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Use of HGSYSTEM/UF_6 and MACCS2 for the Building 9204-2E Safety Analysis Report Consequence Analysis: General Overview and Comparison of Models

D. A. Lombardi
Oak Ridge National Laboratory

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W. R. Brock
Lockheed Martin Energy Systems, Inc.

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by

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
managed by
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I have reviewed this report and concur with its conclusions and recommendations.

3/2/98

Date

Louis Restrepo
Omicron
P.O. Box 93065
Albuquerque, New Mexico 87199-3065
(505) 883-0553

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ABBREVIATIONS AND ACRONYMS

API	American Petroleum Institute
CCDF	complementary cumulative distribution function
DOD	U.S. Department of Defense
DOE	U.S. Department of Energy
EPA	U.S. Environmental Protection Agency
GPE	Gaussian Plume Equation
HF	hydrogen fluoride
HGSYSTEM/UF_6	Heavy Gas-system-Uranium Hexafluoride
ISC3	Industrial Source Complex-Version 3
kg	kilogram
m	meter
MACCS2	MELCOR Accident Consequence Code System-2
mg	milligram
NRC	U.S. Nuclear Regulatory Commission
s	second
SAR	Safety Analysis Report

1. INTRODUCTION

Building 9204-2E is used for assembly, disassembly, and storage of weapons components, and quality operations. The building, built in 1971, is a three story structure approximately 101 m long, 51 m wide, and 21 m high located in the western exclusion area of the Y-12 Plant, Oak Ridge, Tennessee. Assembly activities include piece part cleaning, manual assembly techniques, adhesive bonding, welding, leak testing, machining, electrical testing, etching, painting, and packaging. The disassembly activities involve manual tear down operations, material verification/accountability activities, standard and inert machining operations, cryogenic operations, and containerization of disassembled components for reclamation and disposal. Storage activities involve receipt and verification of weapons stockpile units, repackaging from transportation containers to approved storage containers, and placement of containers in storage areas. Quality operations include non-destructive testing activities such as radiography, ultrasonics, and dimensional inspection activities such as manual testing with hard gauges and open set up, comparator measurements, and numerically controlled coordinate measuring machine operations, and materials testing such as mechanical properties measurement and metallography.

For these activities, several types of hazardous (e.g., toxic, reactive, and corrosive) and radioactive (including fissile) materials are used and stored in Building 9204-2E. Uranium, posing a toxic, radioactive, and sometimes fissile hazard, is the hazardous material of primary concern because of the large inventory of this material in Building 9204-2E. During a fire, criticality event, or other accident, the potential exists for the release of uranium and other hazardous materials from the building to the atmosphere. A Safety Analysis Report (SAR) is being prepared for Building 9204-2E, in which the consequences of such releases to on-site workers and the off-site public are being analyzed.

Consequence estimates from accidental airborne releases are generally calculated using computer models that simulate dispersion and transport of the plume as it travels downwind. More robust computer models also simulate initial rise of the plume due to buoyancy and momentum, the effects of buildings on downwind dispersion of the plume, deposition of material from the plume during downwind transport, chemical reactions and transformations of material within the plume, and other phenomena. For the Building 9204-2E SAR, two candidate atmospheric dispersion candidate models have been identified for use: (1) the Heavy Gas System-Uranium Hexafluoride (HGSYSTEM/UF_6) Model Suite, and (2) the MELCOR Accident Consequence Code System-2 (MACCS2). The purpose of this paper is to provide a general description of the two model suites and compare model results for generic release cases, representative of those that will be analyzed in the Building 9204-2E SAR. Recommendations for use of the model suites in the SAR are also discussed.

2. GENERAL DESCRIPTION OF THE MODEL SUITES

2.1 HGSYSTEM/UF_6

HGSYSTEM was originally developed by Shell Research, Ltd. in the mid to late 1980s to simulate a wide variety of hazardous gas releases, including two-phase aerosol jets of hydrogen fluoride (HF) resulting from ruptures of valves and pipelines on pressurized HF tanks (McFarlane *et al.* 1990; Witlox *et al.* 1990). In 1994, an updated version of HGSYSTEM (Version 3.0) was released by Shell Research Ltd., with several enhancements sponsored by the American Petroleum Institute (API). This version of HGSYSTEM was approved by the EPA as an alternative regulatory model (40 CFR 51, App. W).

In 1992, at the request of the U.S. Department of Energy (DOE), Martin Marietta Energy Systems (now called Lockheed Martin Energy Systems) sponsored a review of 37 existing dispersion models to determine the most appropriate for simulating accidental releases of reactive materials from the gaseous diffusion plants (Sykes and Lewellen 1992). Based on the reviewers' recommendations, DOE decided to incorporate previously developed algorithms, accounting for (1) chemical reactivity, (2) release of heat of reaction, and (3) density variations in the plume, into HGSYSTEM. The new model suite was called HGSYSTEM/UF_6 because of the focus on chemical reactions of uranium hexafluoride in the modeling system. Development of HGSYSTEM/UF_6 was closely coordinated with development of HGSYSTEM Version 3.0 (Hanna *et al.* 1996). All improvements to the Shell HGSYSTEM model have been incorporated into HGSYSTEM/UF_6 (Hanna *et al.* 1996), with the final Shell technical documentation (Post 1994a) and user's guide (Post 1994b) containing descriptions of the uranium modules.

The HGSYSTEM/UF_6 suite consists of several models:

- **AEROPLUME/RK.** This model estimates near-field (i.e., downwind distances ranging from tens to hundreds of meters) dispersion of elevated, two-phase (aerosol and vapor) momentum jets of UF_6 and its reaction products (UO_2F_2 and HF), as well as other non-reactive materials. This model applies to releases from pressurized tanks or cylinders at the point of release to the time when they either (1) strongly interact with the ground and become a dense ground-based plume or (2) become passive (i.e., the density approaches ambient air density and chemical reactions cease). The initials RK stand for the inclusion of a robust Runge-Kutta numerical solver that enables the user to model situations where the plume angle changes rapidly with time, such as dense gas releases with steep jet angles (between −10 and −45° from the horizontal) pointing toward the ground. The Runge-Kutta numerical solver replaces the SPRINT numerical solver employed in HGSYSTEM Version 3, which could not consistently simulate dense gas releases with steep jet angles (Hanna and Chang 1997).

