Invited Paper

Simulation of urban barrier effects on polluted urban boundary layers using the three-dimensional URBMET/TVM model with urban topography – new results from New York City

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ABSTRACT

Urban areas affect prevailing mesoscale and synoptic flow patterns due to a variety of physical processes, including urban heat island induced accelerations, surface roughness induced decelerations, and building barrier effects. Analysis of data collected over New York City (NYC) has shown that the city is capable of significantly altering mesoscale and synoptic flows fields. The urban barrier effect is the most significant factor altering such flows over NYC.

Results from a series of simulations using the URBMET/TVM mesoscale model are presented to illustrate NYC urban barrier effects on mesoscale flow patterns during heat island and sea breeze flow periods. The model reproduced observed urban retardation effects on sea breeze frontal passages and observed nighttime flow diffluence effects around the city.

Simulated meteorological fields were then used as input to a three-dimensional Eulerian dispersion model to study urban impacts on dispersion patterns during sea breeze flow conditions. Results showed that the dispersion model is capable of simulating most of the effects of sea breeze frontal passages on surface concentration fields. However, the omission of urban topographic barrier induced flow effects can result in incorrect concentration predictions in some areas of the domain.

INTRODUCTION

Urban areas affect prevailing mesoscale and synoptic flow patterns due to a variety of physical pro-
cesses, including urban heat island induced accelerations, surface roughness induced decelerations, and building barrier effects. Analysis of data collected over New York City (NYC) has shown that the city is capable of significantly altering the speed and/or direction of movement of thunderstorm cells, sea breeze fronts, and synoptic fronts. Analyses of the above effects, plus additional analysis (during periods without such features) of surface flow patterns, surface convergence fields, tetroon vertical velocities, and double theodolite velocity fields all point to the urban barrier effect as the most significant factor altering mesoscale flow over NYC (Bornstein and LeRoy [1]).

Results from a series of simulations using the URBMET/TVM mesoscale model are presented to illustrate the different contributions to the observed urban barrier effect over NYC arising from the various urban and coastal influences described above. The simulated meteorological fields were then used as input to a three-dimensional Eulerian dispersion model to study urban effects on dispersion patterns.

FORMULATION

The TVM three-dimensional mesoscale vorticity-mode numerical model of Schayes and Thunis [2] originated from the PBL URBMET model of Bornstein et al [3] and is hydrostatic and Boussinesq (and hence incompressible). The model contains a soil sub-surface layer and an atmospheric layer, which is divided into two sub-layers: a constant flux surface layer in which time dependent meteorological profiles are calculated from analytical stability functions dependent only on height, and a transition layer in which the hydrodynamic and thermodynamic equations are solved numerically with finite differences. Surface temperature and moisture values are computed using the surface energy and moisture balance equations, respectively, forced by internally computed solar radiation values.

The transition-layer equations are derived from the exact equations of motion for a Reynolds averaged viscous Newtonian fluid in a rotating coordinate system by assuming that:

> The atmosphere is Boussinesq. Density fluctuations are thus ignored, except in the buoyancy term in the vertical equation of motion, where they are replaced by mesoscale temperature fluctuations. This assumption produces the incompressible form of the continuity equation.
The atmosphere is hydrostatic. Vertical velocities must thus be computed from the continuity equation.

Specific humidity $q$ is a conserved property in the atmosphere.

Radiative flux divergence within the PBL occurs only from water vapor and from naturally occurring carbon dioxide effects on long wave radiative fluxes.

Potential temperature $\theta$ in the PBL can be approximated by

$$\theta \approx T + \Gamma z.$$ 

Mean thermodynamic and dynamic variables may be defined as the sum of several parts. For example, the total mean pressure $p$ may be written as

$$p = p_a + p_0(z) + p_n + p_m,$$

where $p_a$ is the (assumed constant) PBL average pressure and $p_0(z)$ is the hydrostatic variability in the absence of either (upper level) synoptic forcing $p_n$ or mesoscale forcing $p_m$. In TVM/URBMET, synoptic forcing is assumed constant, and thus all spatial and temporal variations arise only from mesoscale effects.

