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Benchmarking Upgraded HotSpot Dose Calculations Against MACCS2 Results

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Abstract

The radiological consequence of interest for a documented safety analysis (DSA) is the centerline Total Effective Dose Equivalent (TEDE) incurred by the Maximally Exposed Offsite Individual (MOI) evaluated at the 95th percentile consequence level. An upgraded version of HotSpot (Version 2.07) has been developed with the capabilities to read site meteorological data and perform the necessary statistical calculations to determine the 95th percentile consequence result. These capabilities should allow HotSpot to join MACCS2 (Version 1.13.1) and GENII (Version 1.485) as radiological consequence toolbox codes in the Department of Energy (DOE) Safety Software Central Registry. Using the same meteorological data file, scenarios involving a one curie release of ^{239}Pu were modeled in both HotSpot and MACCS2. Several sets of release conditions were modeled, and the results compared. In each case, input parameter specifications for each code were chosen to match one another as much as the codes would allow. The results from the two codes are in excellent agreement. Slight differences observed in results are explained by algorithm differences.

Introduction

An upgraded version of HotSpot (Version 2.07) has been developed with the capabilities to read site meteorological data and perform the statistical calculations to determine the 95th percentile consequence result.[1] Specifically, HotSpot Version 2.07 is capable of reading meteorological data in the format required by MACCS2 (Version 1.13.1).[2]

The 95th percentile result from the distribution of consequence results is established by the DOE in Appendix A to DOE-STD-3009-94 as the basis for comparison against the evaluation guideline for nonreactor nuclear facilities.[3] The statistical procedure to determine the 95th result is prescribed to be consistent with that used to determine 95th percentile χ/Q values described in regulatory position 3 of NRC Regulatory Guide 1.145.[4] The χ/Q parameter represents the amount of dilution that the plume has undergone at given distance during atmospheric transport as predicted by the Gaussian plume transport and dispersion model. This statistical treatment relies upon one or more years of representative meteorological data consisting of hourly averages of wind speed and measure of atmospheric stability at minimum. In regulatory position 3 of NRC Regulatory Guide 1.145, a χ/Q value is calculated for each hourly record of meteorological data and sorted. The χ/Q value that is exceeded by 5% of the calculated χ/Q values establishes the 95th percentile result.

The added statistical capabilities for calculating χ/Q values in accordance with Appendix A to DOE-STD-3009-94 should, after necessary SQA review requirements are met, allow HotSpot to join MACCS2 (Version 1.13.1)[a] and GENII (Version 1.485)[b] as radiological consequence toolbox codes in the Department of Energy (DOE) Safety Software Central Registry (i.e., the *Toolbox*).[c] This paper compares consequence results from HotSpot against those from MACCS2. Benchmark cases were performed in which input parameter specifications for each code were chosen to match one another as much as the codes would allow. In addition, a few sensitivity cases were performed to highlight unique capabilities of each code.

Overview of the Gaussian Plume Model

Both HotSpot and MACCS2 use the Gaussian plume model to transport and disperse a release of radiological material to the atmosphere. A review of the model and its inputs is given to show how meteorological data are used.

Atmospheric Turbulence and Measure of Stability

In the Gaussian transport and dispersion model, horizontal and vertical dispersion coefficients (σ_y and σ_z, respectively) are typically determined from established curves showing σ_y and σ_z as a function of atmospheric stability and downwind distance. Atmospheric stability is inferred from measured and/or observed meteorological data.[6]

Atmospheric boundary layer turbulence is thought of as having two sources. First, mechanical turbulence caused by roughness elements, e.g., irregular surface features, vegetation, trees, buildings, etc. that generate turbulence as wind blows over their rough surfaces and turbulent wakes form. As wind speed increases mechanical turbulence increases due to increased wind shear near the surface. Second, buoyancy (or thermally) generated turbulence is caused by the sun's heating of the earth's surface, or by any mechanism that provides a source of warm, buoyant air near the surface. Warm air near the surface can produce large thermal eddy structures and unstable vertical thermal gradients under low wind speed conditions. As the wind speed becomes very strong, however, the large thermal eddy structures are destroyed by wind shear.

