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A Summary of Recent Refinements to the WAKE Dispersion Model, a Component of the HGSYSTEM/UF_6 Model Suite

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CONTENTS

LIST OF FIGURES

Page

LIST OF TABLES

ACRONYMS AND ABBREVIATIONS

ASHRAE	American Society of Heating, Refrigerating and Air Conditioning Engineers
ASCII	American Standard Code for Information Interchange
CFR	*Code of Federal Regulations*
DOE	U.S Department of Energy
EPA	U.S. Environmental Protection Agency
Eqn.	equation
erf	error function
ft	feet
FORTRAN	Formula Translator
GDP	gaseous diffusion plant
GUI	graphical user interface
HGSYSTEM	Heavy Gas-system
HGSYSTEM/UF_6	Heavy Gas-system-Uranium Hexafluoride
ISC3	Industrial Source Complex-Version 3
K	degrees Kelvin
kg	kilogram
m	meter
MACCS2	MELCOR Accident Consequence Code System-2
MB	megabyte
MHz	megahertz
mg	milligram
mph	miles per hour
N/A	not applicable
PGDP	Paducah Gaseous Diffusion Plant
PORTS	Portsmouth Gaseous Diffusion Plant
Q	mass flux rate
s	second
SAR	Safety Analysis Report
UF_6	uranium hexafluoride
χ	concentration

1. INTRODUCTION

The original WAKE dispersion model (Hanna and Chang 1997), a component of the HGSYSTEM/UF_6 model suite, is based on Shell Research Ltd.'s HGSYSTEM Version 3.0 (Post 1994a,b) and was developed by the U.S. Department of Energy (DOE) for use in estimating downwind dispersion of materials due to accidental releases from gaseous diffusion plant (GDP) process buildings. The model is applicable to scenarios involving both ground-level and elevated releases into building wake cavities of non-reactive plumes that are either neutrally or positively buoyant. For a given release, the WAKE model assumes that a fraction, f_c, is captured in the building recirculation cavity and is transported into the far wake region, while the remaining fraction, $1-f_c$, rises above the turbulent wake and is affected by building downwash (see Fig. 1). The original WAKE model is composed of three separate executable components. Ground level concentrations at downwind receptor locations associated with the portion of the release captured in the recirculation cavity are calculated by the WAKE code using formulas developed by Wilson (1995) and Briggs (1995; 1996), while those associated with the fraction of the release which rises above the wake cavity are determined using a modified version of the the U.S. Environmental Protection Agency's (EPA's) Industrial Source Complex-Version 3 (ISC3) dispersion model (EPA 1995). In the original WAKE model, separate files are created containing the results corresponding to each of these two fractions. These results are summed by third, post-processing utility, POSTWAKE, to obtain total ground-level concentration at the receptor.

Over the 2-year period since its creation, the WAKE model has been used to perform consequence analyses for Safety Analysis Reports (SARs) associated with gaseous diffusion plants in Portsmouth (PORTS), Paducah (PGDP), and Oak Ridge (Bloom 1997; Lombardi 1998; Lombardi and Gant 1998). These applications have identified the need for additional model capabilities (such as the treatment of complex terrain and time-variant releases) not present in the original WAKE, ISC3, or POSTWAKE utilities which, in turn, has resulted in numerous modifications to these codes as well as the development of additional, stand-alone postprocessing utilities. Consequently, application of the model has become increasingly complex as the number of executable, input, and output files associated with a single model run has steadily grown.

In response to these problems, a streamlined version of the WAKE model has been developed which integrates all calculations that are currently performed by the existing WAKE, ISC3, and the various post-processing utilities. Unlike the original version of the WAKE model in which the user must run a series of executable utilities that pass information from one to the next via multiple input/output files, the revised WAKE model consists of a single executable file which reads information contained in a single, mandatory, main input file and an optional terrain input file, and generates all necessary output information without requiring any interim user interaction. This internal transfer of information results in greater model execution speed and mathematical precision. This report summarizes the efforts involved in developing this revised version of the WAKE model.

Other refinements have also been made to algorithms used in the original WAKE model. Examples of these include a more rigorous method for estimating exposure times at downwind locations, additional capabilities for characterizing transient releases, and the inclusion of an iterative scheme in the ISC3 model which calculates plume rise based on wind speed at half the plume height rather than at the release height. This report also provides a detailed description of refinements made to the WAKE model since its introduction in 1997.

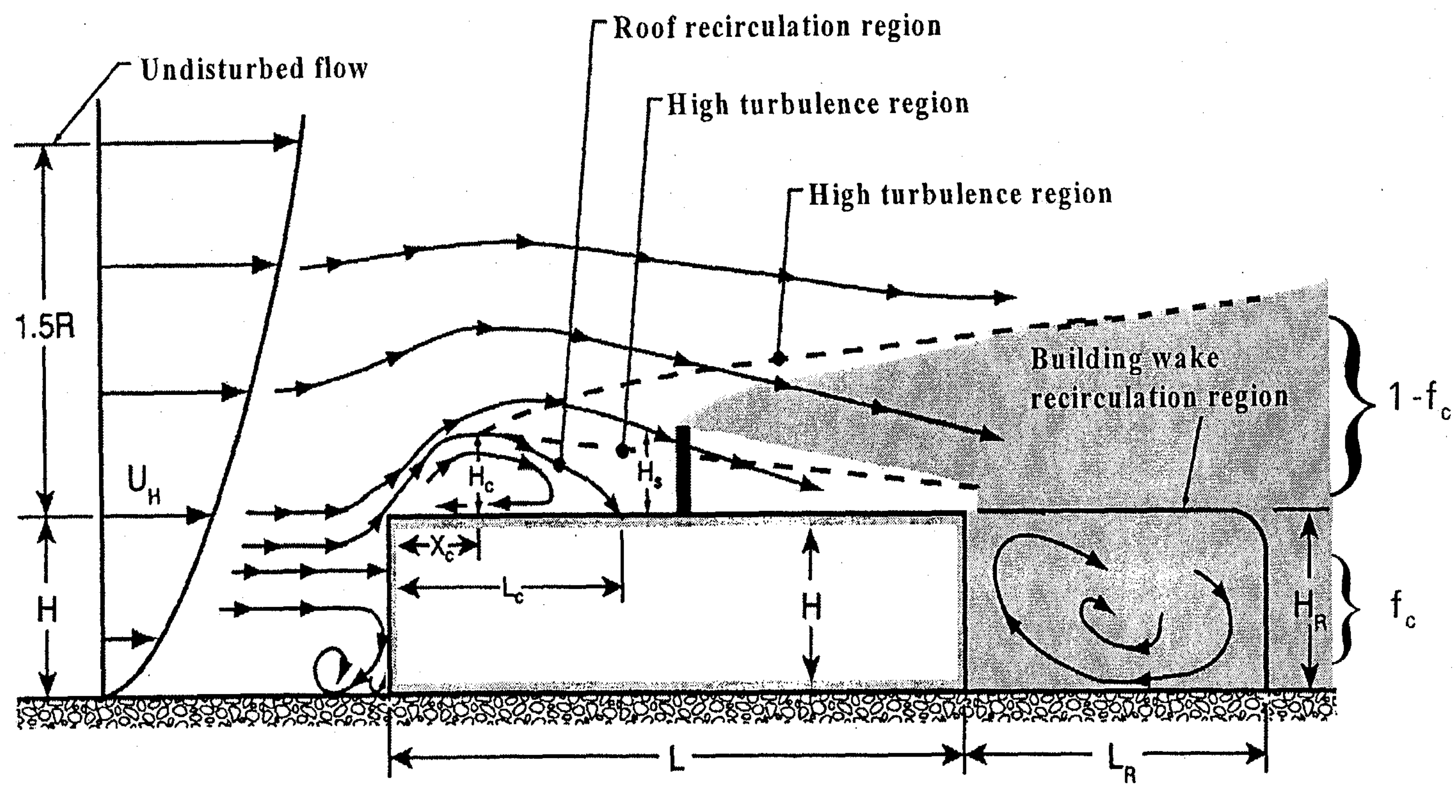

Fig. 1. Flow over a building for a wind normal to the upwind face. ***Source*****: Wilson 1979.**

2. BACKGROUND OF THE ORIGINAL WAKE DISPERSION MODEL

2.1 BACKGROUND OF THE ORIGINAL WAKE DISPERSION MODEL

The HGSYSTEM/UF_6 model suite (Hanna et al. 1996) was developed by DOE from Shell Research Ltd.'s HGSYSTEM Version 3.0 (Post 1994a,b). HGSYSTEM Version 3.0 is approved by the EPA as an alternative regulatory model in Appendix W of 40 *CFR* 51 (1997). HGSYSTEM/UF_6 was originally developed to simulate accidental releases of reactive [specifically, uranium hexafluoride (UF_6)] and non-reactive materials from GDPs located in Portsmouth, Ohio and Paducah, Kentucky. At the time of its development, it was assumed that the primary release scenario of interest would be the rupture of a gas pipeline or liquid tank over open terrain away from the influence of GDP buildings. Further application of the HGSYSTEM/UF_6 model suite revealed the need to consider the additional scenario of an accidental release within a GDP process or transfer building. For this case, the turbulent flow patterns and recirculation cavities created by the building can have a significant effect on buoyant plume lift-off and downwind transport of material released from the building. The original HGSYSTEM/UF_6 model suite contained only simple methods for estimating concentrations due to low-momentum releases of passive gases from buildings (Wilson and Britter 1982). As a result, the WAKE dispersion model (Hanna and Chang 1997) was created for use in estimating downwind concentrations due to elevated releases from buildings of non-reactive plumes which are either buoyant or neutrally buoyant.

