A NEW COMBINED LOCAL AND NON-LOCAL PBL MODEL FOR METEOROLOGY AND AIR QUALITY MODELING

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1. INTRODUCTION

A new version of the Asymmetric Convective Model (ACM) (Pleim and Chang 1992) has been developed to describe sub-grid vertical turbulent transport in both meteorology models and air quality models. The new version (ACM2) combines the non-local convective mixing of the original ACM with local eddy diffusion to better represent the full range of turbulent transport within the convective boundary layer (CBL) (see Fig. 1). The result is smoother near-surface profiles compared to the original ACM, and more well-mixed profiles compared to pure eddy diffusion models.

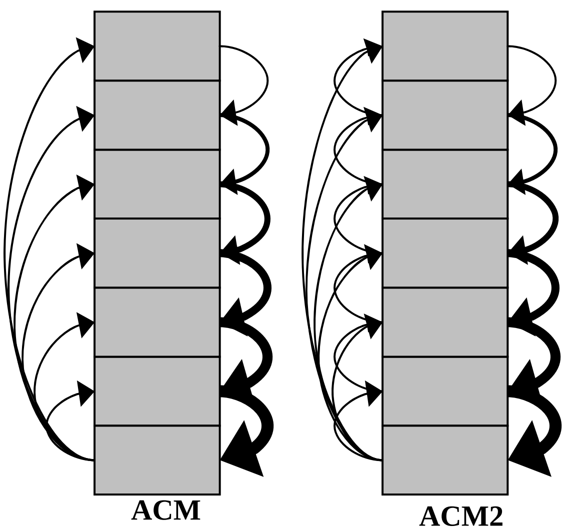

Fig. 1. Schematic representations of the exchange among model layers in the original ACM and the ACM2.

A detailed model description is provided by Pleim (2006a), along with single column testing and comparison to large-eddy simulations. Implementation and evaluation of the ACM2 in MM5 is described in a companion paper (Pleim 2006b). After a summary of the model formulation and the MM5 evaluation, this paper focuses on the implementation of the ACM2 in the Community Multiscale Air Quality (CMAQ) model and some initial testing and evaluation.

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2. MODEL FORMULATION

A brief overview of the model formulation is presented here. For a detailed description the reader is referred to Pleim (2006a). The ACM2 tendency equation for any transported quantity C_i in model layer *i* is given by,

$$\frac{\partial \mathrm{C_i}}{\partial \mathrm{t}} = \mathrm{M2uC_1} - \mathrm{M2d_iC_i} + \mathrm{M2d_{i+1}C_{i+1}}\frac{\Delta z_{i+1}}{\Delta z_i} + \frac{1}{\Delta z_i}\left(\frac{K_{i+\frac{1}{2}}(C_{i+1}-C_i)}{\Delta z_{i+\frac{1}{2}}} + \frac{K_{i-\frac{1}{2}}(C_i - C_{i-1})}{\Delta z_{i-\frac{1}{2}}}\right). \tag{1}$$

The first three terms on the rhs of Eq. 1 represent the non-local scheme that, except for a modification to the convective mixing rates (M2u and M2d), are identical to the equation for the original ACM model. The last term in Eq. 1 represents eddy diffusion where K is the local mixing rate that is proportional to the vertical eddy diffusivity. The non-local rates are defined as

$$M2u = \frac{f_{conv}K_z(z_{1+\frac{1}{2}})}{\Delta z_1\left(h - z_{1+\frac{1}{2}}\right)} \tag{2a}$$

for upward mixing and

$$M2d_i = M2u\left(h - z_{i-\frac{1}{2}}\right)/\,\Delta z_i \tag{2b}$$

for downward mixing. Local mixing is defined as,

$$K(z) = K_z(z)\left(1 - f_{conv}\right)\ . \tag{3}$$

Vertical eddy diffusivity (K_z) is defined by boundary layer scaling similarly to Holtslag and Boville (1993) as,

$$K_z(z) = k \frac{u_*}{\phi(\frac{z_s}{L})} z(1 - z/h)^2 \ , \qquad (4)$$

where k is the von Karman constant (k = 0.4), u_* is the friction velocity, ϕ is the non-dimensional profile function, and h is the PBL height. For unstable conditions (z_s/L < 0), z_s = min(z, 0.1h) and for stable condition $z_s = z$, where L is the Monin-Obukov Length scale.