- **HEGADAS/UF_6.** This model applies to continuous, ground-hovering plumes. The model is used for either (1) area source releases (i.e., spills) or (2) at the point where AEROPLUME predicts that the dense plume will be in direct contact with the ground.

- **PGPLUME.** This model is used in the final passive phase of the plume where the Gaussian plume methodology is applicable. No chemical reactions or thermodynamic processes are modeled in PGPLUME. This model is only used after AEROPLUME determines that the plume has become passive and is not dense.

- **UF_6MIXER.** This model simulates the dispersion of warm, possible reactive plumes that drift out of a building horizontally (e.g., through an open bay door or a hole) directly into the building wake. The model employs recently-developed building wake algorithms (discussed in more detail below), as well as a modified version of HEGADAS/UF_6.

- **WAKE.** This model simulates the release of buoyant plumes from vents on the top or sides of a building using recently-developed building wake effect algorithms (discussed below). No chemical reaction processes are modeled in WAKE.

In addition to the effects of buildings on plume dispersion, several other phenomena were incorporated into HGSYSTEM/UF_6, including: (1) lift-off of the plume centerline from ground-level as buoyancy changes from negative to positive as a result of heat input due to chemical reactions, (2) removal of gases and particles by wet and dry deposition, (3) parameterization of some meteorological variables using recent boundary-layer theory, and (4) accounting for variations in concentration with averaging time.

2.2 MACCS2

MACCS2 is an update to the MACCS, both developed by Sandia National Laboratories. Publicly distributed since 1987, MACCS was developed to estimate the potential impacts to the surrounding public of severe accidents at nuclear power plants. The principal phenomena considered in MACCS are atmospheric transport, diffusion, and deposition under time-variant meteorology, short-term and long-term mitigative actions and exposure pathways, deterministic and stochastic health effects, and economic costs of mitigative actions. MACCS2 was developed as a general-purpose analytical tool applicable to diverse reactor and non-reactor NRC licensed, and DOD- and DOE- operated facilities. The MACCS2 code includes three primary modules listed below and described in more detail in Chanin and Young (1997):

- **ATMOS.** This module calculates dispersion of material downwind from the release point using the Gaussian plume methodology. The model calculates wet and dry deposition of aerosols from the plume, as well as radioactive decay of the released material. The Gaussian plume methodology employed by the module is suitable for simulating neutrally-buoyant plume dispersion, with the model also simulating initial plume rise of positively-buoyant plumes.

- **EARLY.** This module calculates acute radionuclide exposures from cloudshine (radioactivity emitted from the plume during passage), groundshine (radioactivity emitted from deposited material), and inhalation during the initial (emergency) phase of the release. The duration of this phase is determined by the user, with an allowable range of 1 to 7 days. Exposures can be calculated assuming mitigative actions, such as evacuation, sheltering, and dose-dependent relocation.

- **CHRONC.** This module estimates chronic radionuclide exposures over intermediate (7 days to 1 year) and long-term (greater than 1 year) exposures. The module estimates exposures based on relocation practices and land-use restrictions. In addition to exposures, CHRONC estimates the economic cost of accidental releases during the intermediate and long-term phases.

In addition to the three main modules, MACCS2 includes several preprocessors that calculate dose conversion factors and exposure pathways via the food chain.

A key feature written into the MACCS2 code is the ability to assess relative risks of radiological releases in the form of a complementary cumulative distribution function (CCDF), produced through a random sampling of one year of meteorological data. CCDFs may be used to compare relative risks and economic costs among a variety of accident scenarios.

3. SCOPE OF THE COMPARISON

In the general overview of HGSYSTEM/UF_6 and MACCS2, the overall difference in emphasis of each model suite becomes apparent. The models of HGSYSTEM/UF_6 focus primarily on a wide variety of plume dispersion mechanisms, with specific emphasis on the interaction of uranium physical and chemical properties, and plume characteristics. While one of MACCS2 modules (ATMOS) simulates plume dispersion of radioactive material, the primary focus of the code is to incorporate this dispersion module with sophisticated radiological exposure and economic cost algorithms that simulate many post-release mitigative actions. The difference in emphasis of each suite makes comparison of the two codes difficult. For instance, MACCS2 does not simulate the following phenomena included in the HGSYSTEM/UF_6 codes:

- physical and chemical properties of uranium (specifically, UF_6) and HF on plume dispersion, and

- heavy gas dispersion.

On the other hand, MACCS2 does simulate the following phenomena that are not directly included in HGSYSTEM/UF_6:

- radioactive decay of plume material during dispersion,

- human exposure to radioactivity, particularly via the food chain,

- risk assessment capabilities based on CCDF estimates from various release scenarios, and

- economic costs associated with accidental releases of radioactive materials.

In defining the scope of the model comparison, the general nature of accidents that will be analyzed in the Building 9204-2E SAR are important to consider. With this building, uranium is the primary radioactive material that may be released into the atmosphere during an accident. Therefore, radioactive decay during transport is a much less important issue because of uranium's long half-life. Also, most accidents in and around the building would be of relatively short duration (e.g., releases of one hour or less). As such, the sophisticated intermediate and long-term exposure pathway and economic cost algorithms in MACCS2 that were designed to simulate potential nuclear reactor accidents, with associated deposition of fission products over a large area (i.e., simulation of land interdiction events), are not needed in the Building 9204-2E SAR. Additionally, short-duration releases limit the number of mitigative actions that are relevant, with much of the detailed emergency response modeling capabilities of MACCS2 not applicable for the Building 9204-2E SAR. Therefore, basing the comparison on these phenomena is not reasonable.