The basic Reynolds averaged equation of motion in the transition layer for the URBMET were given by Bornstein et al [3]. Both the infra-red radiative flux divergence term in the energy equation and the new higher order turbulence closure scheme (used to obtain vertical eddy diffusivities) are discussed in Schayes and Thunis [2].

The basic equations of motion are rewritten in vorticity form, so that pressure can be eliminated from the equations, as the upper boundary condition on this variable is not well posed in primitive equation mesoscale models. It is also frequently a source of instability, generating waves extraneous to the desired solution. On the other hand, the vorticity approach requires additional integrations to recover velocity components from the required stream functions. The hydrostatic approximation leaves only horizontal vorticity components with only vertical derivatives.

The equations of Bornstein et al [3] were transformed in TVM to a new coordinate system to account for topographic influences. In this new system, only the vertical coordinate is transformed following Pielke [4]. Vertical grid spacing is thus a function of hori-
zontal location, and only the surface level is terrain following.

Note that transformed horizontal velocities still equal corresponding Cartesian values and that this transformation is not time-dependent, as is the sigma-pressure coordinate system. Coincidence of the first grid level with the topography top also simplifies application of lower boundary conditions.

To obtain these equations, it was assumed that the horizontal gradient of the new vertical coordinate can be neglected versus its vertical gradient, which requires terrain slope angles much less than 45° (Pielke, [4]).

The original URBMET model used two different turbulence closure formulations, i.e., the first order closure of O’Brien in which vertical eddy diffusivities are specified as third degree polynomials depending only on SBL characteristics and a higher order integral length scale formulation based on Mellor and Yamada [5].

TVM uses a 1.5 turbulent kinetic energy (TKE) closure. The dissipation and diffusion mixing length formulation is that of Therry and Lacarrere [6], and is able to reproduce features normally only found with higher order models.

Turbulent fluxes are considered to be constant with height in the SBL, whose height $h_g$ is currently fixed at 10 m. Variables in the SBL are assumed to obey Monin-Obukhov similarity theory, which defines surface friction velocity, temperature, and specific humidity scaling parameters. These parameters are computed from horizontal wind speed, temperature, and humidity values at the surface and at $h_g$.

The current formulation uses the Businger [7] forced and mixed convective SBL stability functions. For the very stable case, a modified Webb [9] formulation is used. The Webb formulation slows the rate at which SBL fluxes approach zero in very stable conditions, as $z/L$ exceeds unity.

The water vapor and carbon dioxide infra-red flux divergence term is calculated using the Sasamori [10] scheme, rather than with the emissivities of Atwater [11] used in Bornstein et al [3]. As this process generally dominates that of the solar flux, this latter effect is currently neglected.
Incoming surface insolation is calculated for a horizontal surface following the method of Schayes and Thunis [2], while surface inclination effects are included following Pielke [4]. PBL attenuation includes a specified aerosol absorption factor, variable earth-sun distance, dry-air Rayleigh scattering, and water vapor absorption. Above PBL cloud attenuation can influence solar fluxes.

Boundary conditions are specified at each of the six external model boundaries and at the two internal boundaries (i.e., the surface and SBL top). TVM imposes the following:

> Open lateral boundary conditions, which normally permit perturbations to cross a lateral boundary; however, the variable grid formulation of the current application uses stretched horizontal grid spacings near lateral boundaries to move them away from the region of activity. This stretching, in combination with a complex terrain can allow new perturbations to grow in these regions. This problem is minimized by use of horizontal topography at the outer four grid points at each lateral boundary.

> The model top wind is geostrophic and its vertical temperature and humidity values match those of the synoptic scale. No constraints, in addition to a zero surface-value, are imposed on the vertical velocity component w, which is computed to satisfy continuity. Note that imposition of a zero w at the model top would be an over-specification.