The key to combining local and non-local closure techniques is the definition of the partitioning factor f_{conv}. The partitioning factor controls the degree of local versus non-local behavior. At either extreme, f_{conv} =1 or f_{conv} =0, the scheme reverts to either the ACM1 non-local scheme or local eddy diffusion, respectively. For stable or neutral conditions f_{conv} is set to zero for pure eddy diffusion since the non-local scheme is only appropriate for convective conditions where the size of buoyant eddies typically exceed the vertical grid spacing.

The partitioning factor is derived from the ratio of non-local heat flux to total heat flux at the top of the surface layer (0.1h) according to the model of Holtslag and Boville (1993). The result (Eq. 5) is a simple function of stability (h/L) where f_{conv} ramps up quickly from zero for neutral conditions with increasing instability then leveling off at around 0.5 for very unstable conditions. The partitioning factor is given as,

$$f_{conv} = \left(1 + \frac{k^{-2/3}}{0.1a}\left(-\frac{h}{L}\right)^{-1/3}\right)^{-1} \qquad (5)$$

where a is a constant set to 7.2.

3. METEOROLOGY APPLICATION

The ACM2 was incorporated in MM5v3.7.2 and run for a 5 week period (July 12 – August 18) during the summer of 2004. The domain covered the eastern US at 12 km grid resolution with 34 vertical layers. Physics options included the Pleim-Xiu land surface model (PX LSM) (Xiu and Pleim 2001), the rapid radiation transfer model (RRTM) for long wave radiation (Mlawer et al. 1997), version 2 of the Kain-Fritsch (KF2) cumulus parameterization (Kain 2004), and the Reisner 2 microphysics scheme (Reisner et al. 1998). Four dimensional data assimilation (FDDA) was applied using gridded analyses for nudging winds at all levels and temperature and humidity above the PBL. Also, the indirect nudging of soil moisture using surface analyses of temperature and humidity was used with the PX LSM as described by Pleim and Xiu (2003).

Surface statistics were similar to other model evaluation studies and well within the commonly accepted limits. For example, mean biases for 2-m temperature, 2-m water vapor mixing ratio, and 10-m wind speed were 0.37 K, 0.11 g/Kg, and -0.21 m/s, respectively. Similarly, mean absolute errors were 1.42 K, 1.14 g/Kg, and 1.03 m/s.

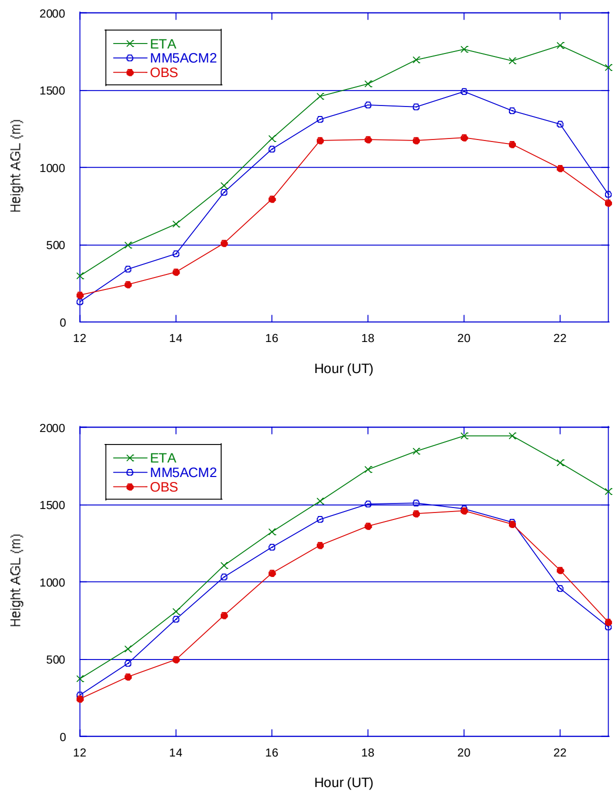

Fig. 2. PBL height averaged over the simulation period from the MM5-ACM2 and Eta models and derived from a radar wind profiler at Pittsburgh, PA (top) and Concord, NH (bottom).

