Development of Short Range Hazard prediction model for toxic air pollutants

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Introduction

Computer simulations of passive gas dispersion can be used to predict the dispersal of a toxic air pollutant in to the atmosphere. These predictions play a significant role in the disaster management and in rescue activities. Most of the chemical warfare agents are considered as dense gasses or liquids due to their physical properties and storage conditions. However, the dispersal of released gas or vapor clouds is often modeled by passive gas simulations (Kingdon, 2007). Such a model is capable of graphically representing the dispersion which allows calculating the concentration of the toxic gas in any location at a given time. Moreover, it can predict the number of human lives at stake.

The dispersal of a passive gas in the atmosphere mainly depends on the type of release, meteorological conditions, geographical parameters and chemical and physical processes. In considering the toxicity of an air pollutant in the atmosphere, it is important to focus on chemical reactions. Particularly, it is straightforward to introduce first order chemical reactions into dispersion models as a reduction or an increment of the effective mass of the toxic pollutant.

$$A \xrightarrow{k} Product$$

For a first order reaction, if A is the toxic pollutant of interest, the concentration at a given time can be calculated as,

$$[A]_t = [A]_{t_0} e^{-kt} \qquad (1)$$

Although, many advanced passive gas dispersion models have been developed, most of them do not account for chemical processes and are very costly. Moreover, certain models that are used by the military sector are not even commercially available. Therefore, our proposed computer simulation software to predict dispersion of a passive toxic gas release fulfills a mandatory requirement in the field of disaster management.

In this project, a computer model for the short range dispersion of toxic gas/vapor clouds resulting from an instantaneous release is developed and evaluated. This includes a diagnostic meteorological preprocessor and a Lagrangian puff/particle dispersion model based on Langevin equation (Andronopoulos, 2009). The program is capable of predicting the dispersal in the planetary boundary layer, calculating concentrations of the toxic pollutant in hazard areas considering first order chemical reactions and graphically representing them on a satellite map.

Computational Procedures

A 3D computational grid system with a constant domain height was chosen in this study. In the horizontal direction, the grid is uniform with adjustable number of cells and dimensions. The vertical coordinate system is terrain following and non-uniform, which

squeezes or expands between the varying topography and constant domain top. Terrain heights at each grid point were calculated by processing Digital Elevation Maps in ArcGis (ESRI, 2009) and were stored in a SQL Server data base. Appropriate mathematical models to calculate meteorological parameters from user input and methods to interpolate them at each grid point were selected from literature and the necessary programs were written using Visual C# 2010. These meteorological parameters include wind vectors, temperature, pressure, humidity and some other micrometeorological parameters. Interpolated wind field should take topographic features into account and obey the principle of conservation of mass. Therefore, a divergence minimization algorithm was developed to perform minimum possible correction to interpolated wind field considering terrain slopes. Complete mathematical derivation will be presented elsewhere (Kumara, 2012).

To simulate the dispersion of air pollutants, the center of a pollutant cloud was treated as a particle where the concentration is distributed in a Gaussian manner in lateral, horizontal and vertical directions. The trajectory of the particle was calculated according to the following equation (Andronopoulos, 2009):

$$x_i^{n+1} = x_i^n + (\acute{u}_i + u_i')\Delta t \tag{2}$$

in which Δt is the time step, n is the time step index, i is the direction index, $\acute{u}_i$ is the mean wind velocity in direction i, and u_i' represents turbulent velocity fluctuations. $\acute{u}_i$ was obtained from mass consistent wind field and u_i' was estimated from one dimensional Langevin equation assuming that the velocity and particle position evolve as a Markov process and there exists a mutual independence between three velocity components. The instantaneous concentration of the air pollutant at a point (x, y, z) was calculated using following equation.