One key phenomenon highly relevant to the Building 9204-2E consequence analysis which is simulated by both HGSYSTEM/UF_6 and MACCS2 is the effect of turbulent wakes created by the building on buoyant plume lift-off and dispersion. Because of the relative importance of building wake effects and buoyant plume lift-off on the results of the consequence analysis, this code comparison will focus on these phenomena and the resulting impact on downwind consequence estimates. As discussed earlier, two models in HGSYSTEM/UF_6 can be used to estimate downwind consequences from releases into building wakes, UF_6MIXER and WAKE. The UF_6MIXER model was developed primarily for ground-level releases of reactive plumes. On the other hand, the WAKE model can be used for both ground-level and elevated releases for non-reactive plumes that are either neutrally- or positively-buoyant, and therefore, this model has a wider flexibility for use in a variety of release scenarios. Because of its enhanced flexibility, the WAKE model was selected from the HGSYSTEM/UF_6 suite to compare to the MACCS2 dispersion module, ATMOS. The treatment of building wakes and lift-off of buoyant plumes by both MACCS2 and WAKE is discussed in more detail below.

4. MODEL TREATMENT OF BUILDING WAKES AND LIFT-OFF OF BUOYANT PLUMES

Figure 1 is a schematic of the complex flow that develops around large buildings. As the wind field impacts the upwind face of the building, streamlines will split with a significant fraction of the flow ascending over the roof of the building. Downwind of the building, streamlines descend toward the ground surface. As the flow is split and streamlines ascend and descend over the building, many turbulent zones are created. A buoyant plume emitted at roof level may be affected by one or more of these turbulent zones as the rising plume passes through the region of the building wake. For instance, if a vent is located within the roof recirculation region near the upwind edge of the building, much of the plume may be recirculated toward the roof level and relatively high concentrations along the roof would be expected (Hosker 1984). Also, as a buoyant plume rises through the roof recirculation cavity or the high turbulence zone, it will be rapidly diluted (to ambient density) causing the height of final plume rise to be less, and the plume vertical width to be larger than a plume released in the absence of a building (Schulman and Scire 1980).

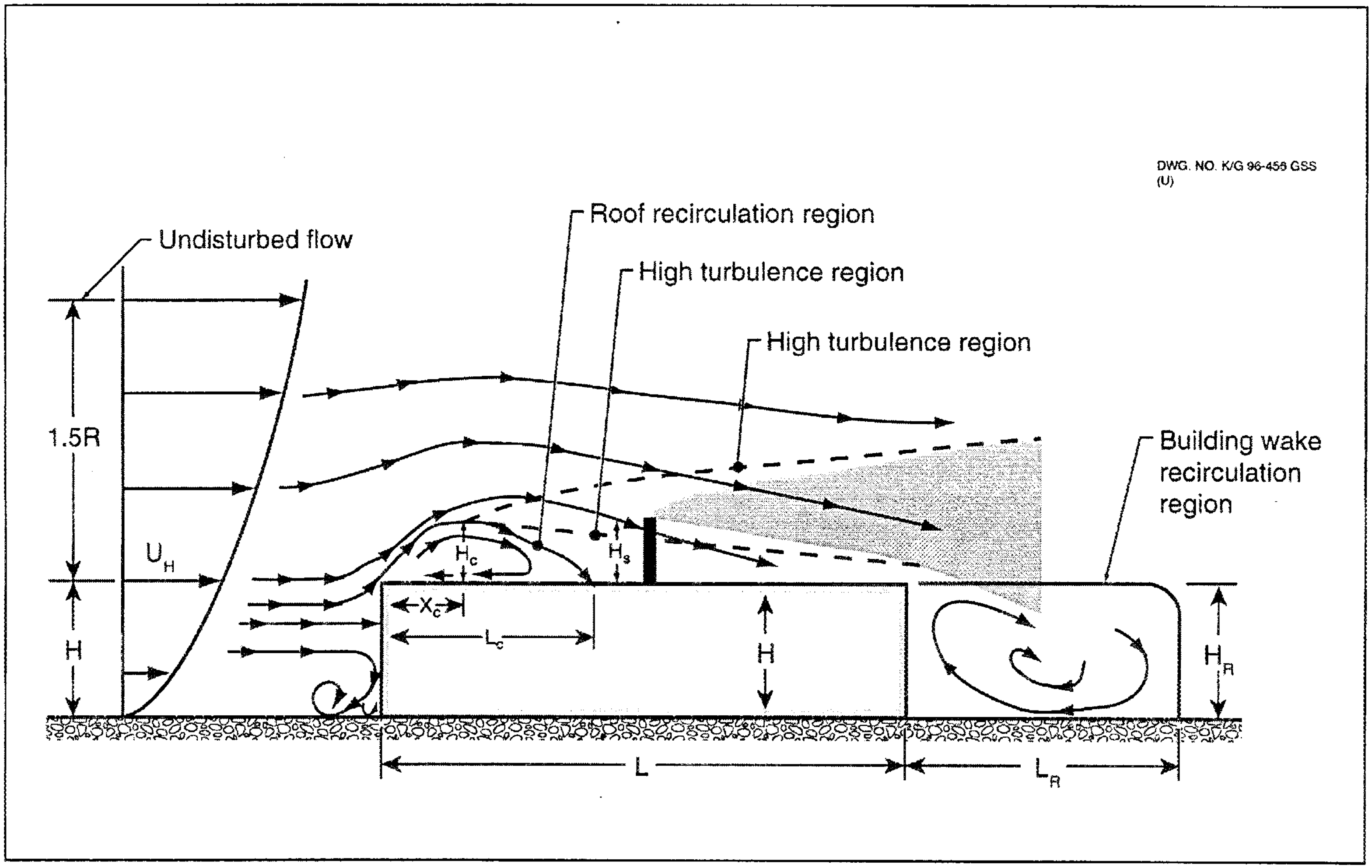

Fig. 1. Flow over a building for a wind normal to the upwind face (Wilson 1979).

