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LAGRANGIAN VS. EULERIAN DISPERSION MODELING: EFFECTS OF WIND SHEAR ON POLLUTION DISPERSION

Chris J. Walcek*
Atmospheric Sciences Research Center, State University of New York, Albany, New York, 12203, U. S. A.

1. INTRODUCTION

In this study, a Lagrangian “puff” dispersion model is compared with an Eulerian model under simplified but typical atmospheric conditions. The purpose of this study is to demonstrate the dispersive effects of wind shear that is normally present near the Earth’s surface, but implicitly ignored by Lagrangian “puff” models. In section 2, the “Eulerian puff” model is described. In section 3, a “Lagrangian puff” formulation is presented. These two methods are compared in Section 4.

2. EULERIAN PUFF MODEL

An individual puff of pollution is simulated by numerically integrating the three-dimensional advection-diffusion equation forward in time (t) on a Cartesian grid:

$$\frac{\partial(C)}{\partial t} = \nabla(K\nabla C) - \nabla(\vec{v}C) \quad . \qquad (1)$$

where C is the pollutant concentration, K is the turbulent diffusion coefficient, and $\vec{v}$ is the velocity vector. For this study eddy diffusion coefficients are horizontally uniform and constant in time, but vary with height (z), and are set to zero at the PBL top (Z_{pbl}), and at the surface (z=0). While these assumptions are probably not appropriate for large domains or long transport distances, it will be shown that even under these simplified conditions substantial deviations from Lagrangian puff theories arise when wind speeds change vertically.

Advection is numerically calculated using the Walcek (2000) sharpened piecewise linear algorithm. Diffusion is simulated using a forward-time, centered space flux-form finite difference approximation. The PBL is vertically divided into 12 layers (Δz=200m). The domain sizes in the west-east and south-north directions are 80 and 120 grid cells, and initially Δy=Δx=500 m. At time t=0, a mass of pollution is placed in one model grid cell 400-600 m above the surface, near the upwind edge of the domain. For all simulations, a background concentration of 1 µg m^{-3} is specified, and the mass of pollution added (Q) is 4.9995 x 10^{11} µg, yielding an initial concentration of 10^{4} µg m^{-3} in the emission cell. Background concentrations (1 µg m^{-3}) are specified as inflow boundary conditions. During the simulation, if the edge of the puff impinges on the edge of the domain, the domain doubles in size in the downwind direction, and concentrations are averaged into the expanded cells so that a larger domain is simulated.

3. LAGRANGIAN PUFF MODEL

The Lagrangian parcel-trajectory model follows standard assumptions employed by classical puff dispersion models (e. g. Draxler and Taylor 1982). For a pollution puff initially released at a point and diffusing in an environment of spatially constant winds and diffusivities, limited vertically by the surface (z=0) and

**Author address:* ASRC, 251 Fuller Rd., Albany, NY 12203-3649; email: walcek@asrc.cestm.albany.edu

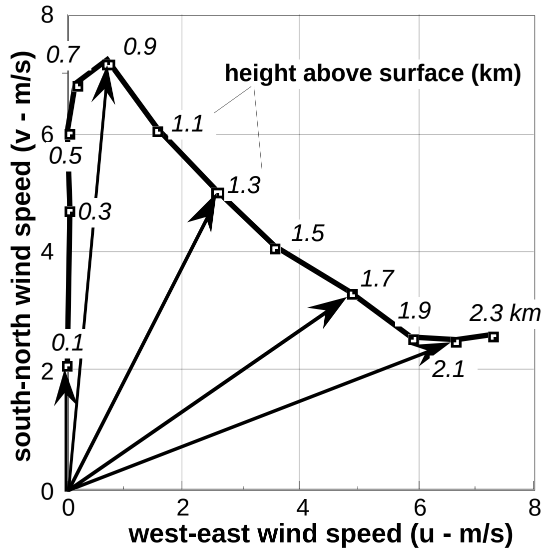

Fig. 1. Wind hodograph of the u *and* v *wind components used in dispersion tests. Heights (km) above surface for each wind vector are shown near each arrow tip.*

PBL top, the concentration around the puff center are analytically calculated using:

$$C = \frac{Q}{(2\pi)^{3/2}\sigma_h\sigma_z}\exp\left(\frac{-(x-x_c)^2-(y-y_c)^2}{2\sigma_h}\right) \mathrm{X} \left[\exp\left(\frac{-(z-z_c)^2}{2\sigma_z}\right)+\exp\left(\frac{-(z+z_c)^2}{2\sigma_z}\right)\right] . \qquad (2)$$

The center of the puff (located at x_c and y_c) is calculated following a trajectory, and z_e is the puff emission height (500 m). σ_h and σ_z are the horizontal and vertical dispersion of pollutant mass around the puff center. The z-dependent exponential terms in Eq. (2) are vertical reflecting terms required since diffusion is not allowed above the top of the PBL or below the surface. If $\sigma = \sqrt{2Kt}$ is used for calculating σ_h and σ_z, Eq. (2) represents an analytical solution to the 3-D advection-diffusion Eq. (1). However, most dispersion models empirically specify horizontal dispersions σ to be consistent with a large body of dispersion measurements, and are not based on Fickian diffusion principles. It is generally recognized that shear-related effects are the dominant factor enhancing dispersion relative to purely turbulent diffusive tendencies (e. g. Smith 1965; Randerson 1972).