The Pasquill-Gifford (P-G) categories for atmospheric dispersion are a simplified way to determine the turbulence intensity level. Turbulence intensity is the underlying factor for determining the amount of spread of a dispersing cloud as it moves downwind. Pasquill first used

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[a] Version 2.4 of MACCS2 has been released by Sandia National Laboratory (SNL) in 2009, but this version has not yet been added to the DOE toolbox.

[b] Version 2.0 of GENII was released by Pacific Northwest National Laboratory (PNNL) in 2002, but this version has not yet been added to the DOE toolbox.[5]

[c] http://www.hss.energy.gov/CSA/CSP/SQA/central_registry.htm

the standard deviations of the vertical and horizontal wind direction fluctuations to determine turbulence intensity.[7] He then expressed the dispersion coefficients, σ_y and σ_z, for the horizontal and vertical spread of a ground level or elevated plume, in terms of these fluctuations. The practical problem with this approach is that the wind direction fluctuations can only be measured with rather specialized instruments (e.g., bidirectional wind vanes). Gifford provided a turbulence typing scheme for relating the temperature gradient to the standard deviations of the wind direction fluctuations.[8] Six categories designated with the letters A-F were used to relate the amount of spread of the dispersing plume as it moved downwind. These categories were based on the results of dispersion experiments that had been carried out during project Prairie Grass in the U.S. during the 1950s.[9]

The stability categories A-F were meant to reflect the state of atmospheric stability. The unstable categories A, B, and C reflect daytime solar heating and the stable categories E and F reflect nighttime conditions. At the time Pasquill and Gifford devised the dispersion categories, the neutral category D was presumed to represent the transitional state between early morning sunrise and the onset of solar heating, or the period around sunset when solar heating disappears and the surface begins to cool by radiative processes. As time has progressed, the important role of wind speed in promoting neutral stability conditions became better understood.

Dispersion Coefficient Sets

The P-G set of dispersion coefficients based on the project Prairie Grass field experiments are shown in Figure 1 in their original form as plotted curves.[7, 10] Tadmor and Gur later developed curve-fit equations that were later corrected for typographical errors by Dobbins.[11, 12] This set of dispersion coefficients is available for MACCS2 use in both equation form and tabular form.