A particularly important parameter for evaluation of PBL models is the temporal evolution of the PBL. Thus, model simulated PBL heights were compared to PBL heights derived from radar wind profile measurements at two sites: Pittsburgh, PA and Concord, NH. The observed PBL heights were hand-analyzed using a combination of signal to noise ratio (SNR) (Angevine et al. 1994), and vertical velocity variance (Bianco and Wilczak 2002). Figure 2 shows diurnal plots of observed and model simulated PBL heights averaged over all available data within the 5-week period. Forecasted PBL heights from NCEP's Eta model are also plotted for reference. On the average the MM5-ACM2 overpredicted the PBL height at Pittsburgh throughout the day but to a lesser degree than the Eta model. The MM5-ACM2 also overpredicted PBL height at Concord in the morning with diminishing bias in the afternoon.

The combination of accurate near-surface temperature, humidity, and wind speed simulation and a relatively small high bias in PBL height predictions supports the realism of the ACM2 for simulation of PBL processes in meteorological models. The controlled 1-d LES comparisons, shown by Pleim (2006a), demonstrate the ability of the ACM2 to accurately simulate vertical profiles of potential temperature, u and v wind components, and inert chemical tracers. Thus, incorporation of the ACM2 into the chemical transport model, CMAQ, should provide more realistic treatment of PBL transport of chemical species.

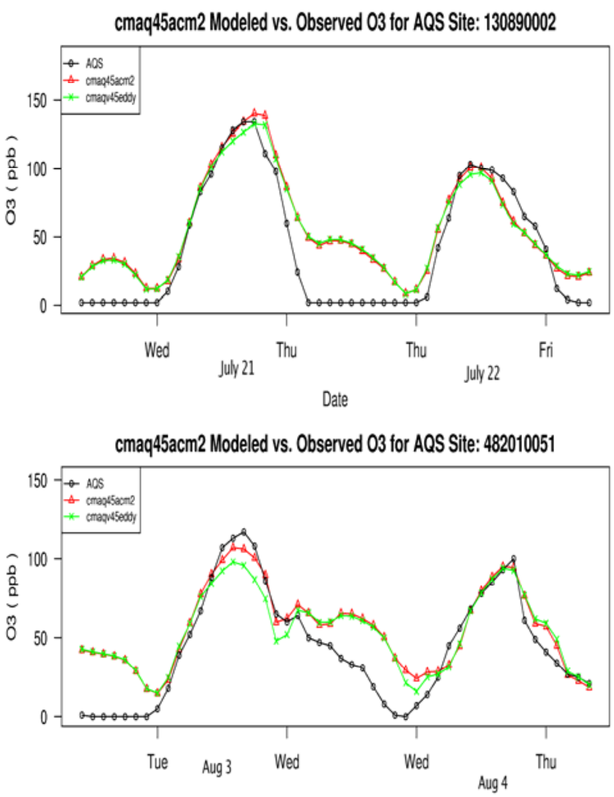

Fig. 3. CMAQ-ACM2 (red) and CMAQ-EDDY (green) ozone concentration compared with AQS measurements (black) near Atlanta (top) and Houston (bottom).

4. CMAQ APPLICATION

The ACM2 has been added to the CMAQ model for release in version 4.6. The ACM2 replaces the previous ACM option and is being used as the default PBL option for the 2006 model release evaluation. The CMAQ still has two PBL options: ACM2 and EDDY, where EDDY is an eddy diffusion scheme described by Byun et al. (1999). Preliminary model comparisons have been made to show the effects of these different PBL options.

4.1 Comparisons to surface observations

CMAQv4.5 with CB4 gas phase chemistry and the AE3 aerosol module was run on a 12 km grid covering most of the eastern US from mid July to mid August, 2004 using both ACM2 and EDDY. Fig. 3 shows examples of 2-day time series comparing both CMAQ-ACM2 and CMAQ-EDDY to ozone measurements at individual AQS sites near Atlanta and Houston during high ozone episodes. While the two model runs produced very similar ozone concentrations, the ACM2 run often produced greater values near the daytime peaks that were, in these cases, closer to the measurements. Directly comparing the two model runs for maximum daily ozone concentrations (Fig. 4) shows that ACM2 predicts ozone concentrations that are about 5-8% higher at the high end of the distribution compared to the run using EDDY.