Complex topography in a hydrostatic PBL model also allows for formation and propagation of (almost) vertically propagating gravity waves in stable conditions. As these waves can reflect at the upper boundary, a filter is used in a damping layer (consisting of the five uppermost domain levels) that gradually attenuates rising perturbations. The filter smooths all prognostic variables (except TKE) at each time step by use of their four neighboring values.

As real topography contains unresolvable features (smaller than two horizontal grid spacings), the same filter is used on observed topographic height values to prevent propagation of "two delta x" waves.

> Time and space varying surface temperature and humidity values are calculated by a soil sub-model using soil heat and moisture fluxes. While water surface temperature is assumed constant, soil surface temperature is calculated from the prognostic "force-
The surface layer turbulent fluxes are imposed at the internal boundary at the bottom of the transition layer (i.e., at the first numerical grid point beyond $h_g$). Following Therry and Lacarrere [6], turbulent energy is set equal to $4u_*$ both in the SBL and at the lowest transition layer numerical grid point.

The numerical scheme contained in TVM employs the fractional time step method described by Bornstein and Robock [15] and Bornstein et al [3]. For each prognostic equation, the three one-dimensional advection equations are thus first successively solved, likewise the three one-dimensional diffusion equations, and finally the remaining body forces or source/sink terms.

Finite difference calculations are performed on the non-uniformly spaced, three-dimensional staggered interlaced Arakawa type C grid of Bornstein et al [3], which locates velocity components at the center of each perpendicular (to the flow component) grid cell face, vorticities on edges above and below corresponding velocity components, and passive scalars at the cell center (as they represent cell averages). TVM locates TKE values at the centers of the upper and lower cell faces, as opposed to the cell center URBMET location. The current location is more reasonable, as TKE is a flux and not a scalar.

While the variable URBMET grid spacing allows for high resolution near the surface and near surface discontinuities, it permits generated waves to propagate at non-constant speeds due to numerical scheme properties. A constant horizontal grid size is thus used in
TVM, except for a few outer points where grid size is extended.

Boundary conditions on the current interlaced grid requires extrapolation of variables outwards across some boundaries. One plane of extra nodal points is therefore defined at positions above the top of the PBL and outside all lateral boundaries. These points are located outside the computational domain at distances equal to the distances between the boundaries and the first interior grid points in the same coordinate direction.

Finite-difference schemes currently used require secondary variables defined at various nodal locations in the computational cell. Such variables are defined by either flux-weighing or linear interpolation of primary variables, as discussed in MacCracken and Bornstein [16] and Bornstein et al [3].

Donor cell differencing, used to first solve the three one-dimensional advection equations, possesses first order time accuracy and the second order space accuracy of centered derivatives. While the scheme does not produce negative values and is conservative, it induces significant artificial viscosity that damps (but stabilizes) solutions. The scheme is, however, well suited for flow confluences simulated by TVM, e.g., near sea breeze fronts and at valley bottoms.

The two one-dimensional horizontal diffusion equations are next solved by an explicit three point forward in time, centered in space (FTCS) finite difference scheme, which possesses second-order space accuracy and first-order time accuracy. For vertical diffusion, the implicit Crank-Nicholson scheme is used. This scheme is numerically stable for any sized time step, and thus allows a larger diffusion time step than the explicit scheme used in Bornstein et al [3]. TVM last solves equations containing all body force and source terms by FTCS differencing.