To simulate releases from buildings, the WAKE model follows procedures recommended by ASHRAE (1993), Schulman and Scire (1993), and Wilson (1995) in that the model splits the plume into two components: (1) the fraction, f_c, that is initially captured in the lee-side recirculation cavity and then transmitted into the far wake region and (2) the remaining fraction, $1-f_c$, which rises through the turbulent wake directly above the building and is subject to building downwash effects. The total, steady-state, ground-level concentration at downwind receptor locations is given by

$$C_{TOT} = C_c + C_a \quad , \qquad (1)$$

where

C_{TOT} = total ground-level concentration associated with release (mg/m^3),
C_c = ground-level concentration from the component of the plume caught in the recirculation cavity (mg/m^3), and
C_a = ground-level concentration from the component of the plume which rises above the recirculation cavity (mg/m^3).

The fraction of the plume captured in the building recirculation cavity, f_c, is calculated by

$$f_c = 0.5 \left(1 + erf \left(\frac{H_B - h_c}{\sqrt{2}\sigma_Z} \right) \right) , \qquad (2)$$

where

H_B = building height (m),
h_c = plume centerline height (m),
erf = error function, and
σ_Z = vertical standard deviation at the end of the recirculation cavity (m) based on formula from Wilson and Britter (1982).

The WAKE model calculates the plume centerline height, h_c, as the sum of the release height and plume rise, where plume rise is assumed to be the minimum of calculated values for gradual and final rise. Gradual plume rise, Δz, for a given downwind distance is calculated by the formula of Briggs (1984)

$$\Delta z = \left(19 \frac{M_o x}{u_S^2} + 4.2 \frac{F_o x^2}{u_S^3} \right)^{1/3} , \qquad (3)$$

where

M_o = momentum Flux (m^4/s^2),
F_o = buoyant Flux (m^4/s^3),
u_S = wind speed at release height (m/s), and
x = downwind distance from source to receptor (m).

The dimensional forms of the momentum and buoyancy fluxes are given by

$$M_o = \frac{w_o^2 A_s T_a}{\pi T_s} , \qquad (4)$$

where

w_o = plume exit velocity (m/s),
A_s = source cross-sectional area ($m^{2)}$,
T_s = plume exit temperature (K), and
T_a = ambient air temperature (K);

and

$$F_o = \frac{g w_o A_s (T_s - T_a)}{\pi T_s} \quad , \tag{5}$$

where

g = acceleration of gravity (9.8 m/s^2).

Note, the value for w_o in Eqn. 4 is non-zero for vertical, uncapped vents only, while in Eqn. 5, w_o can be non-zero for both vertical and horizontal vents.

The final plume rise, Δz_f, is assumed to be the greater of the final momentum-dominated rise, Δz_{mf}, and final buoyant rise, Δz_{bf}. Final momentum-dominated rise is given by a generalized version of a formula from Briggs (1984)

$$\Delta z_{mf} = 4.8 \frac{M_o^{1/2}}{u_S} \quad . \tag{6}$$

Final buoyant-dominated rise for unstable and neutral atmospheric conditions is calculated according to (EPA 1995)

$$\Delta z_{bf} = 21.4 \frac{\mathrm{s}^{1.25}}{\mathrm{m}} \frac{F_o^{0.75}}{u_S} \tag{7}$$

while for stable conditions, final buoyant-dominated rise is given by (Briggs 1984)

$$\Delta z_{bf} = 2.6 \left(\frac{F_o}{u_S S} \right)^{1/3} \quad , \tag{8}$$

where

S = ambient stability factor (s^{-2}).

The ambient stability factor, S, is calculated according to the formula

$$S = \frac{g}{T_a} \frac{\partial \theta}{\partial z} \quad , \tag{9}$$

where

$\partial\theta/\partial z$ = temperature gradient assumed equal to 0.02 and 0.035 K/m for stability classes E and F, respectively (EPA 1995).

Here, the vertical standard deviation, σ_Z, is calculated according to the formula proposed by Wilson and Britter (1982) for nonbuoyant plumes from roof vents

$$\sigma_Z = 0.21 \ R^{0.25} \ (x_B + L_R)^{0.75} \quad , \qquad \textbf{(10)}$$

where

R = building scaling length (m),
x_B = downwind distance from source to building edge (m), and
L_R = length of the recirculation cavity (m).

The building scaling length, R, is given by

$$R = H_B^{2/3} \ W_B^{1/3} \quad , \qquad \textbf{(11)}$$

where

W_B = building width (m).

Note, for $W_B/H_B > 8$, W_B is set equal to $8H_B$ in the above equation. The recirculation cavity length, L_R, is determined according to Schulman and Scire (1993) by

$$L_R = \frac{1.3 \ W_B}{(1 + 0.25(W_B/H_B))} \quad , \qquad \textbf{(12)}$$

The downwind concentration, C_c, is calculated by the WAKE model as the greater value determined from the following two equations. The first, Eqn. (13), was derived from recent wind tunnel data by Wilson (1995), and is used to determine steady-state, ground-level concentrations in the recirculation cavity up to the point at which the plume has become well-mixed (near field) inside the cavity.

$$C_c = \frac{f_c Q}{V_0\left(1 + 13\left(\frac{T_a}{T_s}\right)^{1/2} \frac{w_0}{u_H}\right) + \frac{u_H \ x_s^2}{16}} \quad , \qquad \textbf{(13)}$$

where

Q = mass flux rate of material released at the release point (kg/s),
V_0 = initial volumetric flux rate from source (m^3/s),
w_0 = initial plume speed (m/s),
u_H = Wind speed at top of building (m/s), and
x_s = "stretched-string" distance from source to receptor (m).

The second, Eqn. (14), is a formula suggested by Briggs (1995; 1996) for warm plumes emitted uniformly from a building face, based on wind tunnel data from Hall and Waters (1986) and Hall et al. (1995). This is the equation the WAKE model uses to calculate ground-level concentrations after the plume has become well-mixed (far field).

$$C_c = \frac{f_c Q \exp(-6F_{**}^{0.4})}{u_H R^2 \left(0.037 + 0.03\left(\frac{x}{H_B}\right)^2 + F_{**}^2\left(\frac{x}{H_B}\right)^4 + \left(\pi\frac{\sigma_Y \sigma_Z}{R^2}\right)^3\right)^{1/3}} , \tag{14}$$

where

R = building scaling length (m),
H_B = building height (m),
σ_y = Gaussian horizontal dispersion parameter (m) based on Briggs' equations in Hanna, et al. (1982),
σ_z = Gaussian vertical dispersion parameter (m) based on Briggs' equations in Hanna, et al. (1982), and
F_{**} = non-dimensional buoyancy flux;

with

$$F_{**} = \frac{f_c F_o}{u_H^3 \, W_B} , \tag{15}$$

where

W_B = building width (m).

Eqn. (14) accounts for plume dilution: (1) across the building face and recirculation cavity, (2) due to expansion of the wake in the horizontal direction with downwind distance, (3) due to growth of the wake in the vertical direction caused by buoyancy, and (4) due to dispersion of the plume from ambient turbulence not related to the presence of the building where Gaussian plume methodology is applicable (i.e., once the plume has migrated out of the building wake). Note the term, $\exp(-6F_{**}^{0.4})$, which appears in Eqn. (14), represents buoyant lift-off (i.e., the lift-off correction factor).

The steady-state, ground-level concentrations at downwind locations associated with the fraction of the plume which rises through the turbulent wake, C_a, are calculated using a modified version of the ISC3 dispersion model (EPA 1995) using the standard Gaussian plume equation

$$C_a^* = \frac{Q_a}{2\pi\sigma_Y\sigma_Z u_S}\exp\left[-\frac{y^2}{2\sigma_Y^2}\right]\left(\exp\left[-\frac{(H_E-z)^2}{2\sigma_Z^2}\right] + \exp\left[-\frac{(H_E+z)^2}{2\sigma_Z^2}\right]\right) , \tag{16}$$

where

Q_a = source strength (kg/s),
H_E = effective plume height (m),
u_s = wind speed at stack height (m/s),
y = receptor cross-wind distance from plume centerline (m), and
z = receptor elevation (m).