On the lee side of the building, another larger recirculation cavity may form. Any fraction of a buoyant plume captured in the lee side cavity would be rapidly mixed and transported to the ground along recirculation streamlines. The remaining fraction of the buoyant plume not captured in the cavity would be influenced by the turbulent zone, where streamlines descend near the lee side of the building (downwash). Recent wind tunnel studies conducted by EPA (Snyder 1993; Snyder and Lawson 1994) show that the actual trajectory of a rising plume is substantially affected by building downwash. With certain combinations of wind speed and direction, Scire *et al.* (1995) report that a buoyant plume may actually descend toward the ground surface as a result of the dominance of streamline descent over the effects of buoyancy.

For releases into building wakes, MACCS2 assumes that the initial crosswind and vertical dimensions of the plume are increased due to increased mixing with ambient air caused by the turbulent wake. These dimensions are calculated from user input of initial plume dispersion parameters in the horizontal direction (σ_y–the standard deviation of the concentration distribution in the crosswind direction) and the vertical direction (σ_z–the standard deviation of the concentration distribution in the vertical direction). The MACCS2 user's manual (Chanin and Young 1997) provides a few choices for calculating σ_{y0} and σ_{z0} (initial values at the release point of σ_y and σ_z, respectively), with the most recent method based on Jones (1983):

$$\sigma_{y0} = \frac{W_B}{3} , \; \sigma_{z0} = \frac{H_B}{3} \quad , \tag{1}$$

where,

W_B is the effective width (i.e., the building width perpendicular to the wind direction) of the building (m), and
H_B is the height of the building (m).

The MACCS2 user's guide also states that Jones (1983) suggests when plumes are released into building wakes, the release height should be adjusted to $H/3$. However, in current practice, users are using the actual release height (L. Restreppo, Albuquerque, New Mexico, personal communication to D. A. Lombardi, Oak Ridge National Laboratory, Oak Ridge, Tennessee, December 1, 1997).

To account for the plume capture in the recirculation cavity, MACCS2 will not allow a buoyant plume to rise if the wind speed at the release height is greater than a critical wind speed, u_c, as developed in Briggs (1973):

$$u_c = \left(\frac{9.09F}{L_p} \right)^{1/3} \quad , \tag{2}$$

where, F is the plume buoyancy flux (m^4/s^3), and
L_p is the plume scale length (m), assumed to be the building height in the MACCS2 model.

Application of Equation (2) is "all-or-nothing." If the critical wind speed is exceeded by the wind speed at release height, the plume is assumed to be unable to escape from the building wake and the plume is not allowed to rise. However, although the plume is not allowed to rise, MACCS2 does not simulate mixing in the recirculation cavity nor plume downwash (i.e., the final plume height is equal to the release height), except for the increased initial dimensions of the plume.

The WAKE model uses a revised lift-off methodology proposed by Hanna *et al.* (1997) to account for the smooth transition associated with lift-off phenomena, based on analysis (Briggs 1995, 1996) of wind tunnel experiments involving buoyant plumes released into building wakes (Hall and Waters 1986; Hall *et al.* 1995). Following ASHRAE (1993), Schulman and Scire (1993), and Wilson (1995), the WAKE model splits the plume into two components: (1) the fraction, f_c, of the plume captured in the recirculation cavity and then transported into the far wake region, and (2) the remaining fraction, $(1-f_c)$, of the plume that rises through the turbulent wake directly above the building. The total ground-level concentration, C_{total}, at downwind distances from the release point is summed from these two components (Hanna and Chang 1997):

$$C_{total} = C_c + C_a \quad , \tag{3}$$

where,

C_c is the ground-level concentration (mg/m^3) from the component of the plume caught in the recirculation cavity, and

C_a is the ground-level concentration (mg/m^3) from the component of the plume that rises through the wake above the recirculation cavity.

The development of equations used to calculate C_c are summarized below and detailed in Hanna and Chang (1997). In the near wake, C_c is calculated using formulations empirically-derived from recent wind tunnel data (Wilson 1995):

$$C_c = \frac{Q_c}{wA\left[1 + 13\left(\frac{T_a}{T_s}\right)^{1/2}\frac{w}{u_H}\right] + \frac{u_H x_s^2}{16}} \quad , \tag{4}$$

where,

Q_c is equal to the $f_c Q$ and Q is the mass flux (kg/s) of the material at the release point,
w is the vertical velocity of the plume at the vent (m/s),
A is the cross-sectional area of the vent (m^2),
T_a is the temperature of the ambient air (K),
T_s is the temperature of the plume at the vent (K),
u_H is the wind speed at the top of the building (m/s), and
x_s is the "stretched string" distance from the source to the receptor (m).

In the denominator of Equation (4), the first $w \times A$ (the volume flux from the vent) is included to ensure the predicted concentrations do not exceed the initial concentration in the vent plume. The second term, with T_a/T_s, accounts for reductions in concentrations from the initial rise of the plume out of the jet. The third term calculates the concentrations on the roof and downwind sides of the buildings.

Equation (4) applies until the plume grows such that the estimated concentrations drop to the concentrations calculated using a model for a well-mixed building wake. The well-mixed building equation modified from Briggs (1995, 1996) is used to calculate concentrations at downwind distances beyond this point and is given as:

$$C_c = \left(\frac{Q_c}{u_H R^2} \right) \frac{B_{LO}}{\left[0.037 + 0.03 \left(\frac{x}{H_B} \right)^2 + F_{**}^2 \left(\frac{x}{H_B} \right)^4 + \left(\pi \frac{\sigma_y \sigma_z}{R^2} \right)^3 \right]^{1/3}} , \qquad \textbf{(5)}$$

where,

R^2 is the scaling area in the wake as defined by Wilson (1995) (m^2), with R being the representative scaling length of the building (m),
B_{LO} is the non-dimensional buoyant lift-off term,
x is the downwind distance from the source to the receptor (m),
W_B and H_B are the width and height of the building, respectively (m),
σ_y and σ_z are the Gaussian horizontal and vertical dispersion parameters, respectively (m), and
F_{**} is the non-dimensional buoyancy flux, calculated as:

$$F_{**} = \frac{F}{u_H^3 W_B} . \qquad \textbf{(6)}$$

As stated earlier, Equation (5) is a modified version of 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). Note: the data from Hall *et al.* (1995) is for wind tunnel experiments simulating warehouse fires, which specifically applies to the types of accidents that are anticipated to be analyzed in the Building 9204-2E SAR. The derivation of Equation (5) is detailed in Hanna and Chang (1997) and Hanna *et al.* (1997).

