ADDENDUM

USER'S GUIDE FOR THE

INDUSTRIAL SOURCE COMPLEX (ISC3) DISPERSION MODELS

VOLUME II - DESCRIPTION OF MODEL ALGORITHMS

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TECHNICAL DESCRIPTION FOR THE
REVISED ISCST3 MODEL (DATED 99155)

This document provides a technical description of model algorithms for recent enhancements of the ISCST3 model, including the most recent version dated 99155. The algorithms described in this Addendum include the gas dry deposition algorithms based on the draft GDISCDFT model (dated 96248), and the optimizations of the area source algorithm. Both of these enhancements are associated with the non-regulatory default TOXICS option introduced with version 99155 of ISCST3. A brief description of the user instructions for these new options is presented in the accompanying Addendum to Volume I of the ISC3 model user's guide (ISC3ADD1.WPD).

Gas Dry Deposition Algorithms

The ISCST3 dry deposition algorithm for gaseous pollutants is based on the algorithm contained in the CALPUFF dispersion model (EPA, 1995a), and has undergone limited review and evaluation (Moore, at al. 1995).

The deposition flux, F_d, is calculated as the product of the concentration, χ_d, and a deposition velocity, v_d, computed at a reference height z_d:

$$F_d = \chi_d \cdot v_d \tag{A1}$$

The concentration value, χ_d, used in Equation A1 is calculated according to Equation 1-1 of the ISC3 model user's guide, Volume II (EPA, 1995b), with deposition effects accounted for in the vertical term as described in Section 1.1.6.3 of Volume II. The calculation of deposition velocities is described below for gaseous emissions.

Deposition Velocities for Gases

At a reference height z_d, the deposition velocity (v_d) for gases is expressed (Wesley and Hicks, 1977; Hicks, 1982) as the inverse of a sum of three resistances:

$$v_d = \left(r_a + r_d + r_c \right)^{-1} \tag{A2}$$

where, r_a =   the atmospheric resistance (s/m) through the surface layer,

                 r_d =   the deposition layer resistance (s/m), and,

                 r_c =   the canopy (vegetation layer) resistance (s/m).

An alternative pathway that is potentially important in sparsely vegetated areas or over water is deposition directly to the ground/water surface. Although not involving vegetation, it is convenient to include the ground/water surface resistance as a component of r_c.

The atmospheric resistance term (r_a) is given by Equations 1-81 and 1-82 in Section 1.3.2 of the ISC3 model user's guide, Volume II (EPA, 1995b).

The deposition layer resistance (r_d) is parameterized in terms of the Schmidt number (EPA, 1995a) as:

$$r_d = d_1 S_c^{d_2} / \left(k \, u_* \right) \tag{A3}$$

where, S_c =   the Schmidt number (υ/D_M),

υ =   the kinematic viscosity of air ($^\sim 0.15 \times 10^{-4}$ m^2/s),

D_M =   the molecular diffusivity of the pollutant (m^2/s), and,

d_1, d_2 =   empirical parameters; $d1/k=5$, $d2=2/3$ (Hicks, 1982)

k =   the von Karman constant ($^\sim 0.4$)

u_* =   surface friction velocity (m/s)

The canopy resistance (r_c) is the resistance for gases in the vegetation layer, including the ground/water surface. There are three main pathways for uptake/reaction within the vegetation or at the surface (EPA, 1995a):

(1)   Transfer through the stomatal pore and dissolution or reaction in the mesophyll cells (plant tissue that contains chlorophyll).

(2)   Reaction with or transfer through the leaf cuticle.

(3)   Transfer into the ground/water surface.

These pathways are treated as three resistances in parallel.

$$r_c = \left[LAI / r_f + LAI / r_{cut} + 1 / r_g \right]^{-1} \tag{A4}$$

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where, r_f =   the internal foliage resistance (s/m) (Pathway 1, Transfer through the stomatal pore and dissolution or reaction in mesophyll cells),

          r_{cut} =   the cuticle resistance (s/m), (Pathway 2, Reaction with or transfer through the leaf cuticle, a thin film covering the surface of plants),

          r_g =   the ground or water surface resistance (s/m), (Pathway 3, Transfer into the ground/water surface), and,

          LAI   =   the leaf area index (ratio of leaf surface area divided by ground surface area). The LAI is specified as a function of wind direction and month/season, and is included in the meteorological input file provided by the MPRM preprocessor.

