SUPPLEMENT

DETAILED DESCRIPTION OF THE MODEL UPDATES

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TRANSPORT AND DISPERSION. Because there are no new modifications to the puff dispersion algorithms as described in Draxler and Hess (1998), this section will only present a description of the 3D Lagrangian particle dispersion.

Based on the discretization of the classical Langevin equation (Chock and Winkler 1994), the horizontal turbulent velocity components at the current time [$U'(t + \Delta t)$] are computed based on the turbulent velocity components at the previous time [$U'(t)$], the horizontal velocity standard deviation (σ_u), a random number drawn from a Gaussian distribution with a mean of 0 and standard deviation of 1 (λ), an autocorrelation coefficient (R) that depends on Δt, and the horizontal Lagrangian time scale (TL_u); namely,

$$U'(t+\Delta t) = R(\Delta t)U'(t) + \sigma_u \lambda \left[1 - R(\Delta t)^2\right]^{0.5}. \quad \text{(ES1)}$$

The integration time step Δt is computed from the requirement that the change in the vertical plume dimension or the 3D particle displacement Δz_p,

$$\Delta z_p < 0.5\,\Delta z, \quad \text{(ES2)}$$

where Δz is the vertical grid spacing, and hence

$$\Delta t = (\Delta z)^2 / \left(8\sigma_w^2 \mathrm{TL}_w\right), \quad \text{(ES3)}$$

where σ_w^2 is the vertical velocity variance and TL_w is the vertical Lagrangian time scale, which are discussed in more detail below.

The calculation of the vertical turbulent velocity is also based on the modified Langevin equation in discrete time [Chock and Winkler (1994) and references therein]; namely,

$$W'/\sigma_w(t+\Delta t) = R(\Delta t)\left[W'(t)/\sigma_w(t)\right] + \lambda\left[1 - R(\Delta t)^2\right]^{0.5} + \mathrm{TL}_w\left[1 - R(\Delta t)\right]\partial\sigma_w(t)/\partial z, \quad \text{(ES4)}$$

and as defined by Wilson et al. (1983),

$$\sigma_w(t+\Delta t) = \sigma_w(t) + W'(t)\Delta t\,\partial\sigma_w(t)/\partial z. \quad \text{(ES5)}$$

The velocity variance gradient term on the vertical turbulent velocity is applied to prevent accumulation of particles in low turbulence regions (Legg and Raupach 1982). The importance of this latter term is somewhat reduced if averaging of the diffusivity profile within the boundary layer is applied (see mixing options section below). Moreover, when computing the turbulence an exponential velocity autocorrelation is assumed such that

$$R(\Delta t) = \exp\left(-\Delta t/\mathrm{TL}_i\right), \quad \text{(ES6)}$$

where TL_i is TL_u or TL_w, and TL_u = 10,800 s (~1/f) is assumed to be constant for convenience. Draxler and Hess (1997) used a single constant value for the TL_w, which was usually set to 200 s. The HYSPLIT model now allows TL_w to switch according to atmospheric stability conditions (Hanna 1982). Therefore, TL_w can be set to two different values: one corresponding to stable and another for unstable atmospheric conditions. Hegarty et al. (2013) propose a TL_w of 5 and 200 s for stable and unstable conditions, respectively. These values result in a random walk ($R \approx 0$) vertical dispersion for most of the longer time steps.

MIXING OPTIONS. The HYSPLIT modeling system allows four different options to estimate the standard deviations of the turbulent velocity $\{\sigma_i = [\sigma_w, \sigma_u, \sigma_v]\}$ needed to calculate the particle's vertical and horizontal mixing: i) assuming the vertical mixing diffusivities K_w follow the coefficients for heat (Draxler and Hess 1998) and

$$\sigma_w = \left(K_w/\mathrm{TL}_w\right)^{0.5} \text{ and} \tag{ES7}$$

$$\sigma_u = 0.25\sigma_w, \tag{ES8}$$

ii) based on the horizontal and vertical friction velocities and the PBL height (Kantha and Clayson 2000), iii) using the TKE fields, or iv) directly provided by the meteorological data. In the following section we will expand on options ii and iii since the calculation of K_w used in Eq. (ES7) is thoroughly described in Draxler and Hess (1998) and iv is self-explanatory.