The time dependent and unequal advection and diffusion time steps of Bornstein and Robock [15] in the URBMET simulations were useful because its advection time step was much larger than its explicit vertical diffusion time step. As TVM uses an implicit vertical diffusion scheme, its (input constant) topography induced gravity wave time step is generally the limiting one in its modified URBMET time step scheme. Values range from 30 to 60 sec, dependent on simulated topographic geometry and atmospheric stability.
The most significant difference between the current URMCON urban dispersion model of Bornstein et al [3] and the original Shir and Shieh [17] model is that the original version used observed meteorological data in a domain extending upwards to the base of the lowest elevated inversion. The current simulations, however, use derived meteorological output from the three-dimensional time-dependent mesoscale meteorological model to compute concentrations in a fixed height domain. Both versions assume that pollutant concentrations do not affect meteorological parameters.

As described in Bornstein et al [3], the mesoscale model provides the non-divergent wind fields and vertical diffusivity fields, while an assumed linear chemical reaction rate constant is specified. No flux vertical boundary conditions are assumed. At inflow boundaries, concentrations are assumed equal to a specified background value, while at outflow boundaries, second normal horizontal gradients are set to zero.

A Lagrangian plume trajectory routine simulates near source diffusion for major point sources until they are large enough to be integrated into the Eulerian dispersion grid. Effective plume emission height are computed from a modified Briggs [18] formulation.

The model domain is a 40 x 30 x 10 three dimensional staggered grid, in which parameters are located on the computational cube as in the URBMET model. Although the model can accommodate nonuniform grid spacings, a uniform 1.6 km horizontal grid interval was used to match the NYC/NYU area source SO2 emission grid of Bornstein et al [19].

Effective area source emission height is arbitrarily set equal to 1.5 times area source height. Daily and hourly emission rates were determined using the linear relationship of Halpern et al [20] between the known annual emission rates and tabulated degree day values. Emissions from the 310 largest SO2 point sources were explicitly simulated. The annual emission, effluent temperature, and effluent velocity of each were tabulated for use in the plume rise estimation procedure.

Observations of surface and PBL values were used to initiate the models and for a qualitative evaluation of their results. The SO2 concentrations data were collected at 33 fixed surface sites, and by instrumented trucks, cars, and helicopters. The helicopters also provided temperature and moisture profiles, while a
Air Pollution

surface anemometer network of about 70 sites and several pibal sites provided wind observations.

METEOROLOGICAL MODEL RESULTS

A series of 30 hour simulations were carried out for an urban heat island (maximum surface intensity of about 6 K)/sea breeze period. A constant geostrophic wind speed was specified as 3 m/s from the NW. Surface roughness values ranged from 1 cm for water areas, 0.5 m for rural areas, 3 m for urban areas, to 4 m for six "super' urban grid areas around the tip of Manhattan. Topography was limited to 20 m for urban areas and 70 m for the super urban areas. The computational grid was 24 by 24 in the horizontal (Fig. 1a) and 16 levels to 2 km in the vertical.

The horizontal distribution of daytime horizontal wind velocity at the 25 m level after 18 hours of the "base" simulation (including urban topographic, roughness, and anthropogenic heating effects) at the simulated time of 1500 LST (Fig. 1a) shows that sea breeze frontal movement has been retarded over the city center, as seen in the wave like shape of the front over the city.

Corresponding results from a similar simulation from Bornstein et al [3], that did not include urban topographic effects, does not show a wave like frontal shape over the city (Fig. 2). The corresponding observations do in fact show such a wave like perturbation (Fig. 3), indicating that it arises due to urban topographic effects.

The new "base" simulation nighttime results after 33 hours (at 0600 LST) show a diffuent flow around the warm city and a local minimum of speed over the city (Fig. 1b). The diffuent flow has arisen from the urban topographic barrier effect, as it was not present in the old nighttime results (not shown). The local urban minimum wind speed area, however, is due mostly to the large urban roughness effect, as it was present in the old results.

Urban topographic effects can be quantified by subtracting (from the new base fields) the corresponding values from a second new simulation that is identical to the first new results, except that all urban and super urban topographic heights are set to zero. The resulting daytime "difference" field at 1200 LST (Fig. 4a) shows a convergent upslope flow over the city, as expected with a raised topographic feature.
These perturbation flows generally happen to be in the same direction as the "base" case flows in each local domain area, i.e., see the NW synoptic flow NW of the city, the SSE sea breeze flow S of the city, and the NE Long Island Sound sea breeze flow NE of the city. This concurrence of each of the local flow directions produce the convergence seen in the figure.