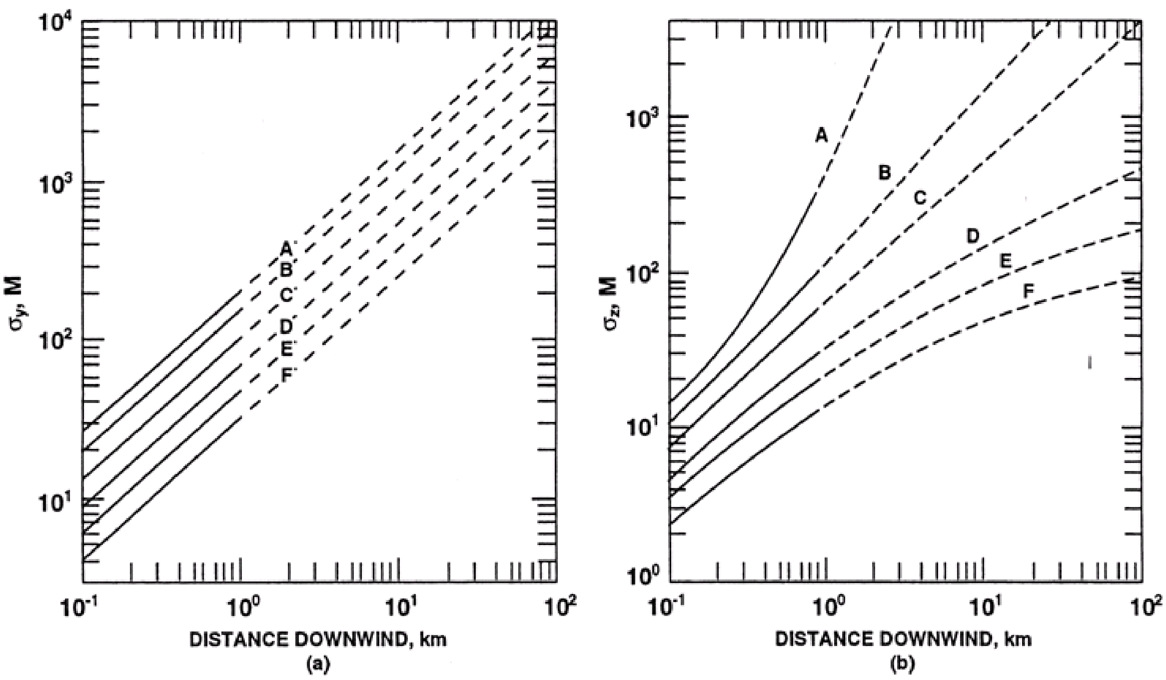

Figure 1 Pasquill-Gifford Curves for Dispersion Coefficients (a) Horizontal and (b) Vertical.

It is easily seen from Figure 1 that less dispersion occurs under stable conditions (e.g., stability category F).

A set of dispersion coefficient formulations was developed by Briggs that combines the Prairie Grass data with data from field experiments of elevated releases taken at Brookhaven National Laboratory (BNL) and the Tennessee Valley Authority (TVA).[10, 13, 14] This set of dispersion coefficient formulations is shown in Table 1 as the Briggs open country set. Also shown in Table 1 are the dispersion coefficient formulations developed by Briggs for urban settings based on experiments taken in St. Louis.[10, 13, 14] Greater dispersion is observed in urban settings due to the increased mechanical turbulence from building structures and from enhanced buoyancy effects from heating of concrete surfaces (urban heat island effect).[10] Both the Briggs open country and Briggs rural sets of dispersion coefficients are available in HotSpot. MACCS2 allows these sets of dispersion coefficients to be input in tabular form.

Open Country		
Atmospheric Stability Class	**σ_y [m]**	**σ_z [m]**
A	$0.22x\ (1+0.0001x)^{-1/2}$	$0.20x$
B	$0.16x\ (1+0.0001x)^{-1/2}$	$0.12x$
C	$0.11x\ (1+0.0001x)^{-1/2}$	$0.08x\ (1+0.0002x)^{-1/2}$
D	$0.08x\ (1+0.0001x)^{-1/2}$	$0.06x\ (1+0.0015x)^{-1/2}$
E	$0.06x\ (1+0.0001x)^{-1/2}$	$0.03x\ (1+0.0003x)^{-1}$
F	$0.04x\ (1+0.0001x)^{-1/2}$	$0.016x\ (1+0.0003x)^{-1}$
Urban		
Atmospheric Stability Class	**σ_y [m]**	**σ_z [m]**
A-B	$0.32x\ (1+0.0004x)^{-1/2}$	$0.24x\ (1+0.001x)^{+1/2}$
C	$0.22x\ (1+0.0004x)^{-1/2}$	$0.20x$
D	$0.16x\ (1+0.0004x)^{-1/2}$	$0.14x\ (1+0.0003x)^{-1/2}$
E-F	$0.11x\ (1+0.0004x)^{-1/2}$	$0.08x\ (1+0.0015x)^{-1/2}$

Table 1 Briggs' Dispersion Coefficients.[1,13]

Gaussian Plume Model

The basic form for the Gaussian plume model for radiological releases is given as follows[15]:

$$\chi(x,y,z)=\frac{Q}{2\pi\sigma_y\sigma_z u}\exp\left[-\frac{1}{2}\left(\frac{y}{\sigma_y}\right)^2\right]\left\{\exp\left[-\frac{1}{2}\left(\frac{z-H}{\sigma_z}\right)^2\right]+\exp\left[-\frac{1}{2}\left(\frac{z+H}{\sigma_z}\right)^2\right]\right\} \qquad \text{Eq. (1)}$$

where:

- χ = time-integrated atmospheric concentration [Ci-s/m^3]
- Q = source term release [Ci]
- x = downwind distance (relative to source location) [m]
- y = crosswind distance (relative to plume centerline) [m]
- z = vertical axis distance (relative to ground) [m]
- H = effective release height (relative to ground) [m]

σ_y = horizontal dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the crosswind axis direction [m]

σ_z = vertical dispersion coefficient (function of x), representing the standard deviation of the concentration distribution in the vertical axis direction [m]

u = average wind speed [m/s]

The last term accounts for reflection of the plume at the ground surface through adding an image source at distance H beneath the ground surface. Equation 1 does not account for depletion of material from the plume due to deposition effects.

