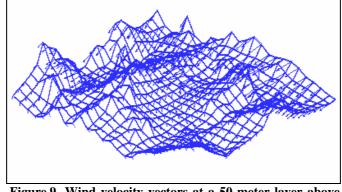


Figure 9. Wind velocity vectors at a 50 meter layer above the surface

Figure 10 shows the particle transport within the Las Vegas valley from a predetermined location. (The red dot denotes the location for the contaminant source)

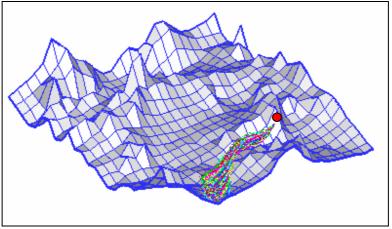


Figure 10. Particle transport trace

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V. Conclusion and future work

In this study, 3D atmospheric meshes have been generated that incorporate complex terrain associated with the Las Vegas Valley. A 3D diagnostic mass-consistent wind field is constructed using a finite element approach. A Lagrangian transport model is coupled with the diagnostic technique to simulate contaminant transport trace within the Las Vegas valley – and provide a near real-time emergency response capability.

Future efforts are being developed that will link the fire stations in a city-wide network to enable communications and data exchange. Application of hp adaptation, permitting more locally refined accuracy in regions of rapidly changing terrain, is being undertaken.

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