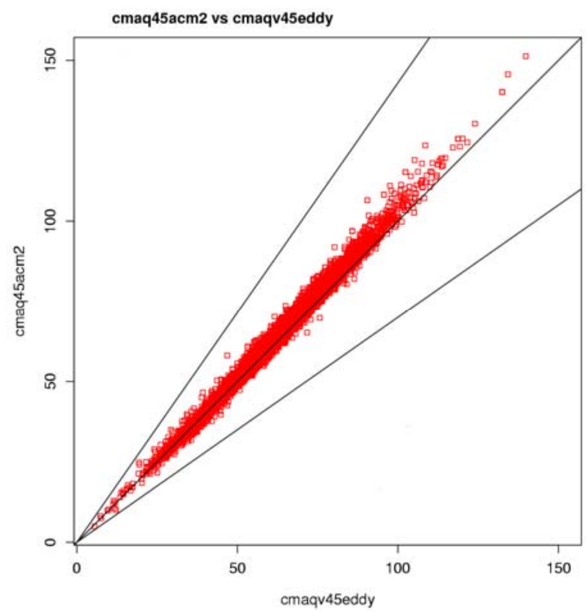

Fig 4. Comparison between maximum daily 1-hr ozone concentrations modeled by ACM2 and EDDY.

For more inert species, such as CO, the ACM2 more often predicts lower concentrations at the surface than EDDY, as shown in Fig. 5. For other species such as sulfate, however, there is little difference between the two runs (not shown). It may be that for species with strong surface emissions, the ACM2 mixes upward more quickly resulting in lower concentrations at the surface but higher concentrations aloft. To test this idea, vertical profiles of CO, NOx and ozone are compared for both model runs.

4.2 Vertical Profiles

Figure 6 shows vertical profiles of CO mixing ratios (ppb) for both CMAQ runs from a grid column over St. Louis for seven hours (16-22Z) on August 1, 2004. Since there is a large ground level emission rate in this urban grid cell both sets of profiles show maximum CO concentrations in the lowest model layer. The ACM2 run, however, produces much more well-mixed profiles in the PBL, especially in the late afternoon, resulting in lesser concentrations at the ground but greater concentrations in the upper two thirds of the PBL. Also, note that the EDDY profiles have a deeper effective mixing depth, due to the quadratic height function used for the definition of eddy diffusivity. The ACM2 uses a cubic height function (Eq. 4) such that the eddy diffusivity becomes much smaller than the eddy diffusivity used in EDDY above about 0.8 *h*.

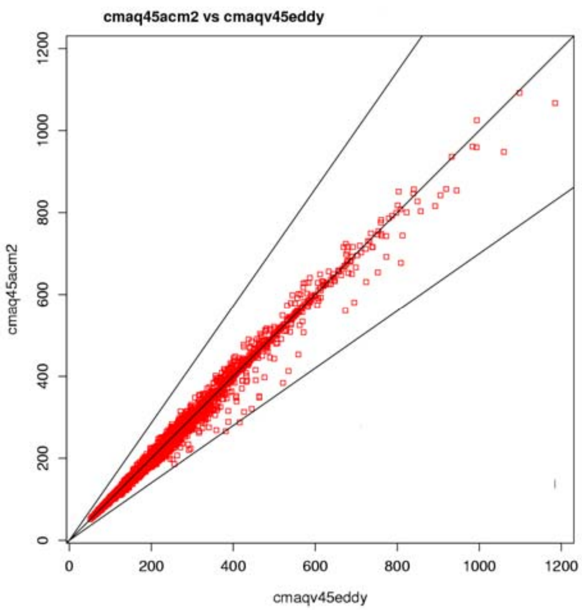

Fig 5. Comparison of hourly CO concentrations from CMAQ runs using ACM2 and EDDY.

The NO_x profiles, shown in Figure 7, show results that are very similar to the CO profiles because of high ground-level emission rates of NO_x. Again, the ACM2 profiles are more well-mixed with lesser concentrations in the lower 1/3-1/2 of the PBL and greater concentrations in the upper portions. The greater ground-level NO_x concentrations for the EDDY run result in lower ground-level O_3 concentrations, as seen in Figure 8, because of NO titration near the ground. Note that the discrepancy in ground-level O_3 concentrations between the two runs is greatest in the late afternoon when turbulent mixing is subsiding and NO_x emissions are near their peak. Also note that the higher effective mixing height for the EDDY run is clearly evident in the afternoon profiles.