$$c(x,y,z) = \frac{Q}{(2\pi)^{\frac{3}{2}}\sigma_x\sigma_y\sigma_z} e^{\left(-0.5\frac{(x_c-x)^2}{\sigma_x^2}\right)} e^{\left(-0.5\frac{(y_c-y)^2}{\sigma_y^2}\right)} \left(e^{\left(-0.5\frac{(z_c-z)^2}{\sigma_z^2}\right)} + e^{\left(-0.5\frac{(z_c+z-2z_g)^2}{\sigma_z^2}\right)} \right) \tag{3}$$

Where, x_c, y_c, z_c are the coordinates of the center of the cloud, $Q$is the mass of pollutant released, z_g is the ground height. σ_i $(i = x, y, z)$ is the standard deviation of the concentration distribution and was calculated by numerical integration.

Equations (1), (2), and the Langevin equation were solved at each time step of the integration to obtain particle position and the variances of the concentration distribution. The dose of a toxic pollutant at a particular point was calculated by integrating equation (3).

Results and Discussion

The model evaluation included checking the accuracy of the meteorology algorithm, divergence minimization algorithm and the dispersion model. In order to evaluate the accuracy of meteorology algorithm, three important micrometeorological parameters known as surface friction velocity, Monin-Obukhov length, and sensible heat flux were compared with a calculated series of data available in well known Indianapolis tracer gas

experiment (Olesen, 2005). Analysis of variances showed that the difference between model predictions and the reported data are insignificant, $F(1,308) = 0.0688,0.793$ for friction velocity, $F(1,292) = 0.0605,0.806$ for Monin-Obukhov length and $F(1,322) = 1.8986,0.169$ for sensible heat flux.

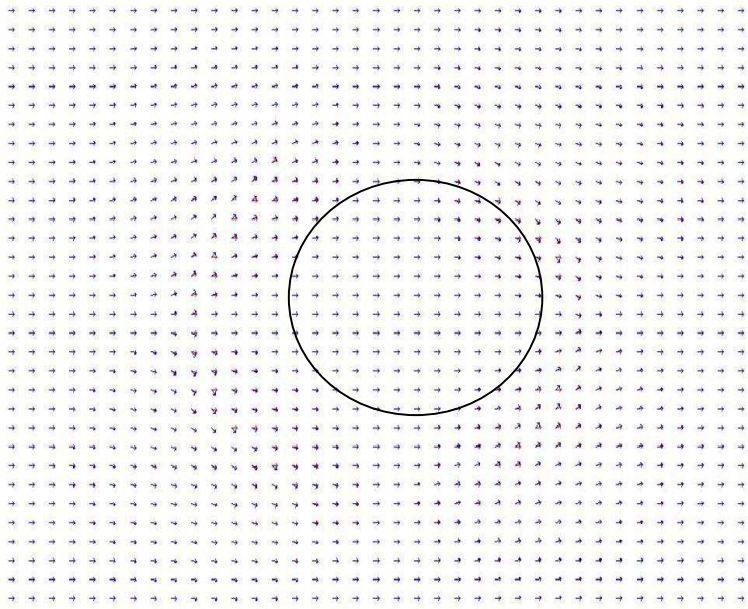

Figure 1: Numerical simulation of a potential flow around a hemi spherical hill. (in each cell two arrows are representing analytical results and our results).

Evaluation of the divergence minimization algorithm was performed by numerically simulating a potential flow around a hemispherical hill and comparing obtained results with an analytical solution. Visual observation (Figure 1) and analysis of variance showed that the numerical and analytical results were in good agreement, $F(1,2448) = 0.4626,0.496$ for horizontal wind profile and $F(1,910) = 0.1145,0.735$ for vertical wind profile. Evaluation of the dispersion model involved a comparison of model predictions with seven instantaneous SF_6 gas releases under various meteorological conditions as reported in Dipole Pride 26 field experiment (Biltoft, 1998). Analysis of the variance showed that the model predictions and reported results for 22.5 minutes after the release were in good agreement.

Conclusion

The model can be extended to predict near field dispersion from industrial sources of passive air pollutants.

References

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