Pathway 1:

The internal foliage resistance (r_f) consists of two components:

$$r_f = r_s + r_m \qquad\qquad (A5)$$

where, r_s =   the resistance (s/m) to transport through the stomatal pore (see below), and,

          r_m =   the resistance (s/m) to dissolution or reaction of the pollutant in the mesophyll (spongy parenchyma) cells, user input by species. For soluble compounds (HF, SO_2, CL_2, NH_3), set to zero; for less soluble compounds (NO_2), it could be > 0)

     Stomatal opening/closing is a response to the plant's competing needs for uptake of CO_2 and prevention of water loss from the leaves. Stomatal action imposes a strong diurnal cycle on the stomatal resistance, and has an important role in determining deposition rates for soluble gaseous pollutants such as SO_2. Stomatal resistance (r_s) is given by (EPA, 1995a):

$$r_s = p_s / (b D_M) \qquad\qquad (A6)$$

where, p_s =   a stomatal constant corresponding to the characteristics of leaf physiology ($\simeq 2.3 \times 10^{-8}$ m^2),

          b   =   the width of the stomatal opening (m), and,

          D_M =   the molecular diffusivity of the pollutant (m^2/s).

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The width of the stomatal opening (b) is a function of the radiation intensity, moisture availability, and temperature. In ISC3, the state of vegetation is specified as one of three states: (A) active and unstressed, (B) active and stressed, or (C) inactive. Irrigated vegetation can be assumed to be in an active and unstressed state. The variation in stomatal opening width during period (A) when vegetation is active and unstressed (Pleim et al., 1984) is:

$$b = b_{max} \left(R_I / R_{max} \right) + b_{min} \tag{A7}$$

where, b_{max} = the maximum width (m) of the stomatal opening ($\sim 2.5 \times 10^{-6}$ m) (Padro et al., 1991),

b_{min} = the minimum width (m) of the stomatal opening ($\sim 0.1 \times 10^{-6}$ m),

R_I = the incoming solar radiation (W/m^2) received at the ground, and is included in the meteorological input file for the model by the MPRM preprocessor, and,

R_{max} = the incoming solar radiation (W/m^2) at which full opening of the stomata occur; assume constant and equal to 600.

During periods of moisture stress, the need to prevent moisture loss becomes critical, and the stomata close. Thus for period (B), active vegetation under moisture stress conditions, assume that $b = b_{min}$. When vegetation is inactive (e.g., during the seasonal dry period), the internal foliage resistance becomes very large, essentially cutting off Pathway 1.

Assuming the vegetation is in state (A), active and unstressed, ambient temperature provides an additional bound on the value of r_s. During cold periods (T < 10°C), metabolic activity slows, and b is set by the code to b_{min}. During hot weather conditions (T > ~35°C) the stomata are fully open ($b = b_{max}$) to allow evaporative cooling of the plant.

Pathway 2:

The resistance due to reaction with or transfer through the leaf cuticle (r_{cut}) is given by (EPA, 1995a):

$$r_{cut} = \left(A_{ref} / A_R \right) r_{cut}(ref) \tag{A8}$$

where, A_{ref} = the reference reactivity parameter of SO$_2$ (~ 8.0),

A_R = the reactivity parameter for the depositing gas, (NO$_2$=8, O$_3$=15, HNO$_3$=18, PAN=4), and,

$r_{cut}(ref)$ = the empirically determined reference cuticle resistance (s/m) of SO$_2$, set equal to 3000 s/m (Padro et al., 1991).

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<u>Pathway 3:</u>

The third resistance pathway for r_c is transfer into the ground/water surface (r_g). In sparsely vegetated areas, deposition directly to the surface may be an important pathway.

$$r_g = \left(A_{ref} / A_R\right) r_g(ref) \tag{A9}$$

where, $r_g(ref)$ =   the reference resistance of SO_2 over ground (~ 1000 s/m) (Padro et al., 1991).