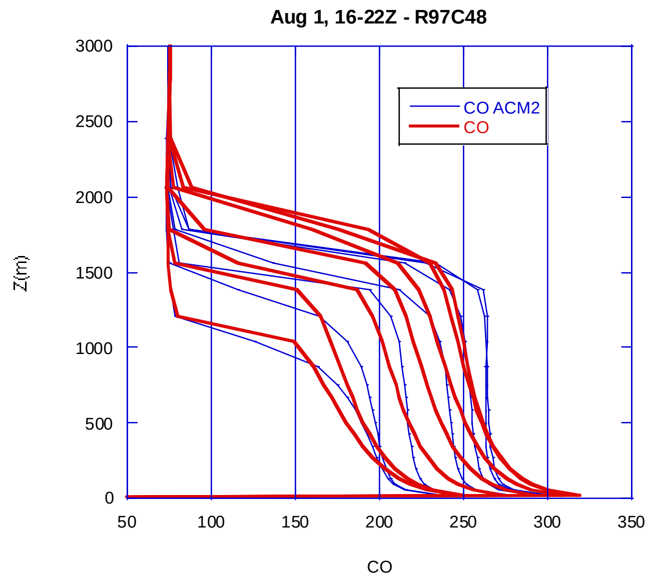

Fig. 6. Vertical profiles of CO mixing ratio over St. Louis for 16-22Z on August 1, 2004. The red profiles were produced by CMAQ using EDDY, and the blue profiles were produced by CMAQ using ACM2.

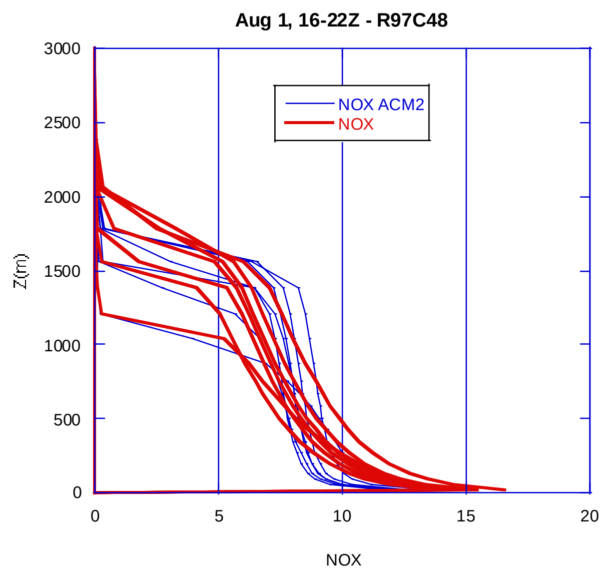

Fig. 7. Vertical profiles of NO_x mixing ratio over St. Louis for 16-22Z on August 1, 2004. The red profiles were produced by CMAQ using EDDY, and the blue profiles were produced by CMAQ using ACM2.

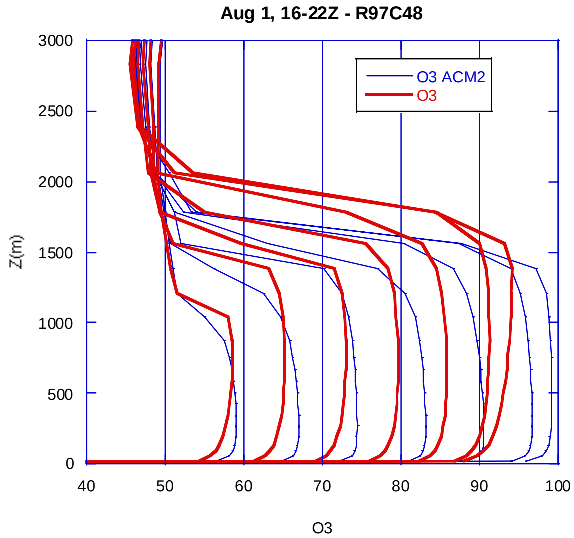

Fig. 7. Vertical profiles of O_3 mixing ratio over St. Louis for 16-22Z on August 1, 2004. The red profiles were produced by CMAQ using EDDY, and the blue profiles were produced by CMAQ using ACM2.