The corresponding nighttime "difference" field at 0300 LST (Fig. 4b) shows the expected divergent downslope flow from the city. Given the generally northwesterly offshore flow during this period, the following effects are noted: along streamline deceleration NW of the city, along streamline acceleration SW of the city, and difluence NE and SW of the city. Both the along streamline speed changes and the difluence contribute to a divergence effect (as shown in the natural coordinate form of the horizontal divergence equation).

AIR QUALITY MODEL RESULTS

The meteorological results from the non-urban topographic simulation were stored on tape and then used as input for the air quality simulations. The pre-frontal northwesterly flow produced surface advection of polluted air to areas SE of the high emission regions in Manhattan and the south Bronx (Fig. 5).

Passage of the sea breeze front decreased surface concentrations in the previously polluted southern coastal NYC locations and increased surface concentrations in the previously clean areas NW of the city (Fig. 6), as the marine air was initially less polluted than the older urban air.

Corresponding observed surface concentration patterns both before (Fig. 7) and after the sea breeze frontal passage (Fig. 8) both show the same features as the simulated patterns. The observed magnitudes and locations of the maximum increases and decreases in concentration due to the frontal passage also agree well with corresponding predicted values.

Hour by hour comparisons between observed and predicted concentration values at several representative sites (Fig. 9) show good agreement at some sites, but poor agreement at other sites. This results as the simulated meteorological input for this dispersion calculation was from the simulation that did not include urban topographic effects. When output from the new meteorological simulations is used as input to the dispersion model in the near future, good agreement be-
CONCLUSION

Results from a series of simulations using the URBMET/TVM mesoscale model were presented to illustrate NYC urban barrier effects on mesoscale flow patterns during heat island and sea breeze flow periods. The model reproduced observed urban retardation effects on sea breeze frontal passages and observed nighttime flow diffluence effects around the city. The specified urban topographic barrier simulated a daytime upslope convergence into the city and a nighttime downslope divergence effect out of the city.

Simulated meteorological fields were then used as input to a three-dimensional Eulerian dispersion model to study urban impacts on dispersion patterns during sea breeze flow conditions. Results showed that the dispersion model is capable of simulating most of the effects of sea breeze frontal passages on surface concentration fields. However, the omission of urban topographic barrier induced flow effects can result in incorrect concentration predictions in some areas of the domain.

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**Fig. 1a.** Simulated 25 m level "base case" flow field over NYC at 1500 LST.
Fig. 1b. Simulated 25 m level "base case" flow field over NYC at 0600 LST of the second simulation day.
Fig. 2. Simulated 37.5 m level flow field over NYC at 0600 LST of the second simulation day for case with no urban topography.

Fig. 3. Observed sea breeze frontal isochrones, where 16 is 1600 LST
Fig 4a. Simulated 25 m level "difference" flow field over NYC at 1200 LST, with corresponding "base" case flow vectors shown.
Fig 4b. Simulated 25 m level "difference" flow field over NYC at 0300 LST of second simulation day, with corresponding "base" case flow vectors shown.
Fig. 5. Simulated surface sulfur dioxide concentrations (pphm) at 0800 EST for case with no urban topography.

Fig. 6. Simulated surface sulfur dioxide concentrations (pphm) at 1800 EST for case with no urban topography.
Fig. 7. Observed surface sulfur dioxide concentrations (pphm) at 0830 EST.

Fig. 8. Observed surface sulfur dioxide concentrations (pphm) at 1830 EST.
Fig. 9. Observed (dots) and predicted (circles and line) hourly surface sulfur dioxide concentrations at four monitoring stations.