Here, the magnitude of the source term, Q_a, for this part of the plume is given by $(1-f_c)Q$. ISC3 incorporates the downwash algorithms of Schulman and Scire (1980) which are preferred by EPA for refined regulatory dispersion modeling of buoyant point source emissions affected by building wakes (40 *CFR* 51, App. W). Note, the ISC3 code does not calculate concentrations at downwind locations inside the building wake (i.e., for $x < 3H_B$). Therefore, the version of ISC3 used in the WAKE model was modified so that ground level concentrations for $x < 3H_B$ are set equal to the ground-level concentration at $x = 3H_B$. Concentrations predicted by ISC3 are based on empirical relationships which assume a steady-state or constant duration release (i.e., 600 s or more). To account for the effects of plume meander for release durations other than 600 s, the concentrations predicted by the ISC3 module of the original WAKE model, C_a^*, were corrected using the following expression recommended by Hanna, et al (1996)

$$C_a = C_a^* \, (600\,\mathrm{s} \; / \; T_a)^{0.2} \quad , \qquad \textbf{(17)}$$

where

T_a = averaging time other than 600 s (s).

In the original WAKE dispersion model (Hanna and Chang 1997), a separate, post-processing utility, POSTWAKE, was used to sum the concentrations predicted by the WAKE and ISC3 modules (C_c and C_a, respectively) in order to determine the total concentration C_{TOT} and toxic load at downwind receptors, where the toxic load at a downwind distance, x, is given by the formula

$$TL(x) = \int_{T_{EXP}} C_{TOT}^{n}(x,t)\, dt \quad , \qquad \textbf{(18)}$$

where

$\int_{T_{EXP}}$ = integral over exposure period of length T_{EXP} s, and

n = species-specific exponent determined by toxicologists (McGuire 1991).

In addition, POSTWAKE can be used to estimate downwind concentrations associated with finite duration releases. This is accomplished by first determining the exposure duration, i.e., the total amount of time, T_{EXP}, required for the plume to pass over the receptor. In theory, T_{EXP} differs from T_{DUR} due to the fact that, as the plume travels downwind, the effects of dispersion cause the plume to elongate or spread in the downwind direction. The natural exposure time limit, T_{EXP}, is calculated based on downwind distance, mean convective velocity, and release duration according to the following equation

$$T_{EXP} = T_{DUR} + m\frac{\sigma_X}{u_C} \quad , \qquad (19)$$

where

T_{DUR} = release duration (s),
m = integer characterizing the amount of leading and trailing edge of the concentration vs time profile included (usually set equal to 4),
σ_X = along-wind dispersion parameter (m) (Ermak 1986; Blewitt et al. 1987), and
u_C = mean convective velocity (m/s) (Ermak 1986; Blewitt et al. 1987).

Due to the effects of plume rise, the velocity of the plume varies as a function of downwind travel distance. The average or mean convective velocity, u_c, of by the plume during its travel from source to receptor is defined as the downwind distance to the receptor divided by the time required for the plume to reach the receptor location. Note that in some cases, the maximum value for T_{EXP} may be limited by a maximum exposure time, T_{EXPMAX}, imposed for the accident scenario. Using the value for T_{EXP}, POSTWAKE then calculates downwind concentration as function of time as the product of the steady-state concentration value, C_{TOT}, and the correction factor, ϕ, (Bloom et al. 1989). For $t < T_{DUR}$, ϕ is given by

$$\Phi = erf\left(\frac{x + u_C t}{\sqrt{2}\sigma_X}\right) + erf\left(\frac{-x + u_C t}{\sqrt{2}\sigma_X}\right) \quad , \qquad (20)$$

and, for $t > T_{DUR}$,

$$\Phi = erf\left(\frac{x + u_C t}{\sqrt{2}\sigma_X}\right) - erf\left(\frac{x + u_C (t - T_{DUR})}{\sqrt{2}\sigma_X}\right) + erf\left(\frac{-x + u_C t}{\sqrt{2}\sigma_X}\right) - erf\left(\frac{-x + u_C (t - T_{DUR})}{\sqrt{2}\sigma_X}\right) \quad . \qquad (21)$$

Finally, average concentration values, as well as toxic loads are calculated for the finite duration release by numerically integrating these time-dependent concentrations over the entire exposure period of length T_{EXP}.

2.2 EXECUTION OF THE ORIGINAL WAKE DISPERSION MODEL

Actual application of the original WAKE model requires multiple steps. The first is the creation of an input file (extension "WKI") which contains data describing the source facility, (building dimensions, stack height, etc.), source release characteristics (emission rate, exit velocity, temperature, etc.), ambient meteorological conditions (wind speed, temperature, stability class, etc.), and receptor locations. The WAKE executable file reads the information contained in this file and generates four separate output files: (1) a report file (extension "WKR") which summarizes run results, (2) an output file (extension "WKO") which contains concentrations predicted by the WAKE model for the portion of the plume captured in the building recirculation cavity, and two files used as input to ISC3 containing (3) information describing the facility and release characteristics for the portion of the plume which rises above the recirculation cavity (extension "ISC"), and (4) data which describe meteorological conditions (extension "MET").

Next, the ISC3 executable file is run using the "ISC" and "MET" files. This results in the creation of an output file (extension "ISO") which contains (in addition to a large volume of intermediate results) concentrations at downwind receptor locations associated with the fraction of the plume which rises above the recirculation cavity. Finally, results contained in the "WKO" and "ISO" files are merged by running POSTWAKE. Output from POSTWAKE consists of (1) a main output file (extension "OUT") containing peak, averaged ground-level concentrations and toxic loads at downwind receptor locations corresponding to an exposure time, T_{EXP}, and (2) a supplemental output file (extension "OUX") which lists additional values calculated during the modeling process including along-wind dispersion coefficients, and plume mean convective wind speed and steady-state, ground-level concentrations at receptor locations.

3. REFINEMENTS TO THE WAKE DISPERSION MODEL

Since its initial development during the fall and winter of 1995-1996, the WAKE dispersion model has been used to estimate consequences associated with potential, accidental releases from multiple DOE facilities (PORTS 1997; PGDP 1997; Lombardi 1998; Lombardi and Gant 1998). During this period, a number of refinements have been made to the model which have (1) added additional capability and versatility to the model, (2) resulted in more accurate estimates of concentrations and doses seen by individuals at designated receptor locations, and (3) made execution of the WAKE model more user-friendly. The following sections provide a detailed description of these refinements.

3.1 ADDITIONAL MODEL CAPABILITIES

Recent application of the WAKE dispersion model in the SAR process for DOE facilities (PORTS 1997; PGDP 1997; Lombardi 1998; Lombardi and Gant 1998) has resulted in the inclusion of additional capabilities which were not present in the original version of the model. These include a method for approximating the effects of complex terrain on predicted concentrations, as well as the ability to simulate a time-variant or transient release. The modifications are described in the following sections.

3.1.1 Treatment of Atmospheric Dispersion in Areas of Complex Terrain

Recent analyses have identified a need for the ability to evaluate atmospheric dispersion associated with the release of toxic material in hilly environments. Previously this has been accomplished via the use of an additional postprocessor utility, PSTWAKE (Bloom 1997). PSTWAKE is a modified version of the POSTWAKE utility developed by Hanna and Chang (1997) which uses algorithms based on those developed by Briggs (Hanna et al. 1982) for estimating the effects of complex terrain on plume dispersion. Under unstable and neutral atmospheric conditions (Stability Classes A-D), the plume centerline associated with the fraction of the plume which rises above the building recirculation cavity is assumed to follow the terrain to some extent. Here, the quantity, H_E - z, used by ISC3 in the Gaussian dispersion equation (see Eqn. 16), has been constrained such that it is equal to or greater than half the effective plume height, H_E. For stable atmospheric conditions (Stability Classes E and F), the plume height of the fraction of the plume which rises above the recirculation cavity is assumed to remain constant; hence, the possibility exists for the plume to impinge on terrain. The effects of complex terrain on the fraction of the plume captured in the building recirculation cavity are modeled by not allowing the plume to lift-off [i.e., the lift-off correction factor (see Eqn. 14) is set equal to 1.0]. As with its predecessor, POSTWAKE, PSTWAKE is also used to combine results from the WAKE and ISC3 models. Note, for cases in which terrain elevations are zero, the results calculated by the PSTWAKE utility reduce to those calculated by POSTWAKE.

The PSTWAKE utility has recently been modified by W. D. Goode and S. G. Bloom (Lombardi 1998). These modifications include (1) the use of a separate, optional input file for specifying terrain elevations (extension "GRD"), (2) continued application of the lift-off correction factor for cases in which the terrain is flat, (3) creation of a new output file, (extension "ISX") echoing parameters obtained from the "ISO" file for each receptor point, and (4) the printing of the fraction of the plume caught in the recirculation cavity and the maximum plume height to the "OUT" file. PSTWAKE has also been modified to include the algorithms found in POSTWAKE for calculating concentrations for finite duration releases.