In Equation (5), B_{LO}, describes the decrease in ground-level concentration due to buoyant lifting of the plume in the building wake, which is determined by:

$$B_{LO} = \exp\left(-6 F_{**}^{0.4} \right) . \qquad \textbf{(7)}$$

In Equation (5), the denominator under B_{LO} has four terms (i.e., those terms in brackets). The first three terms account for plume dilution (1) across the building face and recirculation cavity, (2) due to expansion with downwind distance, and (3) due to growth caused by buoyancy. The fourth term accounts for dispersion of the plume due to ambient turbulence not related to the presence of the building, where the Gaussian plume methodology is applicable.

To estimate ground-level concentrations resulting from the part of the plume that rises through the building wake, C_a [Equation (3)], the Industrial Source Complex - Version 3 (ISC3) (EPA 1995) dispersion model is used. Values of C_a are calculated using default regulatory methods for building downwash defined by the EPA (40 CFR 51, App. W). The Schulman and Scire (1980) downwash algorithms incorporated into ISC3 are preferred by EPA for refined regulatory dispersion modeling of buoyant point source emissions affected by building wakes (40 CFR 51, App. W). A detailed discussion of the Schulman and Scire downwash algorithms is given in the ISC3 *User's Guide* (EPA 1995). The source term for the part of the plume above the wake, Q_a, is calculated as:

$$Q_a = (1 - f_c)\, Q \quad . \tag{8}$$

5. DESCRIPTION OF RELEASE CASES AND MODEL INPUT PARAMETERS

Three release cases were considered to compare model results. The model input parameters for each case are listed in Table 1 and discussed in more detail below. The release cases were selected to provide a range of release conditions that generally represent a variety of accidents analyzed in the Building 9204-2E SAR. However, to facilitate comparison, the cases analyzed represent relatively simple release scenarios (e.g., steady-state release from only one vent with no deposition of material as the plume travels downwind).

- Case 1: a non-buoyant, ground-level release with no building wake effect. This case simulates the release of material in an open area, far from any buildings. The plume is assumed to be at the same temperature and density as the ambient atmosphere.

  For this case, the ambient atmosphere was assumed to be stable (class F) with a light wind speed (1 m/s) and a temperature of 283 K (50°F). This stability class and wind speed result in maximum concentrations for ground-level, non-buoyant releases and typically occur at the Y-12 Plant about 9% of the time (Sharp 1997). The ambient temperature represents a typical value at the Y-12 Plant.

- Case 2: a non-buoyant elevated release into a building wake. This case simulates the release of material from a capped (i.e., no vertical momentum flux) vent flush with the roof of Building 9204-2E. As with Case 1, the plume is assumed to have the same temperature and density as the ambient atmosphere. Building dimensions are representative of Building 9204-2E.

  For this case, the ambient atmosphere was assumed to have neutral stability (class D) with moderate wind speeds (4 m/s). These meteorological conditions result in relatively high ground-level concentrations for elevated releases and occur relatively often (i.e., about 5%) of the time at the Y-12 plant.

Table 1. Release conditions for three MACCS2-WAKE model comparison case runs

Parameter	Case 1: non-buoyant ground-level release with no building wake effect	Case 2: non-buoyant elevated release with building wake effect	Case 3: buoyant elevated release with building wake effect
Building height, m	N/A[a]	20.7	20.7
Effective building width[b], m	N/A[a]	113	113
Effective building length[c], m	N/A[a]	60.0	60.0
Release height, m	0	20.7	20.7
Vent diameter, m	N/A[a]	2.00	2.00
Plume temperature at vent, K	283	850	850
Plume exit velocity at vent, m/s	N/A[a]	10.0	10.0
Plume heat at exit, W	0	0	7.45×10^6
Ambient air temperature, K	283	283	283
Ambient wind speed at 10 m, m/s	1	4	4
Atmospheric stability class	F (stable)	D (neutral)	D (neutral)

[a]N/A = this model input parameter is not applicable for this release scenario.
[b]The effective building width was calculated as the square root of the sum of squares of the building length (101 m) and the building width (51 m).
[c]The effective length was calculated as the length of the building perpendicular to the effective width.

- Case 3: a buoyant elevated release into a wake created by Building 9204-2E. Similar to Case 2, this case simulates the release of material from a capped vent flush with the roof of Building 9204-2E. However, for this case, the plume is assumed to be buoyant relative to the ambient atmosphere with a relatively high plume temperature such as would occur during a fire release. As with Case 2, class D and 4 m/s meteorological conditions were used.

For Case 3, the heat, H (in Watts - note: the MACCS2 manual uses Q for heat; however, H is used for this paper to avoid confusion with the Q that is the mass flux of the released material), of the plume at the release is needed for the MACCS2 input file to calculate plume buoyancy. The heat of the plume was calculated as:

$$H = C_p (T_p - T_a) \dot{m} \quad , \tag{9}$$

where,

C_p is the specific heat (constant pressure) of the plume at the release point, assumed to be equal to that of air (1.004 KJ/kg-K),

T_p is the temperature of the plume,

T_a is the ambient air temperature, and

$\dot{m}$ is the mass flux of the entire plume (air + released material) at the release point, defined as:

$$\dot{m} = \frac{\pi\, p\, d^2\, w\, MW}{4\, R\, T_p} \quad , \tag{10}$$

where,

p is the ambient pressure (1 atm),

d is the diameter of the release vent (m),

w is the plume exit velocity at the release point (m/s),

MW is the molecular weight of the plume assumed to be approximately equal to dry air (29 kg/kgmole), and

R is the ideal gas law constant (0.0820g atm-m^3/kgmol-K).