Over water, deposition of soluble pollutants can be quite rapid. The liquid phase resistance of the depositing pollutant over water is a function of its solubility and reactivity characteristics, and is given by (Slinn et al., 1978):

$$r_g = H / \left(\alpha_* \, d_3 \, u_*\right) \tag{A10}$$

where,   H   =   the Henry's law constant, which is the ratio of gas to liquid phase concentration of the pollutant, $(H \sim 4 \times 10^{-2}$ (SO_2), 4×10^{-7} (H_2O_2), 8×10^{-8} (HNO_3), 2×10^{0} (O_3), 3.5×10^{0} (NO_2), 1×10^{-2} (PAN), and 4×10^{-6} (HCHO)),

α_* =   a solubility enhancement factor due to the aqueous phase dissociation of the pollutant $(\alpha_* \sim 10^3$ for SO_2, ~ 1 for CO_2, 10 for O_3), and

d_3 =   a constant (~ 4.8×10^{-4}).

If sufficient data are not available to compute the canopy resistance term, r_c, from Equation A4, then an option for user-specified gas dry deposition velocity is provided. Selection of this option will by-pass the algorithm for computing deposition velocities for gaseous pollutants, and results from the ISCST3 model based on a user-specified deposition velocity should be used with extra caution.

<u>Optimizations for Area Sources</u>

When the non-regulatory default TOXICS option is specified, the ISCST3 model optimizes the area source algorithm to improve model runtimes. These optimizations are briefly described below.

In the regulatory default mode, the ISCST3 model utilizes a Romberg numerical integration to estimate the area source impacts, as described in Section 1.2.3 of the ISC3 model user's guide, Volume II (EPA, 1995b). While the Romberg integration performs well relative to other approaches for receptors located within or adjacent to the area source,

its advantages diminish as the receptor location is moved further away from the source. The shape of the integrand becomes less complex for the latter case, approaching that of a point source at distances of about 15 source widths downwind. Recognizing this behavior, the TOXICS option in ISCST3 makes use of a more computationally efficient 2-point Gaussian Quadrature routine to approximate the numerical integral for cases where the receptor location satisfies the following condition relative to the side of the area source being integrated:

$$XU - XL < 5*XL \tag{A11}$$

where, XL = the minimum distance from the side of the area source to the receptor, and

XU = the maximum distance from the side of the area source to the receptor.

If the receptor location does not satisfy the condition in Equation A11, then the Romberg numerical integration routine is used. In addition, for receptors that are located several source widths downwind of an area source, a point source approximation is used. The distance used to determine if a point source approximation is applied is stability dependent, and is determined as follows:

$$X > FACT * WIDTH \tag{A12}$$

where, X = the downwind distance from the center of the source to the receptor,

FACT = a stability-dependent factor (see below), and

WIDTH = the crosswind width of the area source.

Values of FACT:		
Stability Class	Rural	Urban
A	3.5	3.5
B	5.5	3.5
C	7.5	5.5
D	12.5	10.5
E	15.5	15.5
F	25.5	15.5

When area sources are modeled with dry depletion, the TOXICS option also allows the user to specify the AREADPLT option, which applies a single effective dry depletion factor to the undepleted value calculated for the area source. The effective dry depletion

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factor, which replaces the application of dry depletion within the area source integration, is intended to provide potential runtime savings to the user. Since dry depletion is distance-dependent, the effective dry depletion factor is calculated for an empirically-derived effective distance. The effective distance is calculated as the distance from the receptor to a point within the area source that is one-third the distance from the downwind edge to the upwind edge. For receptors located upwind of the downwind edge, including receptors located within the area source, the effective distance is one-third the distance from the receptor to the upwind edge of the source.

In addition to the area source optimizations described above, when the TOXICS option is specified, the dry depletion integration is performed using a 2-point Gaussian Quadrature routine rather than the Romberg integration used for regulatory applications.

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