Hourly data from the meteorological data file provides the values for u. The meteorological data file also provides the atmospheric stability class which is the basis for the σ_y and σ_z values.

For a ground-level release (i.e., H = 0) with the receptor of interest at ground level (i.e., z = 0), the concentration on the plume centerline (i.e., y = 0) is given by following simplified for m of the Gaussian plume equation.

$$\chi(x,0,0)=\frac{Q}{\pi\sigma_y\sigma_z u} \qquad \text{Eq. (2)}$$

Benchmark and Sensitivity Cases

Using the same meteorological data file, scenarios involving a one curie release of ^{239}Pu were modeled in both HotSpot and MACCS2 to benchmark the HotSpot results against those of MACCS2. The Briggs open country set of dispersion coefficients were used in the following three benchmark cases.

- Ground-level release with no deposition
- Ground-level release with deposition (deposition velocity[d] input of 1 cm/s)
- 60-m stack release with deposition (deposition velocity input of 0.1 cm/s)

In addition to the benchmark cases, a few sensitivity cases were performed to highlight unique capabilities of each code. The sensitivity cases for MACCS2 involved using the Tadmor-Gur dispersion coefficients in place of the Briggs open country dispersion coefficients that were used in the benchmark cases. Recall that the project Prairie Grass experiments provide the basis for the Tadmor-Gur dispersion coefficients. The short grassy surfaces associated with these experiments have been characterized with a surface roughness length of 3 cm.[e] The *surface roughness length* is a measure of the amount of atmospheric mechanical turbulence that is induced by the presence of surface roughness elements such as vegetation and man-made

[d] The deposition velocity represents the ratio of the deposition flux and the ground-level air concentration.

[e] As a general rule, the surface roughness length is considered to be approximately 0.1 times the average height of roughness elements located in the transport region of interest.

structures. For the MACCS2 sensitivity cases, surface roughness lengths of 3 cm and 100 cm were used. For the 100 cm case, an adjustment to the σ_z parameter is made corresponding to the ratio of 100 cm to 3 cm raised to the 0.2 power[10] ([100/3]^0.2 = 2.0).

In the benchmark cases, the capability of HotSpot to model the increase in wind speed with elevation was effectively disabled so that the wind speed in the meteorological data file was used directly without adjustment. The wind speed profile is typically considered to follow a power-law relationship (Figure 2) with the power-law exponent a function of atmospheric stability class. Different sets of power-law exponents have been developed for rural and urban terrain. HotSpot requires the reference height for the wind speed to be input. For a ground level release, no adjustment in wind speed is made if the reference height is specified to be 2 m (Figure 2). For an elevated release, no adjustment in wind speed is made if the reference height for wind speed is set equal to the release height. For the benchmark cases, the HotSpot reference height for wind speed was set to 2 m for the ground-level release cases and to 60 m for the stack release case. An additional sensitivity case was run for the 60 m stack release in which HotSpot reference height for wind speed was set to 10 m. A reference height of 10 m corresponds to the basis for the wind speed data in the meteorological data file that was originally developed for MACCS2, following the recommendation given the MACCS2 user's manual.[2] MACCS2 does not adjust the wind speed for the height of release.[f]

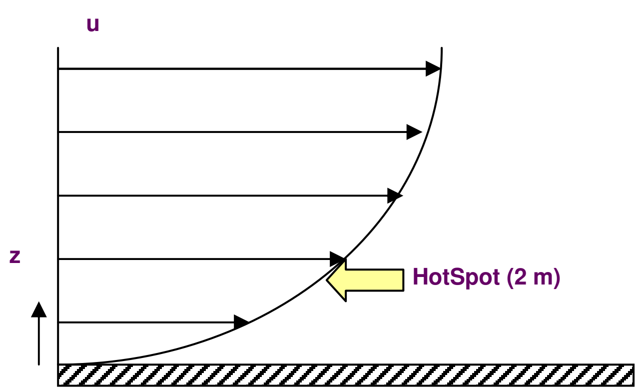

Figure 2 Wind Speed Profile.