The calculated value of H is given in Table 1.

6. RESULTS OF THE MODEL COMPARISON

Dispersion factors, sometimes referred to as normalized concentrations or χ/Q (where χ is the concentration and Q is the mass flux of the released material), were calculated for each case using both MACCS2 and WAKE. Figures 2 through 4 show the comparison of estimated χ/Q values from each model for each case. Dispersion factors are presented, rather than actual concentrations, to isolate the differences in dispersion methodologies between the two models by removing the dependence on source term. For the cases analyzed, isolating the dispersion factor is possible because both models estimate the ground-level concentrations to be linearly proportional to the release rate of the material.

Values of χ/Q were estimated at 100 m increments in a downwind distance range between about 100 m and 2000 m from the release point. These distances represent a reasonable range where maximum consequences at the Y-12 Plant site boundary may occur. Receptors were positioned directly downwind of the source to provide maximum estimates at the plume centerline.

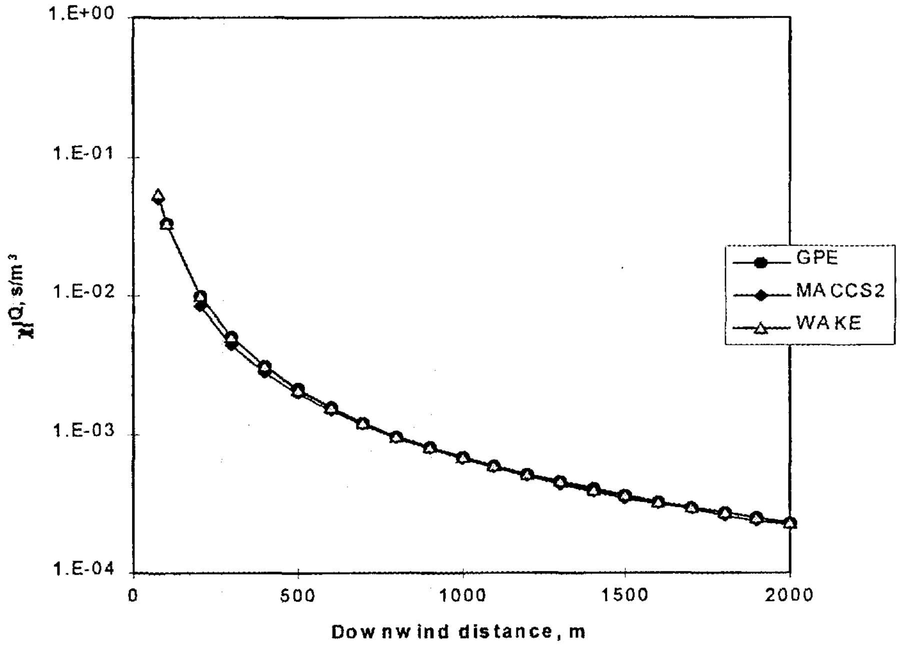

Fig. 2. Comparison of dispersion results between MACCS2, WAKE, and the Gaussian Plume Equation (GPE) for Case 1: non-buoyant release with no building wake effect. For this case, the atmosphere is stable (class F) with a light wind speed (1 m/s).

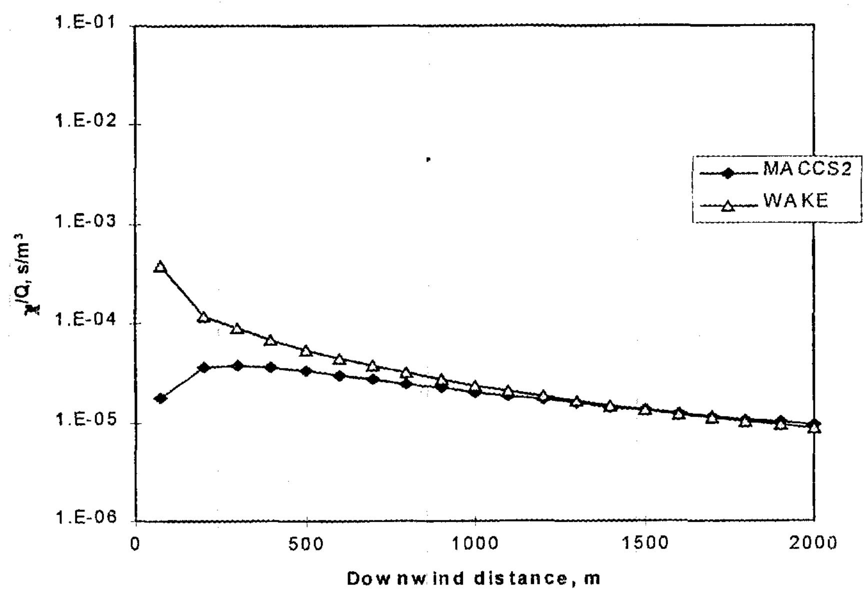

Fig. 3. Comparison of dispersion results between MACCS2 and WAKE for Case 2: non-buoyant release with building wake effect. For this case, the atmosphere has neutral stability (class D) with a moderate wind speed (4 m/s).