3.1.2 Treatment of Transient Releases

The original WAKE model was somewhat limited in applicability in that it was only capable of simulating sources whose material release rates were constant. In order to remove this limitation, two additional post-processing utilities, COMBINE and PPSTWAKE, were developed as a means for estimating downwind concentrations associated with transient releases of material into building wake regions. These are based on the assumption that a time-variant release can be simulated by superimposing results generated for a series of separate, steady-state release periods of constant duration. Previously, this process involved multiple runs of the WAKE, ISC3, and PSTWAKE utilities in order to generate the "OUX" files containing the concentrations, $C_{(tot,i)}$, associated with each release period. The first of these utilities, COMBINE (Lombardi and Goode 1997), reads the concentrations contained in each of the "OUX" files and reformats the information in a form suitable for use by PPSTWAKE (to a file with extension "PRN"). The names of up to six "OUX" files containing the concentrations calculated for each release period by PSTWAKE are specified via a separate input file ("COMBINE.IN").

PPSTWAKE is then used to numerically integrate the contributions for each of these release periods. This is accomplished by first dividing the exposure period, T_{EXP}, into a set of finite intervals (normally 2000-4000). For each of these intervals, PPSTWAKE then applies the algorithms of Bloom et al. (1989) to calculate the contribution from each release period to the total downwind concentration. These are then summed to obtain the total downwind concentration for the current time interval. Finally, the total downwind concentrations for each interval are integrated to obtain peak, average concentration and toxic load values at receptor locations associated with transient releases. PPSTWAKE reads input information from the "PRN" file created by COMBINE and writes results to a separate output file (extension "OUT").

3.2 REFINEMENTS TO MODEL ALGORITHMS

The following sections describe refinements that have been made to algorithms found in the WAKE dispersion model and its associated post-processing utilities.

3.2.1 Inclusion of a Numerical Iterative Method for Calculating Plume Rise at Receptor Locations

In the original version of ISC3 used by the WAKE dispersion model, plume rise was calculated based on the wind speed at the height of the release. However, the plume rise data used to develop the plume rise equations found in ISC3 were correlated using (1) the wind speed measured at a height halfway between the release height and the plume centerline and, in some instances, (2) the mean wind speed seen by the plume during travel to its final height (Briggs 1997). This suggests that use of the wind speed at half the plume height would be more appropriate than wind speed at release height for determining final plume rise. This assumption was confirmed by additional guidance (Hanna 1994), stating that ground-level concentrations would be better simulated using a wind speed at half the plume height for stacks shorter than those of tall power plants.

For buoyant plumes, the wind speed at half the final plume height is usually greater than the wind speed at the release height, resulting in greater dilution of the plume as it travels downwind. However, use of a higher wind speed in calculating plume rise also results in a lower final plume height. In general, the increase in ground-level concentration due to the lower plume heights associated with a higher wind speed more than offsets the dilution of the plume associated with the higher windspeed. Hence, use of the wind speed at the release height, for buoyant plumes, normally results in non-conservative estimates of ground-level concentrations.

To compensate for this lack of conservatism, the ISC3 model used in WAKE has been revised to calculate plume rise based on wind speed at half the plume height. This is accomplished via a Newton-iterative process which has been added to the PCALC and PHEFF subroutines of ISC3 (Lombardi 1998; Lombardi and Gant 1998). Similar iterative methods have been applied to calculate plume rise and wind speed in other recently developed dispersion models, for example, the Hybrid Plume Dispersion Model developed by Hanna and Chang (1993). Note, the calculated wind speed at half the plume height is also used as input to the dispersion equation (Eqn. 16) where ground-level concentrations are calculated.

3.2.2 Refinements to Method for Treatment of Transient Releases

As described in Sect. 3.1.2, concentrations and doses associated with transient releases are calculated by the post-processing utility, PPSTWAKE by integrating the concentrations estimated for each release period over a calculated exposure time, T_{EXP}, at each downwind location. Originally in was assumed that the plume associated with the first release period was the first to reach a given, downwind receptor, and, that the plume associated with the last release period was the last to pass the receptor. While this may be true in most instances, in theory, because of plume "spreading" due to the effects of downwind dispersion, the possibility exists (especially in cases where a short duration release is followed by a release of a much longer duration) for the leading edge of the plume associated with a later release period to reach the receptor location first. In addition, when concentrations obtained for the case of a steady-state release of duration T_{DUR} were compared to those obtained for an identical transient release consisting of six release periods of duration $T_{DUR}/6$, the WAKE model produced different results. These differences were later found to be linked to the method in which the exposure time was calculated in the PPSTWAKE utility. Therefore, for transient releases, modifications were made so that the exposure time, T_{EXP}, is now calculated as the difference between (1) the shortest time required for the leading edge of the plume (associated with any release period) to reach a receptor and (2) the longest time required for the trailing edge of the plume (associated with any release period) to pass the receptor.

Additional refinements were made to the method in which average concentrations and toxic loads were determined for the case in which the calculated exposure time, T_{EXP}, is greater than a user-specified value, T_{EXPMAX}. In these instances, when integrating over the entire exposure duration, T_{EXP}, use of the time period of length T_{EXPMAX} which produces the largest "average" concentration and toxic load values is desired. Previously, this time period was calculated by first determining the individual release period which resulted in the highest steady-state concentration at the receptor and the corresponding time, T_0, at which the center of this plume reached the receptor. Average concentrations and toxic loads were then found by integrating over a period of length, T_{EXPMAX}, centered about time, T_0. Improvements made to the code now enable it to scan the entire exposure period, T_{EXP}, to determine the contiguous time period of length T_{EXPMAX} which results in the highest "average"concentration and toxic loads at the receptor.

Due to the nature of the Gaussian formulation used by ISC3 for the portion of the plume which rises above the building recirculation cavity, contaminants are instantaneously transported downwind as soon as a release occurs. Hence, the possibility exists for a release period to contribute to downwind receptor concentrations before the release period actually begins. In the original WAKE model this could result in overly conservative concentration and toxic load estimates. Therefore, additional logic has been added to the integration process described above which prevents contributions from a release period at a downwind location for times less than the time at which the release period begins.

3.2.3 Additional Refinements to WAKE Model Algorithms

Previously, the concentrations input into PSTWAKE and PPSTWAKE to calculate peak, averaged concentrations and toxic loads for release durations other than 600 s had the power-law correction (Eqn. 17) applied to steady-state concentrations calculated by ISC3 (i.e., the fraction associated with the portion of the plume that rises above the building recirculation cavity). In order to make these inputs more consistent with the formulation of the work of Witlox et al. (1990), this correction is no longer applied.

Recent studies by Lines et al. (1997), found that standard, steady-state dispersion models such as the WAKE dispersion model can be used to calculate concentrations under stable atmospheric conditions for wind speeds greater than or equal to 1 mile per hour (mph). This differs from previous EPA guidance which suggests that the minimum wind speed should be greater than or equal to 2 mph. Based on this new guidance, subroutines in the WAKE and ISC3 modules have been revised to allow wind speeds of 1 mph or greater for stable atmospheric conditions.

The following additional assumptions/revisions have been made: (1) for releases below the height of the building, it is now assumed that the plume is entirely caught in the building wake and that the stack is "capped" and (2) based on guidance found in Hanna et al. (1996), the maximum instantaneous concentration (corresponding to an exposure time of 18.75 s) is calculated by multiplying the steady-state concentration (i.e., that based on a 600-s exposure time) by a factor of 2.0.

3.3 MODIFICATIONS TO STREAMLINE CODE EXECUTION

Perhaps the most apparent change to a user of the WAKE model has been the creation of a single executable file that is used to perform all necessary calculations. As seen in Sects. 2.2, 3.1.1, and 3.1.2, application of the WAKE model (which includes the WAKE, ISC3, POSTWAKE, PSTWAKE, COMBINE and PPSTWAKE utilities) can be a rather cumbersome process as the user is faced with the task of having to manage multiple input, output and executable files. Therefore, as a means of making execution of the WAKE model more "user-friendly" and accurate due to the fact that there is no longer a need to pass data between separate executable files, a single, "WAKE," executable file has been developed which performs all calculations previously made by the WAKE, ISC3, POSTWAKE, PSTWAKE, COMBINE, and PPSTWAKE executable files.

In creating a single WAKE executable file, the number of input files required by the user has been reduced to two: (1) a main input file similar in form to the original WAKE executable input file and (2) the optional "GRD" file specifying receptor elevations (see Sect. 3.1.1). In addition, many of the intermediate output files formerly created by each of the ISC3, POSTWAKE, etc. utilities have been retained for user reference. A list of all files (input and output) associated with the WAKE model is given in Appendix B.

4. VERIFICATION AND VALIDATION OF THE REVISED WAKE MODEL

The accuracy of predictions made by atmospheric dispersion models such as WAKE can be evaluated via two processes: (1) verification (comparison to solutions obtained analytically or from other models) and (2) validation (comparison to actual measured field data). The former, a relatively simple task to perform, only evaluates how well the model performs in theory; while the latter, an expensive, time-consuming and often difficult process, actually measures the model's performance under a known set of atmospheric and release conditions. Studies were conducted in which both methods were employed to assess the performance of the revised WAKE model. The results from these studies are discussed in the following sections.