5. CONCLUSIONS

The ACM2 is a new PBL scheme that is equally applicable to meteorology and air quality modeling. The ACM2 combines local and non-local closure techniques to account for both small-scale shear driven turbulence and larger-scale convective turbulence. In concept, the ACM2 is similar to several other PBL models that are formulated with local and non-local terms. Such models, which are essentially eddy diffusion schemes with an additional gradient adjustment term (e.g. Troen and Mahrt 1986, Holtslag and Boville 1993, Noh et al. 2003), have been used extensively in meteorology models such as MM5, WRF, and GFS. However, application of this type of model to air quality is problematic because the non-local gradient adjustment term was originally derived for sensible heat and is proportional to surface flux. Extensions to water vapor and momentum have been made for some models but application to trace chemical concentrations that may or may not have surface fluxes, does not seem viable. While the ACM2 performs similarly to these PBL schemes for heat flux, it is more applicable to a wide range of other quantities including air quality chemical species. Therefore, by using the ACM2 for both meteorology and chemical transport modeling, consistency in PBL transport techniques is achieved in the air quality modeling system.

7. REFERENCES

Angevine, W.M., A.B. White, and S.K. Avery, 1994: Boundary layer depth and entrainment zone characterization with a boundary layer profiler. *Boundary Layer Meteor.*, **68**, 375-385.

Bianco and Wilczak, 2002: Convective Boundary Layer Depth: Improved Measurement by Doppler Radar Wind Profiler Using Fuzzy Logic Methods. *J. Atmos. and Oceanic Technol.***, 19,** 1745–1758.

Byun, D. W., J. Young, J. Pleim, M. T. Odman, and K. Alapaty, 1999: Numerical transport algorithms for the Community Multiscale Air Quality (CMAQ) chemical transport model in generalized coordinates, in *Science Algorithms of the EPA Models-3 Community Multiscale Air Quality (CMAQ) Modeling System.* D. W. Byun and J. K. S. Ching, eds., National Exposure Research Laboratory, U.S. EPA, Research Triangle Park, NC. Chap 7.

Holtslag, A. A. M. and B. A. Boville, 1993: Local versus non-local boundary layer diffusion in a global climate model, *J. Climate*, **6**, 1825-1842.

Kain, J.S., 2004: The Kain–Fritsch convective parameterization: An update. *J. Appl. Meteor.*, **43**, 170–181.

Mlawer, E.J., S.J. Taubman, P.D. Brown, M.J. Iacono and S.A. Clough, 1997: RRTM, a validated correlated-k model for the longwave. *J. Geophys. Res.*, **102**, 16663-16682.

Noh, Y., W. G. Cheon, S. Y. Hong, and S. Raasch, 2003: Improvement of the K-profile model for the planetary boundary layer based on large eddy simulation data, *Boundary-Layer Meteorol.,* **107**, 401-427.

Pleim, J. E., 2006a: A Combined Local and Non-local Closure Model for the Atmospheric Boundary Layer. Part 1: Model Description and Testing, *J. of Appl. Meteor. and Clim.*, in press.

Pleim, J. E., 2006b: A Combined Local and Non-local Closure Model for the Atmospheric Boundary Layer. Part 2: Application and Evaluation in a Mesoscale Meteorology Model, *J. of Appl. Meteor. and Clim.*, in press.

Pleim, J. E., and J. S. Chang, 1992: A non-local closure model for vertical mixing in the convective boundary layer, *Atmos. Environ.,* **26A**, 965-981.

Pleim, J. E., and A. Xiu, 2003: Development of a land surface model. Part II: Data Assimilation. *J. Appl. Meteor*., **42**, 1811-1822.

Reisner, J., R. M. Rasmussen, and R. T. Bruintjes, 1998: Explicit forecasting of supercooled liquid water in winter storms using the MM5 mesoscale model. *Quart. J. Roy. Meteorol. Soc*., **124 B**, 1071-1107.

Troen, I. and L. Mahrt, 1986: A simple model of the atmospheric boundary layer: Sensitivity to surface evaporation, *Boundary-Layer Meteorol.* **37**, 129-148.

Xiu, A., and J. E. Pleim, 2001: Development of a land surface model part I: Application in a mesoscale meteorology model. *J. Appl. Meteor*., **40**, *192-209*.

Disclaimer

The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement DW13921548*. This work constitutes a contribution to the NOAA Air Quality Program. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.*