The determination of σ_i following Kantha and Clayson (2000) assumes that in a stable or neutral boundary layer,

$$\sigma_w^2 = 1.7u_*^2\left(1 - z/z_i\right)^{3/2}, \tag{ES9}$$

$$\sigma_u^2 = 4.0u_*^2\left(1 - z/z_i\right)^{3/2}, \text{ and} \tag{ES10}$$

$$\sigma_v^2 = 5.0u_*^2\left(1 - z/z_i\right)^{3/2}, \tag{ES11}$$

where z is the vertical position, z_i is the boundary layer height, and u_* is the horizontal friction velocity. In the stable or neutral surface layer,

$$\sigma_w^2 = 1.7u_*^2, \tag{ES12}$$

$$\sigma_u^2 = 4.0u_*^2, \text{ and} \tag{ES13}$$

$$\sigma_v^2 = 5.0u_*^2. \tag{ES14}$$

In the unstable boundary layer,

$$\sigma_w^2 = w_*^2\left(z/zi\right)^{2/3}\left(1 - z/zi\right)^{2/3}\left[1 + 0.5\left(H_{\mathrm{pbl}}/H_{\mathrm{sfc}}\right)^{2/3}\right], \tag{ES15}$$

where w_* is the vertical component of the friction velocity and H_{pbl} is the heat flux at the inversion and H_{sfc} the flux at the surface. The $H_{\mathrm{pbl}}/H_{\mathrm{sfc}}$ ratio is assumed to be constant at about 0.2. From Garratt (1992), the horizontal variances are simply a constant function of the convective velocity scale,

$$\sigma_u^2 = \sigma_v^2 = 0.36w_*^2. \tag{ES16}$$

In the unstable surface layer,

$$\sigma_w^2 = 1.74u_*^2\left(1 - 3z/L\right)^{2/3}, \tag{ES17}$$

where L corresponds to the Obukhov stability length. Furthermore, Eq. (ES16) still holds under this stability condition to estimate the horizontal variances.

On the other hand, if the TKE field is available, then the velocity variances can be computed from its definition,

$$E = 0.5\left(\sigma_w^2 + \sigma_v^2 + \sigma_u^2\right), \tag{ES18}$$

and Eqs. (ES9)–(ES14), resulting in the following constant relationships to the TKE:

$$\sigma_w^2 = 0.32E, \tag{ES19}$$

$$\sigma_u^2 = 0.74E, \text{ and} \tag{ES20}$$

$$\sigma_v^2 = 0.85E. \tag{ES21}$$

Then, from the definition (ES18) and Eqs. (ES15)–(ES17),

$$\sigma_w^2 = 2E/\left(1 + G\right) \text{ and} \tag{ES22}$$

$$\sigma_u^2 = \sigma_v^2 = 0.5G\sigma_w^2, \tag{ES23}$$

and where in the unstable surface layer G is defined as

$$G = 0.41\left(w_*^2/u_*^2\right)/\left(1 - 3z/L\right)^{2/3} \tag{ES24}$$

and in the unstable boundary layer

$$G = 0.72\Big/\left\{\left(z/zi\right)^{2/3}\left(1 - z/zi\right)^{2/3}\left[1 + 0.5\left(H_{\mathrm{pbl}}/H_{\mathrm{sfc}}\right)^{2/3}\right]\right\}. \tag{ES25}$$