4.1 VERIFICATION OF THE REVISED WAKE MODEL RESULTS

Two separate analyses were performed in order to verify the accuracy of WAKE model calculations. The first task was to verify values predicted by the WAKE code for important parameters as well as final concentration and toxic load values via comparison to hand calculations. The second involved the comparison of results obtained using the modified WAKE model to results previously obtained using the original WAKE model and the MACCS2 model (Lombardi and Brock 1998).

4.1.1 Verification of Revised WAKE Model Predictions vs Analytical Solutions

Verification of results calculated using the revised WAKE model to analytical solutions obtained via hand calculations is necessary in order to ensure the accuracy of algorithms used by the revised WAKE model for estimating downwind concentrations and toxic loadings (as well as the intermediate parameters used to determine these values). The "final" results generated by the WAKE model are the result of a detailed series of calculations involving estimation of plume capture, building wake effects, standard Gaussian dispersion parameters as well as adjustments for the effects of complex terrain and finite release duration. Hence, the logical approach was to break down the verification procedures into a series of steps designed to test calculations performed by each component or module of the WAKE model (WAKE, ISC3, PSTWAKE, and PPSTWAKE) separately. This was accomplished via analysis of a set of hypothetical release scenarios which were designed to represent a realistic range of release and meteorological conditions. Note, the calculated values for intermediate parameters associated with the work of Witlox et al. (1990) are assumed to have been verified previously.

4.1.1.1 Verification of WAKE module results

The first of these scenarios was designed to test the performance of the WAKE module in calculating values associated with the fraction of the plume trapped in the recirculation cavity, f_c, for a steady-state release from a single source. The input parameters associated with this scenario are presented in Table 1. Values for various intermediate parameters calculated for cases in which the surrounding terrain is assumed to be both flat and complex, are presented in Table 2. Table 3 presents the final downwind concentration associated with the fraction of the plume caught in the recirculation cavity for selected downwind distances and elevations. In all cases, values calculated by the WAKE module are in agreement with those obtained analytically.

4.1.1.2 Verification of ISC3 module results

With the exception of those related to the modifications described previously in Sects. 2.1, 3.1.1, and 3.2.1, all calculations performed by the ISC3 module for concentrations, as well as intermediate parameters, associated with the fraction of the plume which rises above the building recirculation cavity, are assumed to have been verified previously by the code authors (EPA 1995). Therefore only verification of the performance of the algorithms recently incorporated into to the ISC3 module was necessary, the most significant being the iterative scheme used to calculated plume rise based the wind speed at plume half height detailed in Sect. 3.2.1. The plume rise algorithms used by ISC3, incorporate estimates for stack downwash (Schulman and Scire 1980), which is determined numerically, via a numerical solution to a polynomial equation. This procedure, coupled with the iterative method described in Sect. 3.2.1, makes verification of model results by hand calculations an extremely tedious and involved process. Hence, an alternate method for verifying the iterative scheme was devised in which the WAKE model was first allowed to calculate the final plume height and corresponding wind speed (at the plume half height). Using the values for final plume rise and the associated wind speed at half the final plume height obtained from this calculation to define the wind speed measurement height and the measured wind speed itself, a second run was made with the assumption that if the iterative scheme is functioning properly, the values calculated for plume rise and wind speed at downwind locations from this run should match those from the previous model run. Initial input for this case, Scenario 1a, was based on a modified version of that used in Scenario 1b (defined in Table 1) in which the release velocity and temperature were increased to 10.0 m/s and 800K, respectively in order to exaggerate the effects of plume rise. The results from this analysis for several downwind locations, given in Table 4, show that the iterative scheme used to wind speed functions as expected.

As discussed in Sects. 3.2.1 and 2.1, additional modifications made to the ISC3 modules include a revised method for handling complex terrain and the assumption that concentrations within a distance, L_R, downwind of the building, are equal to the concentration at the end of the cavity. Verification of the method in which complex terrain calculations are handled can be made by comparing steady-state concentrations calculated by the ISC3 module for a known set of conditions to those obtained analytically using Eqn. 16. Using values for effective plume height, wind speed at plume half-height, σ_Y, σ_Z, etc., calculated for Scenarios 1a and 1b (see Table 1), concentrations at various downwind distances and elevations were evaluated. The results, presented in Table 5, verify that the methods described in Sect. 3.1.1 for

Table 1. Input parameters associated with hypothetical release Scenario 1

Parameter	Value	
Effective building width (m)	110.0	
Distance from source to building edge (m)	20.0	
Release height (m)	20.0	
Ambient temperature (K)	283.0	
Source release rate (kg/s)	1.0	
Release duration (s)	Infinite	
Release temperature (K)	300.0	
Plume exit velocity (m/s)	1.0	
Vent diameter (m)	2.0	
Measurement height of wind speed (m)	10.0	
	Scenario 1a value	Scenario 1b value
Ambient wind speed at 10 m (m/s)	4.0	1.0
Atmospheric stability class	D (neutral)	F (stable)

Table 2. Calculated values for the fraction of the plume caught in recirculation cavity: simple terrain

	Scenario 1a		Scenario 1b	
Parameter	WAKE value	Analytically verified value	WAKE value	Analytically verified value
Building scaling length R, (m)	35.30	35.30	35.30	35.30
Recirculation cavity length L_R, (m)	59.96	59.96	59.96	59.96
Wind speed at release height u_H, (m/s)	4.438	4.438	1.464	1.464
σ_Z (m^2)	13.69	13.69	13.69	13.69
Plume buoyancy flux F_o, (m^4/s^2)	0.5553	0.5553	0.5553	0.5553
Dimensionless buoyancy flux F_{**}	2.370×10^{-5}	2.370×10^{-5}	1.604×10^{-4}	1.605×10^{-4}
Plume momentum flux M_o, (m^4/s^2)	0.9433	0.9433	0.9433	0.9433

Table 2 (continued)

Parameter	Scenario 1a		Scenario 1b	
	WAKE value	Analytically verified value	WAKE value	Analytically verified value
Gradual plume rise Δz, (m)	6.243	6.242	17.57	17.56
Final buoyant plume rise Δz_{bf}, (m)	3.102	3.102	17.65	17.65
Final momentum plume rise Δz_{mf}, (m)	1.050	1.050	3.184	3.184
Fraction of plume caught in recirculation cavity, f_c	0.4104	0.4104	0.09968	0.09976
Lift-off correction factor, $\exp(-6F_{**})^{0.4}$ (flat terrain)	0.9188	0.9188	0.8336	0.8335
Lift-off correction factor, $\exp(-6F_{**})^{0.4}$ (complex terrain)	1.0000	1.0000	1.0000	1.0000
Near field concentration at 10 m Downwind, elevation = 0.0 ft (mg/m^3)	1.012×10^3	1.012×10^3	5.570×10^2	5.573×10^2
Near field concentration at 10 m Downwind, elevation = 20.0 ft (mg/m^3)	1.101×10^3	1.101×10^3	6.681×10^2	6.686×10^2
Far field concentration at 10 m Downwind, elevation = 0.0 ft (mg/m^3)	1.447×10^2	1.447×10^2	9.668×10^1	9.674×10^1
Far field concentration at 10 m Downwind, elevation = 20.0 ft (mg/m^3)	1.575×10^2	1.575×10^2	1.160×10^2	1.161×10^2
Near field concentration at 200 m Downwind, elevation = 0.0 ft (mg/m^3)	2.783×10^1	2.783×10^1	1.848×10^1	1.850×10^1
Near field concentration at 200 m Downwind, elevation = 50.0 ft (mg/m^3)	3.029×10^1	3.029×10^1	2.217×10^1	2.220×10^1
Far field concentration at 200 m Downwind, elevation = 0.0 ft (mg/m^3)	4.370×10^1	4.371×10^1	2.953×10^1	2.955×10^1
Far field concentration 200 m Downwind, elevation = 50.0 ft (mg/m^3)	4.757×10^1	4.757×10^1	3.543×10^1	3.545×10^1

Table 3. Calculated concentrations, C_c for the fraction of the plume caught in the recirculation cavity at selected downwind receptor locations

Downwind distance from building edge to receptor (m)	Receptor elevation (ft)	Scenario 1a		Scenario 1b	
		Calculated concentration (mg/m^3)		Calculated concentration (mg/m^3)	
		WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	0.0	1.012×10^3	1.012×10^3	5.570×10^2	5.573×10^2
10.0	20.0	1.101×10^3	1.101×10^3	6.681×10^2	6.686×10^2
200.0	0.0	4.370×10^1	4.371×10^1	2.953×10^1	2.955×10^1
200.0	50.0	4.757×10^1	4.757×10^1	3.543×10^1	3.545×10^1

Table 4. Calculated values for plume height and wind speed associated with the fraction of the plume which rises above the recirculation cavity

Downwind distance from building edge to receptor (m)	Scenario 2a plume height (m)	Scenario 2a wind speed at half plume height (m/s)	Scenario 2b plume height (m)	Scenario 2b wind speed at half plume height (m/s)
1.0	37.804	1.4641	37.803	1.4641
20.0	44.122	1.5452	44.121	1.5453
60.0	65.500	1.9203	65.499	1.9203
100.0	77.462	2.1059	77.461	2.1059
200.0	77.789	2.1108	77.789	2.1108
500.0	77.789	2.1108	77.789	2.1108

Table 5. Effects of complex terrain on calculated concentrations associated with the fraction of the plume which rises above the recirculation cavity

Downwind distance from building edge to receptor (m)	Receptor elevation (ft)	Scenario 1a concentration, C_a (mg/m^3)		Scenario 1b concentration, C_a (mg/m^3)	
		WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	20.0	2.196×10^2	2.196×10^2	9.159×10^2	9.159×10^2
200.0	50.0	8.709×10^1	8.709×10^1	4.687×10^2	4.687×10^2

handling complex terrain perform properly. Similarly, verification of concentration estimates at downwind distances less than L_R, can be made by examining the concentrations calculated by ISC3 at various downwind distances. Table 6 lists concentrations calculated by the ISC3 module (again based on input parameters for Scenarios 1a and 1b). These results confirm the steady-state concentrations calculated by the model, at distances less than or equal to L_R, are equal to the calculated concentration at a distance L_R downwind of the building.