Results

Results are presented in terms of the 95th percentile TEDE result output by each code for distances from 100 m to 5000 m. The TEDE includes the 50-year committed effective dose equivalent (CEDE) from inhalation of radionuclides from the plume and inhalation of resuspended material (that initially deposited on the ground from the plume), the effective dose equivalent (EDE) from direct external exposure to radioactive material in the plume (cloudshine), and the EDE from exposure to radioactive material deposited on the ground

[f] The algorithm in MACCS2 for determining the plume rise of buoyant release does make use of wind speed correction with height.[16]

(groundshine).[1, 17] The CEDE is directly proportional to the χ/Q value.[1, 17] Typically the CEDE is the dominant pathway for dose, particularly for alpha-emitters like plutonium.[17]

Graphical Presentation of Results

The results for the two ground level release cases are shown in Figure 3 (no deposition) and Figure 4 (deposition). Similar behavior is exhibited in both set of results. Excellent agreement is shown between results that are based on the Briggs open country dispersion coefficients. The MACCS2 results using the Tadmor-Gur dispersion coefficients and 3 cm surface roughness length are slightly lower. The MACCS2 results using the Tadmor-Gur dispersion coefficients and 100 cm surface roughness length are even lower. For the no-deposition case, the results for the 100 cm surface roughness run are nominally a factor of two lower than the 3 cm surface roughness run, consistent with Equation 2 and the calculation presented earlier for the adjustment to the σ_z parameter for surface roughness length of 100 cm. With deposition modeled, the difference is a nominally a factor of two close to the source; but the difference decreases gradually as distance increases. In the MACCS2 model, the amount of deposition is proportional to the ground-level air concentration; such that more deposition occurs in the 3 cm surface roughness length run than with the corresponding 100 cm surface roughness length run.[17]