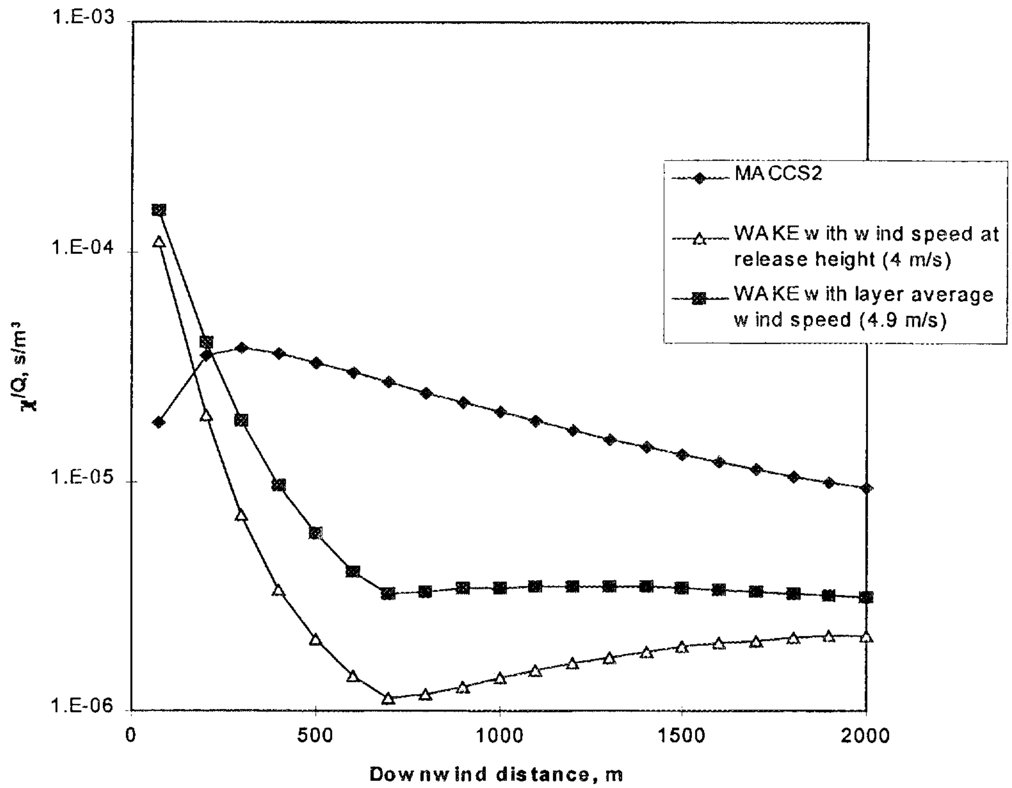

Fig. 4. Comparison of dispersion results between MACCS2 and WAKE for Case 3: buoyant release with building wake effect. For this case, the atmosphere has neutral stability (class D) with a moderate wind speed.

For Case 1 (non-buoyant, ground-level release not affected by a building wake), the estimated dispersion factors agree very well (i.e., within 5% for downwind distances beyond 200 m from the release) between the two models (see Fig. 2). Model results were also compared to the Gaussian Plume Equation (GPE) to show that with a non-buoyant, ground-level release, both MACCS2 and WAKE use the basic Gaussian plume methodology.

The MACCS2 model allows the user to specify σ_y and σ_z. However, WAKE only allows the use of σ_y and σ_z values as calculated by empirical fits of Turner (1994) (portion of the plume with estimates using ISC3) and Briggs (1973) (portion of the plume using the Briggs equation) to the Pasquill-Gifford rural stability curves (Gifford 1960). Note: for Case 1, downwind χ/Q values are calculated by the WAKE model using only the modified ISC3 code (i.e., the Wilson and Briggs equations are not used). For the MACCS2 runs, dispersion parameters for stability classes D and F were selected to closely follow the Pasquill-Gifford stability curves to facilitate comparison. These dispersion parameters were used in the MACCS2 simulations for all three cases.

For Case 2 (non-buoyant plume released into the building wake), the WAKE model estimates greater χ/Q values out to downwind distances of about 1600 m (see Fig. 3). WAKE estimates are greater than MACCS2 by a factor of 10 near the source, but converge to within a factor of 2 at a downwind distance of about 400 m. The WAKE results are greater initially because the model allows for a fraction of the plume (50% in this case) to be captured by the building recirculation cavity, and thereby be mixed to the ground quickly. The MACCS2 model only allows for initial spreading of σ_z, which close to the source does not result in appreciable ground-level concentrations because the plume is elevated. At downwind distances greater than about 1000 m, when the plume is relatively well mixed in the vertical direction, estimated χ/Q values from both MACCS2 and WAKE are in good agreement.

The most substantial differences in results occur with Case 3 (buoyant plume released into the building wake). For Case 3, the MACCS2 model estimates greater χ/Q values at all downwind distances (see Fig. 4). Two plots are shown for WAKE model results using (1) wind speed at the release height (4 m/s) and (2) wind speed averaged between the surface and 100 m above the ground (4.9 m/s). As discussed earlier, the WAKE model uses the wind speed at the release height in its calculations. With the buoyant plume case, using the wind speed at the release height rather than the greater layer-averaged wind speed, results in higher plume rise because the plume does not bend-over as would be the case for a greater wind speed. Therefore, ground-level χ/Q values are less with a lower wind speed because increasing the plume height has a greater effect on reducing ground-level estimates than reduced entrainment of ambient air has on increasing ground-level estimates. As shown in Fig. 5, the plume would rise to a final height of just under 100 m using the release height wind speed of 4 m/s. However, the wind speed at 100 m calculated using the wind power law formula (EPA 1995) would be about 5.7 m/s, with an average wind speed in this layer equal to 4.9 m/s. Using this layer-averaged wind speed, the plume would rise to a final height of about 80 m (Fig. 5).

Values of χ/Q estimated using MACCS2 are 2 to 8 times greater than WAKE estimated at distances beyond 200 m, even with the higher WAKE results calculated from the layer-averaged wind speed. Although the plume is relatively buoyant (F is equal to 65.5 m^4/s^3), MACCS2 does not allow the plume to rise (i.e., the final plume height is equal to the release height of 20.7 m–see Fig. 5) because the wind speed at the release height (4 m/s) is greater than the critical wind speed of about 1.1 m/s calculated using the Briggs old lift-off formula (discussed earlier). Because the old lift-off formula is essentially an "all-or-nothing" calculation, the plume is completely caught in the recirculation cavity. The WAKE model, which allows the plume to be split into the portion that goes into the recirculation cavity and that which rises through the building wake, allows relatively substantial plume rise with only about 5% of the plume caught in the recirculation cavity. Also, this small fraction caught in the recirculation cavity would become well-mixed with relatively high χ/Q values close to the source. Therefore, estimates of χ/Q with the WAKE model are higher than MACCS2 at downwind distances less than 200 m from the release point. The MACCS2 user's guide recommends that the model not be used to estimate doses at downwind distances closer than 500 m from the release because of its limited treatment of building wake effects (Chanin and Young 1997).