4.1.1.3 Verification of combined, steady-state results

After the accuracy of values calculated by both the WAKE and ISC3 modules had been verified, the next step in verifying the accuracy of steady-state values predicted by the WAKE model was to confirm that values calculated for the total concentration, C_{TOT}, and toxic load, TL(x), at downwind receptor locations are accurate. Table 7 lists values for C_{TOT}, as defined in Eqn. 1, at downwind receptor locations corresponding to Scenarios 1a and 1b. In addition, selected toxic load values, as defined by Eqn. 18, corresponding to these concentrations and a steady-state exposure time, T_{EXP}, of 600 s are presented in Table 8.

Table 6. Steady-state concentrations, C_a, associated with the fraction of the plume which rises above the recirculation cavity, where L_R = 59.96 m

Downwind distance from building edge to receptor (m)	Scenario 1a concentration (mg/m^3)	Scenario 1b concentration (mg/m^3)
1.0	1.395×10^2	5.325×10^2
5.0	1.395×10^2	5.325×10^2
10.0	1.395×10^2	5.325×10^2
30.0	1.395×10^2	5.325×10^2
50.0	1.395×10^2	5.325×10^2
60.0	1.395×10^2	5.325×10^2
61.0	1.390×10^2	5.288×10^2
100.0	1.145×10^2	4.611×10^2
200.0	6.736×10^1	3.085×10^2
500.0	2.878×10^1	1.974×10^2
1000.0	1.306×10^1	1.228×10^2

Table 7. Calculated values for steady-state concentration, C_{TOT}, at selected downwind receptor locations

Downwind distance from building edge to receptor (m)	Receptor elevation (ft)	Scenario 1a concentration (mg/m^3)		Scenario 1b concentration (mg/m^3)	
		WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	0.0	1.151×10^3	1.152×10^3	1.089×10^3	1.089×10^3
10.0	20.0	1.321×10^3	1.321×10^3	1.584×10^3	1.585×10^3
200.0	0.0	1.111×10^2	1.111×10^2	3.381×10^2	3.381×10^2
200.0	50.0	1.347×10^2	1.347×10^2	5.041×10^2	5.041×10^2

Table 8. Calculated toxic load values associated with steady-state concentration, C_{TOT}, for selected downwind receptor locations

Downwind distance from building edge to receptor (m)	n	Receptor elevation (ft)	Toxic load: Scenario 1a [$(mg/m^3)^n$-s]		Toxic load: Scenario 1b [$(mg/m^3)^n$-s]	
			WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	1	0.0	6.907×10^5	6.906×10^5	6.535×10^5	6.534×10^5
10.0	2	0.0	7.951×10^8	7.949×10^8	7.117×10^8	7.116×10^8
200.0	1	0.0	6.664×10^4	6.660×10^4	2.029×10^5	2.029×10^5
200.0	2	0.0	7.401×10^6	7.406×10^6	6.859×10^7	6.859×10^7

Having confirmed the accuracy of calculations made by the WAKE code for the case of a single source, it is possible to verify calculations made for a steady-state release from multiple sources. This was accomplished by analyzing a third scenario, defined by the values given in Table 9, in which two sources were considered. Concentrations and toxic load values obtained from this analysis are given in Table 10.

Table 9. Input parameters associated with hypothetical release Scenario 3

Parameter	Source 1 value	Source 2 value
Effective building width (m)	110.0	110.0
Ambient temperature (K)	283.0	283.0
Release duration (s)	Infinite	Infinite
Ambient wind speed at 10m (m/s)	4.0	4.0
Atmospheric stability class	D	D
Measurement height of wind speed (m)	10.0	10.0
Distance from source to building edge (m)	0.0	20.0
Release height (m)	10.0	20.0
Source release rate (kg/s)	2.0	1.0
Release temperature (K)	400.0	300.0
Plume exit velocity (m/s)	5.0	1.0
Vent diameter (m)	1.0	2.0

Table 10. Calculated values at selected downwind receptor locations associated with Scenario 3: multiple source, steady-state release

Downwind distance from building edge to receptor (m)	Concentration, C_{TOT} (mg/m^3)		Toxic load (mg-s/m^3)		Toxic load [(mg/m^3)^2-s]	
	WAKE value	Analytically verified value	WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	5.117×10^4	5.117×10^4	3.070×10^7	3.070×10^7	1.502×10^{12}	1.502×10^{12}
200.0	3.072×10^2	3.072×10^2	1.843×10^5	1.843×10^5	3.048×10^7	3.048×10^7

4.1.1.4 Verification of WAKE model results for finite duration releases

As detailed in Sect. 2.1, the WAKE model can be applied to scenarios involving finite duration releases. The majority of calculations associated with such releases are performed in the POSTWAKE module (formerly the POSTWAKE post-processor). The most important of these is the determination of values for the intermediate parameters: the exposure duration, T_{EXP}, and initial and ending time of exposure, T_1 and T_2. Using the input paramaters associated with Scenario 1a (see Table 1), and substituting a value of 100 s for the release duration, rather than the 600 s associated with that of an infinite-duration release, the following values for these quantities, shown in Table 11, were calculated.

Table 11. Calculated values for parameters associated with a finite duration release of 100 s

Downwind distance from building edge to receptor (m)	T_{EXP} (s)		T_1 (s)		T_2 (s)	
	WAKE value	Analytically verified value	WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	105.9	105.9	8.779	8.779	114.7	114.7
60.0	113.6	113.6	20.32	20.32	133.9	133.9
200.0	120.0	120.0	54.96	54.96	175.0	175.0

In addition to these intermediate results, values for the correction factor, ϕ (Bloom et al. 1989), as well as the concentration and toxic load values calculated by WAKE, associated with this 100-s release, were also verified by comparison to values obtained using MATHCAD (Mathsoft 1997) software. The results of this comparison are presented in Table 12.

4.1.1.5 Verification of WAKE model results for transient releases

The final WAKE model results requiring verification are those associated with transient releases. As explained in Sect. 3.1.2, it is assumed that a time-variant release can be simulated by superimposing results obtained for a series of steady-state releases. Integration of these steady-state results are performed in the PPSTWAKE module (formerly the PPSTWAKE post-processor). The accuracy of this procedure was verified by comparing results obtained for the case of a 100-s release (see Sect. 4.1.1.4) to those obtained using equivalent input parameters to describe building and meteorological conditions, but with the release modeled as four, 25-s duration periods, with emision rates, stack exit velocities, and stack exhaust temperatures of 1.0 kg/s, 1.0 m/s, and 300K, respectively. The results of this analysis, presented in Table 13, show that the results obtained for the steady-state and transient releases are in agreement.

4.1.2 Comparison to Previous Model Studies

A previous study, Lombardi and Brock (1998), compared results obtained using the original WAKE dispersion model to those calculated by the MACCS2 (Chanin and Young 1997) computer code for various release scenarios. For each of these scenarios, Lombardi and Brock (1998) presented two sets of WAKE model results. The first corresponded to the case in which the wind speed at release height (4.0 m/s) was used in plume rise calculations, while the second analysis was conducted using the layer average wind speed (4.9 m/s). To further verify performance of revised code, the revised WAKE model was used to analyze a scenario involving a buoyant, elevated release subject to building effects [Case 3 as defined in Lombardi and Brock (1998)]. Results from this analysis are shown, along with the those of Lombardi and Brock (1998), in Fig. 2.