STABILITY AND MIXING DEPTH CALCULATION OPTIONS. Draxler and Hess (1998) present two options to estimate the boundary layer stability parameters (i.e., u_*, w_*, and L) that determine the calculation of the standard deviation of the turbulent velocities (σ). The preferred one uses the fluxes of heat and momentum provided by the meteorological model, if available. Otherwise, the temperature and wind gradients of each gridpoint sounding are used to estimate stability. On the other hand, the simulated PBL affects the dispersion and the resulting air concentrations by changing the rate of dispersion as well as providing a cap to vertical mixing of pollutants. Currently the modeling system includes the following options for estimating z_i: i) use the meteorological model (uses the z_i value from the meteorological model) and ii) from the temperature profile (computes z_i the height at which the potential temperature is at least 2° greater than the minimum potential temperature). The computation is made from the top down (Draxler and Hess 1998), iii) from the TKE profile (uses the meteorological model's TKE profile to estimate z_i at the height at which the TKE either decreases by a factor of 2 or falls to a value of less than 0.21), and iv) set to a constant value (to match external observations the mixing depth can also be set to a constant value).

DYNAMIC MANAGEMENT SPLIT/MERGE AND MIXED-MODE APPROACH FOR PARTICLES AND PUFFS. When the model is run in 3D particle mode, a fixed number of particles are released and followed for the duration of the computational period. A sufficient number of particles need to be released so that at the end of the simulation, after particles have spread out, adjacent concentration grid cells have enough particles to be able to properly represent the concentration gradients. However, for very-long-duration or high-resolution simulations, a very large number of particles may be required and the computational times may become prohibitive. To ameliorate this issue, the HYSPLIT system includes hybrid particle–puff combinations—such as Gaussian horizontal and top-hat vertical puff (Gh-THv), top-hat horizontal and vertical puff (THh-THv), Gaussian horizontal puff and vertical particle distribution (Gh-Pv), or top-hat horizontal puff and vertical particle distribution (THh-Pv)—as alternatives to the 3D particle mode to describe the transport and dispersion.

Puff split procedures (Rolph et al. 1992) are called at fixed intervals and merging is always called hourly. Puff splitting occurs horizontally when the size of the puff reaches a certain fraction of the meteorological grid size producing four (five) new top-hat (Gaussian) puffs with radius equal to half of the original puff. In the vertical, splitting also occurs when the size of the puff covers more than two meteorological vertical levels producing two new puffs. On the other hand, merging is most sensitive to the setting of the minimum horizontal distance allowed between puff centers before the merge occurs. Increasing this distance from one to four standard deviations of the Gaussian distribution causes almost all the puffs to be merged with at least one other puff. Because merging is called after splitting, most puffs that are merged are already in the same vertical position; hence, there is little sensitivity to variations in the vertical distance allowed between puffs before merging them.

When the total number of puff/particles approaches the array limits, further splitting is restricted until the merge procedures have freed up additional array space. Care is taken to ensure that there is adequate array space to allow for new emissions, if they are specified. Each time the splitting shuts down, the parameter that describes the minimum horizontal distance between puffs to allow merging is automatically incremented to increase the effectiveness of puff merging. Furthermore, the model offers the option that for those remaining puffs that are eligible to split but cannot as a result of the split restriction are prevented from increasing in size (both horizontal and vertical) until the split restriction has been removed. In addition, at the first occurrence of the split restriction, the size to which a puff is permitted to grow before splitting is increased in proportion to a user-defined parameter. Very-long-duration simulations, simulations using very-fine-resolution meteorological data, or those that have an insufficient initial allocation of the puff array space can result in split or perhaps even emission shutdown. If any of these occur, the results may be noisy and inaccurate.

TIME-VARYING EMISSIONS. *Wind-blown dust.* HYSPLIT contains two different wind-blown dust emission algorithms. The first method was developed for applications in Asia, the Middle East, and northern Africa, while the newest procedure was developed for use over North America and expanded for the entire globe.

In the original dust emission algorithm (an option no longer available), the vertical dust flux was described as a fraction of the horizontal transport following the Marticorena et al. (1997) source description to compute the particulate matter with diameters of less than 10 μm (PM10) dust injections. The detailed soil characteristics required to apply this approach proved to be impractical in locations where data are unknown; hence, the following simplified method was applied to calculate the emission flux Q (Westphal et al. 1987):

$$Q = 0.01U_*^4 A, \tag{ES26}$$

where A represents the dust emission area. Dust emissions only occur during dry days and at locations where a constant threshold friction velocity (28 cm s^{-1}) is exceeded (Escudero et al. 2006).