7. CONCLUSIONS AND RECOMMENDATIONS

Three release cases, generally representative of those that may be analyzed in the Building 9204-2E SAR Accident Analysis, were simulated using MACCS2 and HGSYSTEM/UF_6 (specifically, the WAKE model). Agreement between the two codes was very good (i.e., almost identical) for the first release case (non-buoyant ground-level release

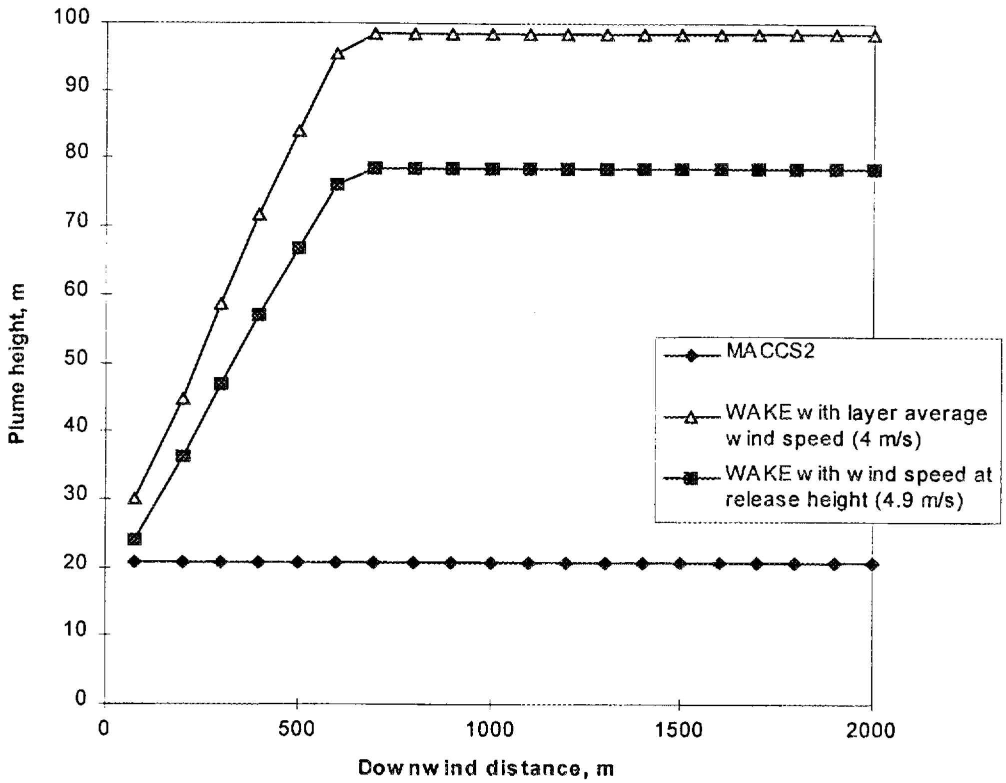

Fig. 5. Comparison of plume height results between MACCS2 and WAKE for Case 3: buoyant release with building wake effect. For this case, the atmosphere has neutral stability (class D) with a moderate wind speed.

without building wake effects) and good (i.e., within a factor of 2 at downwind distances beyond 400 m) for the second release case (non-buoyant elevated release into a building wake). For Case 2, consequence estimates from the WAKE model were greater than those from MACCS2 at downwind distances less than 1400 m because the WAKE model accounts for partial plume capture and turbulent mixing of the captured plume in the lee side recirculation cavity. There was appreciable difference (i.e., a factor of 2 to 8) between the codes for the third release case (buoyant plume released into the building wake) with MACCS2 results greater than WAKE at downwind distances less than or equal to 2000 m. The difference in results is primarily attributable to WAKE using an updated lift-off term.

In the development of WAKE and other HGSYSTEM/UF_6 models, the emphasis has been on using state-of-the-science dispersion methods, allowing for a large variety of release conditions, in combination with robust uranium physical and chemical property algorithms. The development of MACCS2 has focused on providing sophisticated exposure and economic consequence estimates for a large variety of radionuclides, as well as statistical analysis of results to facilitate comparison of mitigative actions in reducing risk. The strengths of each code have value for the Building 9204-2E SAR. The HGSYSTEM/UF_6 models have particular utility for this SAR because accidents associated with this building would release primarily uranium and other chemicals that may react with atmospheric water vapor, but are not radioactive (e.g., HF). Also, building wake effects and plume lift-off will have particular relevance to the Building 9204-2E accident analysis, in which, as discussed above, HGSYSTEM/UF_6 has significant strengths over, not only MACCS2, but a large majority of dispersion models used for accident analyses. Alternatively, MACCS2's exposure assessment methods are useful for the Building 9204-2E SAR. Therefore, HGSYSTEM/UF_6 is recommended to be used for the dispersion calculations and MACCS2 exposure assessment methods are recommended to be used to make final consequence estimates. The exposure methods from MACCS2 are relatively simple algebraic equations that can be translated to computer spreadsheets without additional development for analyzing results from the HGSYSTEM/UF_6 dispersion models. Also, the CCDF risk calculation method used by MACCS2 can be translated to computer spreadsheets and used in the Building 9204-2E consequence analysis. Some MACCS2 simulations are also recommended to be used for simple release cases to verify the accuracy of the MACCS2 methodologies used in computer spreadsheet calculations. An additional advantage of using computer spreadsheets is that all calculations will be flexible in accommodating a variety of assumptions for sensitivity studies, and will be readily reproducible by independent reviews. This combination of using the dispersion calculations of HGSYSTEM/UF_6 with the consequence analysis methodologies of MACCS2 should provide an effective, accurate, and defensible analysis for the Building 9204-2E SAR.

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