Table 12. Calculated concentration and toxic load values associated with a finite duration release of 100 s

Downwind distance from building edge to receptor (m)	ϕ		Concentration, C_{TOT} (mg/m^3)		Toxic load (mg-s/m^3)		Toxic load [(mg/m^3)^2-s]	
	WAKE value	Analytically verified value	WAKE value	Analytically verified value	WAKE value	Analytically verified value	WAKE value	Analytically verified value
10.0	0.9440	0.9440	1.087×10^3	1.087×10^3	1.151×10^5	1.151×10^5	1.303×10^8	1.308×10^8
200.0	0.8262	0.8262	9.176×10^1	9.178×10^1	1.101×10^4	1.101×10^4	1.120×10^6	1.120×10^6

Table 13. Comparison of results associated with a steady, 100-s duration release to those obtained for a transient release consisting of four, 25-s duration releases

Downwind distance from building edge to receptor (m)	Concentration, C_{TOT} (mg/m^3)		Toxic load (mg-s/m^3)		Toxic load [(mg/m^3)^2-s]	
	Steady-state release	Transient release	Steady-state release	Transient release	Steady-state release	Transient release
10.0	1.087×10^3	1.087×10^3	1.151×10^5	1.151×10^5	1.303×10^8	1.303×10^8
200.0	9.176×10^1	9.176×10^1	1.101×10^4	1.101×10^4	1.120×10^6	1.120×10^6

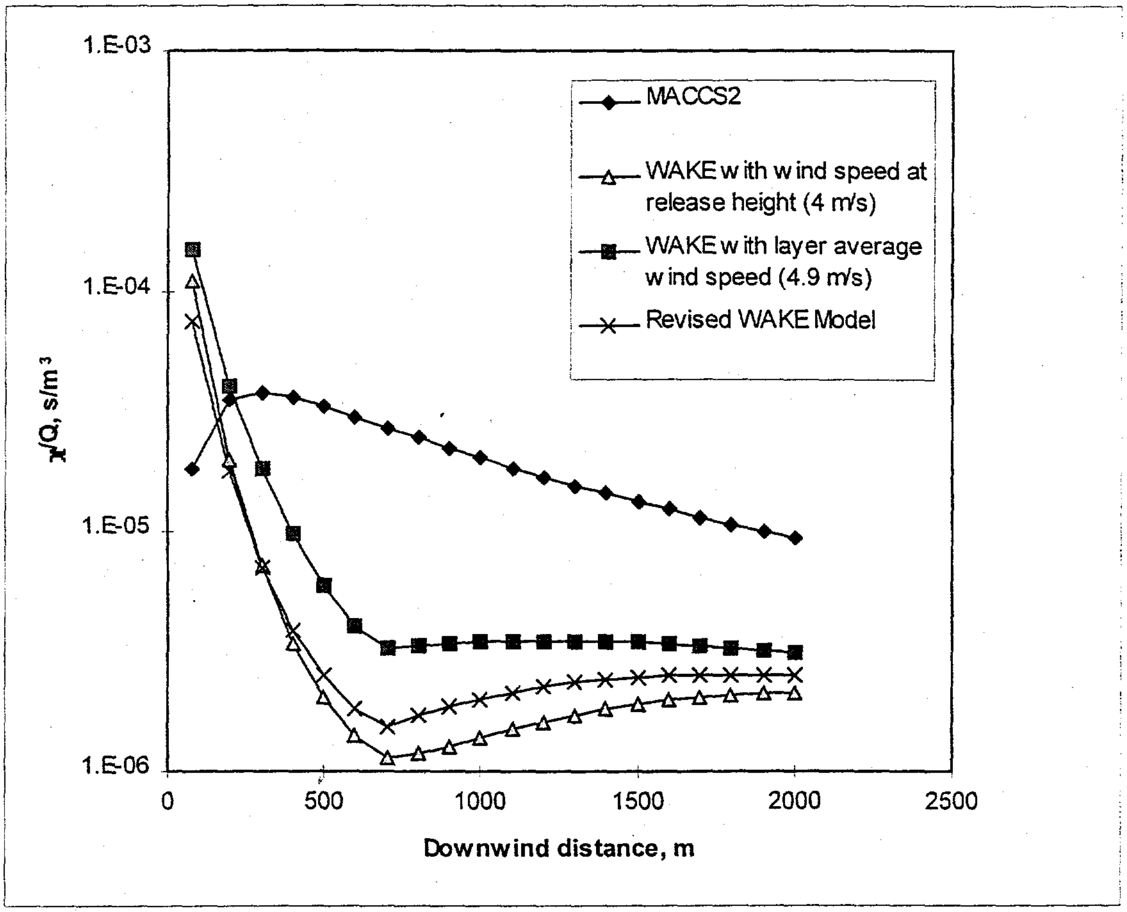

Fig. 2. Comparison of results calculated by the revised WAKE model, MACCS2, and the original WAKE model for a buoyant release with building wake effects.

As explained in Sect. 3.2.1, the amount of buoyant plume rise, and hence the associated ground level concentration, is inversely related to the value for wind speed used in plume rise calculations. Compared to effective plume height values calculated by Lombardi and Brock (1998) based on a uniform wind speed of 4.9 m/s, the final plume rise values calculated by the revised WAKE model, using the iterative scheme discussed in Sect. 3.2.1, were higher for all downwind distances. Therefore, as anticipated, χ/Q values predicted by the revised WAKE model were lower than those estimated by Lombardi and Brock (1998) (based on a wind speed of 4.9 m/s) at all downwind locations. Similarly for distances less than 300 m, effective plume heights calculated by the revised WAKE model were higher than those predicted by Lombardi and Brock (1998) based on a 4.0-m/s wind speed. Here again, χ/Q ratios calculated by Lombardi and Brock (1998) were higher than those determined by the revised WAKE model. However, for distances greater than 300 m downwind, the iterative scheme used in the revised WAKE model resulted in plume heights lower than those predicted by the original WAKE code using a wind speed of 4.0 m/s. Again, as expected, the χ/Q values calculated by Lombardi and Brock (1998) were now less than than those determined by the revised WAKE model.

4.2 VALIDATION OF THE REVISED WAKE MODEL RESULTS

Accurate, meaningful model validation is a difficult, expensive and time consuming procedure. Consequently, as of this writing, no formal validation studies have been conducted in which results predicted by the entire, revised WAKE model have been compared to actual field measurements. However, calculations performed by specific model algorithms have been compared, in previous studies, to actual measured data. Examples include the wind tunnel sensitivity studies conducted by Hall and Waters (1986) on the non-dimensionalized form of concentration values calculated according to Eqn. 14. Additional data by Hall et al. (1995), available in the letter from Briggs (1996), also serve as benchmarks for values calculated by Eqn. 14.

The ISC3 model is recommended by the EPA as a refined dispersion model for use in simple terrain. Consequently, numerous evaluation/validation studies of the model have been performed. These include studies by Cox et al. (1985a, b; 1986; 1987) and Lee (1975).

5. CONCLUSIONS AND RECOMMENDATIONS

The WAKE model was originally developed as a component of the HGSYSTEM/UF_6 Model Suite (Hanna et al. 1996) for use in estimating downwind consequences associated with the releases of UF_6 from GDP process buildings. Since its creation, it has been applied in the SAR process at multiple DOE sites. These applications have identified the need for additional capabilities that were not part of the original WAKE model (Hanna and Chang 1997). Furthermore, over the past two years, a number of significant refinements have been made to model algorithms. Hence, in order to provide the model user with a comprehensive summary of these modifications, a detailed description of recent model changes has been included in this report.

Previously, these additional model capabilities have been implemented through the use of multiple, post-processing utility codes such as PSTWAKE, COMBINE, and PPSTWKE, each associated with there own set of input/output file(s). Consequently, as the number of executable, input, and output files needed to perform model calculations has grown, so has the degree of complexity involved in conducting actual analyses. Therefore, to remove the complexity associated model calculations, as well reduce the chances for errors inherent when multiple input/output files are involved, all calcualtions performed by existing executable files (WAKE, ISC3, POSTWAKE, etc.) have been combined into a single executable file. Furthermore, calculations performed by this "revised" WAKE dispersion model have been checked and verified solutions obtained analytically or using software packages such as EXCEL (Microsoft, 1997) and MATHCAD (Mathsoft 1997).

While the revised WAKE dispersion model represents a significant improvement to the original model developed by Hanna and Chang (1997), there remain additional modifications that can be incorporated into future versions of the model that both improve the speed of model calculations, and enhance the ease of model use. For example, the ISC3 model (EPA 1995) is used by the WAKE model to calculate concentrations associated with the portion of the plume which rises above the recirculation cavity. Many of the algorithms and subroutines present in ISC3 are never used in calculations made by the WAKE model. Hence, future versions of the WAKE model could be further streamlined by extracting only the necessary portions of the ISC3 model. Similarly, inclusion of a graphical user interface could be used to both aid data input as well as visualize model results.

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APPENDIX A

INPUT FILE DESCRIPTION AND USER'S GUIDE FOR THE REVISED WAKE DISPERSION MODEL

This appendix is intended to provide the user with the basic tools and understanding necessary to execute the WAKE dispersion model. It includes a detailed description of model input files as well as instructions for executing the model.