4. RESULTS

For this comparison, winds shown in Fig. 1 are taken from a routine 0 UT 14 June 2000 Albany, NY radiosonde launched about 1 hour before local sunset on a relatively clear, sunny and moderately windy afternoon. Surface temperatures during the late afternoon and stability analysis of the radiosonde temperatures showed that the height of the PBL was approximately 2400 m above the surface. Fig 1 shows that winds are out of the south near the surface, while in the upper PBL, winds veer to a west-to-easterly flow. All simulations follow puff dispersion and advection for four hours.

Fig. 2 shows surface-level calculations of the shape and peak concentration of the Lagrangian and Eulerian puff models for hourly increments after release. The area of maximum surface impact according to the Eulerian calculations remains almost due north of the release point, reflecting the impacts expected if the puff followed a trajectory using emission height winds, which are directed to the north. In contrast, the Lagrangian puff model, using mass-weighted winds to define the trajectory, moves the puff northward initially, but after the puff becomes approximately uniformly mixed, the puff follows the mean PBL winds flowing from southwest to northeast. After four hours, the puff is displaced about 75 km downwind, and the location of the maximum surface impact is about 25 km east of the actual impact area. After 4 hours, peak concentrations calculated from pure diffusion theory disagree by over a factor of 10 from the Eulerian model, and the puff is skewed into a shape that is similar to the crescent shaped wind profile shown in Fig. 1. Interestingly, the centers of mass for both the Lagrangian and Eulerian puffs are identical and are located at the center of the Lagrangian position, but according to the Eulerian model maximum surface impacts are north of the release point, while a bulk of the puff mass in the upper PBL is east of the surface puff location. At longer times, the Eulerian model shows that the crescent-shaped puff grows and is translated by the PBL winds, but the shape remains preserved in this shear-dependent shape as long as wind speeds and directions remain fixed.

5. CONCLUSIONS

Using an accurate numerical method for simulating the advection and diffusion of pollution puffs it is demonstrated that point releases of pollution grow into a shape reflecting the vertical wind shear profile experienced by the puff within a time scale of a less than four hours. For distances beyond several 10s of kilometers from a release point, shear-related dispersion effects are probably the dominant mechanism affecting the area and magnitude of surface impacts. For assessing long-range pollutant dispersion, the common assumption that pollutants disperse as horizontally spherical “puffs” in the atmosphere is inherently inaccurate since shear-induced horizontal spreading of pollution is not a homogeneous “turbulent-like” diffusion process. A Lagrangian puff model can simulate an area impacted by a pollution puff only if larger shear-dependent horizontal puff dispersions are assumed. However, even if impacted areas are reasonably simulated, peak concentrations will be severely underestimated since atmospheric puffs influenced by even small amounts of wind shear are nonspherical. If horizontal dispersion coefficients in a Lagrangian puff model are adjusted so that peak concentrations are

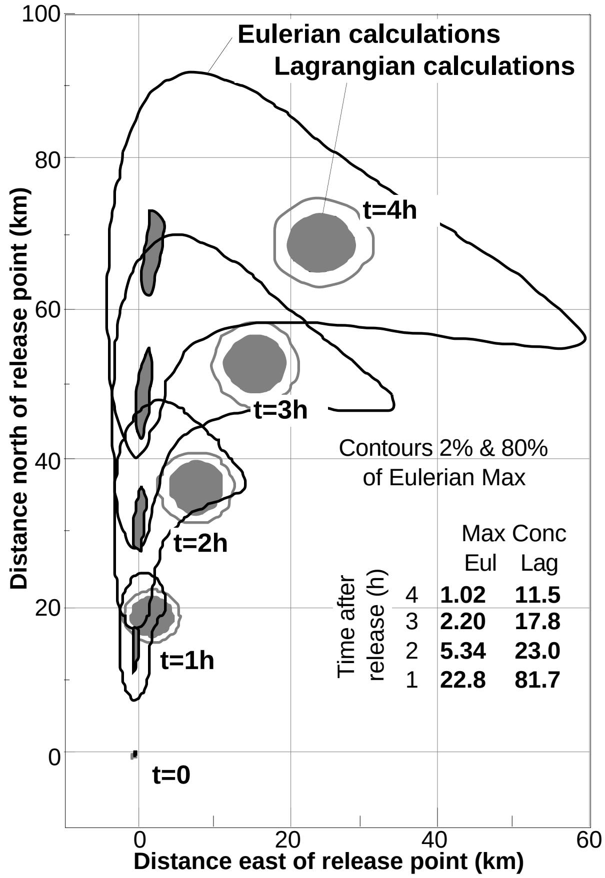

Fig. 2. Surface concentrations (μg m^{-3}) at hourly intervals within a puff initially emitted 0.5 km above the surface in a 2.4 km deep PBL advected with winds shown in Fig. 1 and diffused by turbulence. Gray contours are Lagrangian solutions. Black contours are calculated using the Eulerian model. Contours are 2% and 80% of the maximum Eulerian concentrations, tabulated at lower right.

correctly simulated, then the calculated pollution impact area will be severely skewed. In shear environments, no choice of horizontal dispersion coefficients in a single-puff Lagrangian model will yield reasonable correlations with puffs that are skewed into nonspherical shapes by atmospheric wind shear.

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