ABSTRACT

The California Air Resources Board (ARB) Request for Proposals (RFP), entitled "Determination of the Horizontal Diffusion Coefficient for Use in Air Quality Models," identified three advection solvers that are already available for use within the SARMAP Air Quality Model (SAQM) and called for the theoretical formulation, experimental quantification, and within-SAQM sensitivity testing of diffusivity formulations that will yield net levels of pollutant dispersion that accurately mimic reality. Such a diffusivity formulation must account for the dominant atmospheric advective (e.g., wind shear) and turbulent transfer processes, compensate for smoothing or filtering present in the modeled wind fields, and correct for the unintended mixing processes accompanying present-day numerical advection schemes.

This study revealed that:

- the gridded MM-5 wind fields do cause some spatial smoothing of surface wind gradients, but retain 50-80% of the observed gradients, and are therefore quite useful for correcting the pollutant transport scheme for wind-/concentration-gradient effects;

- such wind gradient-related transport terms yield small changes in surface ozone concentrations;

- as the MM-5 wind fields already include most wind directional shear with height, an important mechanism in lateral dispersion, avoidance of "double-counting" of such shear influences demands that explicitly-modeled dispersion rates and diffusivities exclude such shear influences -- a fact which greatly reduces the usefulness of most tracer experiment results, as real-world experiments include all mechanisms;

- a numerical simulation using the synthetic turbulence model, KSP, suggested that an appropriate lateral diffusivity for 10km wide plumes in an atmosphere free of directional shear is of order $u^* \cdot \sigma_y$, where u^* is the friction velocity and σ_y is the plume's lateral standard deviation;

- extension of this concept throughout the PBL leads to a physical, non-dimensional diffusivity of $k_H = 0.2 \cdot i_y \cdot \varepsilon$, where i_y is the local turbulent intensity, σ_v/U, and ε is the local Courant number, $U \cdot \Delta t / \Delta x$;

- the long-wave numerical diffusivities of the Bott (BOT) and Yamartino (YAM) advection schemes are comparable, larger than those of the Accurate Space Derivative (ASD) scheme, and are modeled in terms of the local Courant number, ε, and the fourth-derivative of the local concentration distribution;

- the short-wave (i.e., $\lambda/\Delta x = 2$ and 3) performance of the three advection schemes differs markedly, includes some non-diffusive and/or non-linear effects (e.g., anti-diffusion, hole-burning), and is not presently modeled as a diffusivity; and,

- SAQM peak daily ozone decreases 10-15 ppb when a plausible level of lateral diffusion is included, and the numerical-diffusion-corrected predictions of the three transport schemes generally agree to within a few ppb, though some differences are as large as 10%.