A.1 INPUT FILE DESCRIPTIONS

Unlike previous versions of the WAKE dispersion model, whose execution required multiple input files associated with the WAKE, ISC3, POSTWAKE, etc. utilities, only two input files are associated with the revised WAKE model, one required and one optional. Both files are in standard, ASCII text format. The main (required) input file which contains information describing the source, release and meteorological conditions, and downwind receptor locations should be named according to the following convention: "XXXXXXXX.WKI", where "XXXXXXXX" is an arbitrary eight-character run identifier and "WKI" is a mandatory file extention. The second (optional) file is used only in cases where the effects complex terrain are considered and is used to specify receptor elevations. This file is identified by the following convention: "XXXXXXXX.GRD", where "XXXXXXXX" is the same eight character run identifier previously described and "GRD" is the mandatory file extention.

A.1.1 Description of the WKI Input File

The "WKI" input file required by the revised WAKE dispersion model is similar in appearance to that used by the original version of the WAKE model (Hanna and Chang 1997), with the major difference being the inclusion of multiple values per record for selected parameters (emission rate, stack exit velocity, and stack exit temperature) used to describe individual release periods associated with time-varying releases. Currently, a maximum of six release periods can be analyzed during a single model run. Like the original WAKE model, information for up to 100 stacks may be specified. Similarly, up to 200 receptor locations can be specified. Note, these limits for the number of release periods, sources and receptor locations are based on previous experience and can be readily modified via changes to "PARAMETER" statements found in the WAKE model source code. As before, input parameters designated as "character" fields should be left justified, whereas those designated as real or integer values are specified in free format. A complete record-by record desciiption of the "WKI" file is given in Table A.1.

Table A.1. Description of WKI input file

Parameter description	Units	Format
Pollutant name	N/A	Character (4)
Building height	m	Real
Downwind building length	m	Real
Projected building width	m	Real
Lateral offset of building centerline from receptor centerline; >0 to the right of receptor centerline, <0 to the left (only applicable to ISC3 calculations)	m	Real
Number of release periods (Currently limited to 6)	N/A	Integer
Note, the following 9 records are repeated until the end-of-stack-input indicator is read		
Stack name (at most 8 characters with no embedded spaces)	N/A	Character (8)
Pollutant emission rates associated with each release period	kg/s	Real[1]
Stack height above ground	m	Real
Stack diameter	m	Real
Stack exit velocities associated with each release period	m/s	Real[1]
Stack exit temperatures associated with each release period	K	Real[1]
Stack capped indicator: 1 = stack is not capped, 2 = stack is capped	N/A	Integer
Horizontal distance between stack and the downwind edge of building	m	Real
Lateral distance of stack from building centerline; > 0, to the right of building centerline; < 0, to the left of building centerline (only applicable to ISC3 calculations)	m	Real
End-of-stack-input indicator = "ENDS"	N/A	Character (4)
Release duration associated with each release periods (< 0 means infinite duration)	s	Real[1]
Ambient wind speed	m/s	Real
Measuring height of ambient wind speed	m	Real
Ambient temperature	K	Real
Stability indicator (1-6; 1=A, 4=D, 6=F, etc.)	N/A	Integer
Rural/urban indicator (1=rural, 2=urban)	N/A	Integer
Maximum allowed exposure time (1800.0 recommended)	s	Real
Total (fore and aft) number of σ_x's used to estimate exposure time (4 recommended)	N/A	Integer
Reference exposure time on which health effects estimates are based (3600.0 recommended)	s	Real
Exponent for calculating toxic load (ignored for U and HF which are automatically set equal to 1 and 2, respectively)	N/A	Integer
Distance from downwind edge of building to receptor	m	Real[2]

[1]These records should contain values for each release period.

[2]This record is repeated for each additional receptor (currently limited to a maximum value of 200).

A.1.2 Description of the GRD Input File

The optional "GRD" input file is only required for cases in which the effects of complex terrain are considered. As with the "WKI" file, "Character" fields should be left justified, while real and integer values are specified in free format. Table A.2 provides a description of all records in the "GRD" file.

Table A.2. Description of .GRD input file

Parameter description	Units	Format
Alpha-numeric header (for reference only)	N/A	Character (80)
Number of downwind receptor locations	N/A	Integer[1]
Distance from downwind edge of building to receptor[2]; Receptor elevation	m, ft	Real, Real [3]

[1]This value must equal the number of downwind receptor locations specified in the ".WKI' file.
[2]This value must equal the downwind distance specified in the ".WKI' file.
[3]This record is repeated for each downwind receptor (currently limited to a maximum value of 200). In addition, the first record is used to define the base elevation at the downwind edge of the building (i.e., downwind distance = 0.0, and elevation = local ground level elevation of building).

A.2 EXECUTION OF THE REVISED WAKE MODEL

In order to execute the revised WAKE model, the user must first create a valid "WKI", and, if necessary, the corresponding "GRD" input file. Next, if running under a WINDOWS 95 or similar environment, the user must create a DOS shell in order to execute the model. Once these tasks are completed, all necessary calculations associated with a given input file, *FILENAME.WKI*, are performed by simply typing the following line at the MS-DOS prompt:

WAKE *FILENAME*

Unlike the original WAKE model which required the user to enter additional commands to run the ISC3, POSTWAKE, COMBINE, etc. components, no additional user-specified commands are necessary as all calculations performed by each of these modules are automatically executed.

A.3 DESCRIPTION OF MAJOR TASKS PERFORMED BY MODEL SUBROUTINES

Appendix A of Hanna and Chang (1997) contains a listing of the major tasks performed by WAKE, ISC3, and POSTWAKE utilities. As described previously in this report, these tasks, as well as those performed by the PSTWAKE, COMBINE, and PPSTWAKE utilities have been incorporated as modules (or groups of subroutines) into a single executable file. The following section presents a brief summary of the major tasks performed by each module of the revised WAKE dispersion model.

The WAKE module and its associated subroutines are responsible for the following tasks:

- processing and verification of input information
- determination of the dimensions of the recirculation cavity
- determination of the fraction of the plume captured in the building recirculation cavity
- calculation of steady-state, downwind concentrations associated with the fraction of plume captured in the building recirculation cavity
- calculation of plume lift-off correction factor
- initialization of all arrays and variables used by other WAKE modules

The ISC3 module and its associated subroutines are responsible for the following tasks:

- determination of wind speed at plume half-height via an iterative scheme
- calculation of steady-state, downwind concentrations associated with the fraction of plume which rises above the building recirculation cavity

The POSTWAKE module and its associated subroutines are responsible for the following tasks:

- integration of downwind concentrations associated with the fractions of plume captured in and rising above the building recirculation cavity
- correction of downwind concentrations due to the presence of complex terrain
- correction of steady-state, downwind concentrations values for finite duration releases

The PPSTWAKE module and its associated subroutines are responsible for the following tasks:

- integration of downwind concentration and toxic load values for time-variant or transient releases

A.4 PROGRAM NOTES

Like the original WAKE dispersion model described in Hanna and Chang (1997), the revised WAKE model was compiled and linked using the Lahey F77L-EM/32 V5.2 FORTRAN compiler. Hanna and Chang (1997) recommend a minimum hardware setup of a 486DX personal computer with 4 MB of memory and 10 MB of free disk space. While such a configuration should still be sufficient to perform calculations using the revised WAKE model, it is recommended that the minimum hardware setup be upgraded to include the following: personal computer with a 100-MHz or greater PENTIUM processor (or equivalent), 16 MB of memory, and 50 MB of free disk space.

APPENDIX B

SUMMARY OF INPUT/OUTPUT FILES REQUIRED/GENERATED BY THE WAKE DISPERSION MODEL

The following is a list and brief description of the files that are either required or generated during the course of WAKE model run. In addition to these files, a number of "scratch" files are generated and automatically deleted during the course of a normal model run. These files should never be apparent to the user unless the program terminates abnormally. The files associated with the WAKE dispersion model which are identified by their three character extension include the following:

DGP: Output file associated with transient releases containing intermediate results (ratios of midpoint concentration to steady-state concentrations, etc.) at downwind locations for each release period.

GRD: Optional input file for specifying receptor elevations for scenarios involving complex terrain.

ISC: Intermediate file generated by WAKE module containing the primary input information used by the ISC3 module.

ISO: Intermediate output file containing an unabridged listing of results generated by the ISC3 module associated with the fraction of the plume which rises above the building recirculation cavity. Used as input to the POSTWAKE module in calculating total concentrations and toxic loads associated with the release.

ISX: An abridged version of the "ISO" file containing a summary of values calculated by the ISC3 module for the fraction of the plume which rises above the building recirculation cavity.

MET: Intermediate file generated by WAKE module containing meteorological information used as input by ISC3 module.

OUT: Primary model output file containing intermediate and final results of the analysis.

OUX: Output file containing calculated values for steady-state concentrations and intermediate parameters grouped according to release period.

WKI: Main model input file.

WKR: Output "report" file generated by the WAKE module. Includes an "echo" of input parameters used in the model run as well as values calculated by the WAKE module for a number of derived parameters used to calculate concentrations associated with the fraction of the plume captured in the building recirculation cavity.

WKX: Intermediate output file containing values for steady-state concentrations calculated by the WAKE module for the fraction of the plume captured in the recirculation cavity.

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