In the newest approach, potential dust source locations are defined on a monthly basis based upon a climatology constructed from the Moderate Resolution Imaging Spectroradiometer (MODIS) Deep-Blue Aerosol Optical Depth's (AOD) values (Ginoux et al. 2010). Dust emissions are presumed to occur at locations, defined at a minimum resolution of 0.25°, where the friction velocity exceeds the threshold friction velocity U_{*t}. The value of U_{*t} was computed from the AOD climatology at each location assuming that the probability U_* will exceed that value is the same as the probability that the AOD will exceed 0.75. Naturally, each grid point has a different probability density function (PDF) and therefore each grid point has a unique U_{*t}. Furthermore, the slope of the higher AOD values and their corresponding friction velocities in the PDF defines a dust emission density K that, when multiplied by $(U_* - U_{*t})$ and A, gives the emission rate from that location; in other words,

$$Q = KA\left(U_* - U_{*t}\right). \tag{ES27}$$

In addition to the values obtained for North America (Draxler et al. 2010), new coefficients for the emission algorithm (K and U_{*t}) were recomputed using the friction velocities from NCEP's GFS meteorological data, allowing for a global application of this approach (Wang et al. 2011).

Plume rise. The HYSPLIT modeling system also includes a very simplified plume rise algorithm based on the method of Briggs (1969) with updates from Arya (1999). Plume rise is computed assuming an air parcel's rise is based only on the buoyancy terms using the heat release, the wind velocity, and the friction velocity. For unstable conditions the following expression is applied to calculate vertical displacement from the source:

$$\Delta z = 1.3\mathrm{FB}\big/\left(UU_*^2\right), \tag{ES28}$$

where FB is the buoyancy flux calculated from the heat release H,

$$\mathrm{FB} = 7.6\times10^{-7}H. \tag{ES29}$$

On the other hand, for stable conditions and $U > 0.5$ m s^{-1},

$$\Delta z = 2.6\mathrm{FB}\big/\left(U\times\mathrm{SSP}\right)^{1/3}, \tag{ES30}$$

where SSP is the static stability parameter. And for calm conditions ($U < 0.5$ m s^{-1}),

$$\Delta z = 5.3\mathrm{FB}^{0.25}\big/\left(\mathrm{SSP}\right)^{3/8}. \tag{ES31}$$

BACKWARD-IN-TIME DISPERSION AND FOOTPRINT. The estimation of the source region (footprint) that could contribute to the air concentration measured at a receptor point is accomplished by emitting a number of 3D particles (N_{tot}) of equal mass that undergo backward transport and dispersion and determining the total amount of time Δt each particle p spends in a volume element (i, j, k) using the expression [see Lin et al. (2003) for more details]

$$f = \frac{m_{\mathrm{air}}}{h\bar{\rho}}\frac{1}{N_{\mathrm{tot}}}\sum_{p=1}^{N_{\mathrm{tot}}}\Delta t_{p,i,j,k}, \tag{ES32}$$

where m_{air} is the molar mass of air and $\bar{\rho}$ is the average density below an atmospheric column of height h.

DEEP CONVECTION PARAMETERIZATION. A very simplified parameterization based on the convective available potential energy (CAPE) (Gerbig et al. 2003) has been incorporated into HYSPLIT. CAPE enhanced mixing results in particles in the cloud layer being randomly redistributed within that layer if they reside in a grid cell where CAPE exceeds a user-set threshold value.

IN-CLOUD WET SCAVENGING PARAMETERIZATION. The in-cloud wet removal of a pollutant is based on the following equation:

$$\frac{dC}{dt} = \Lambda C, \tag{ES33}$$

where C is the concentration and Λ is the scavenging coefficient given by

$$\Lambda = Ar^B, \tag{ES34}$$

where r is the rainfall rate and A and B are scavenging parameters. Default values for these parameters are based on Sportisse (2007, his Table 11).

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