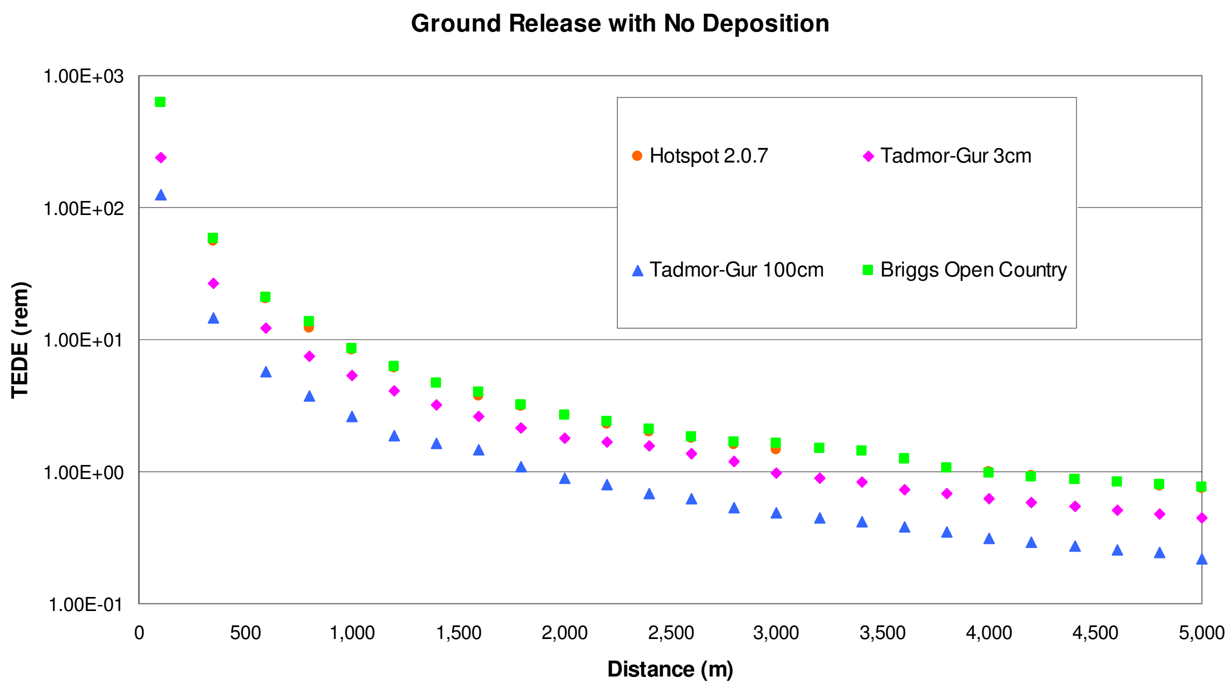

Figure 3 TEDE Results for Ground Level Release with No Deposition.

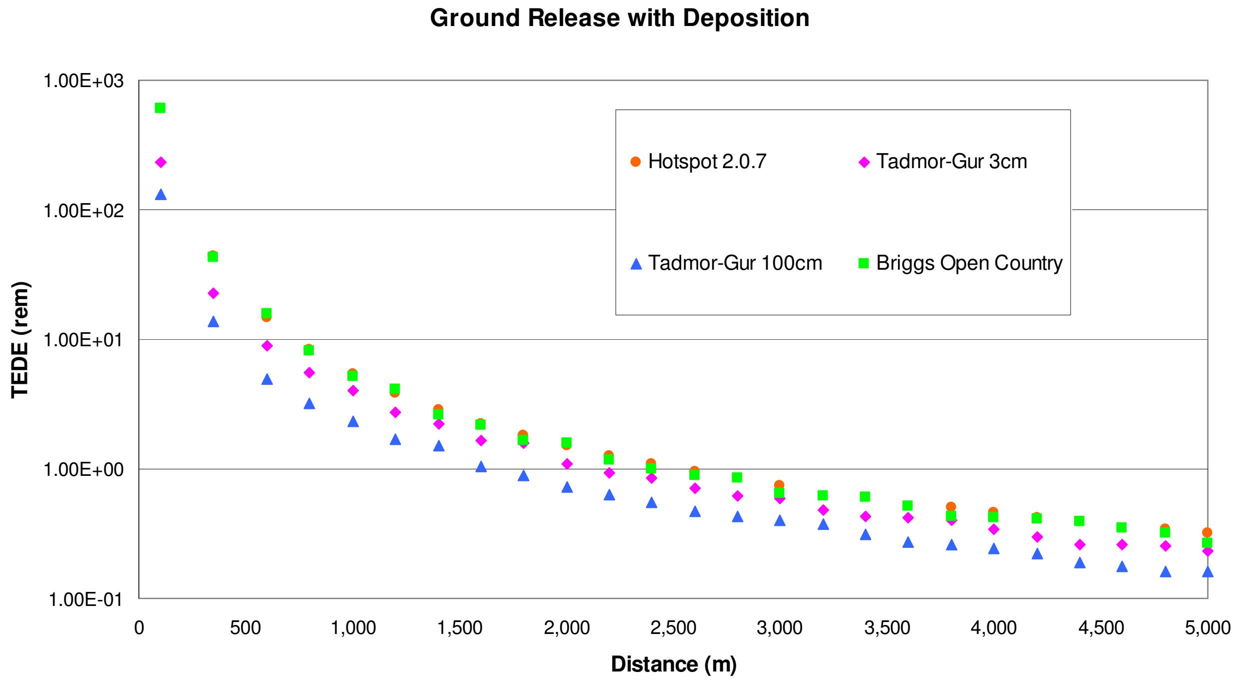

Figure 4 TEDE Results for Ground Level Release with Deposition.

The results for the two stack release cases are shown in Figure 5 (no adjustment of wind speed in HotSpot) and Figure 6 (wind speed adjusted in HotSpot). The wind speed adjustment in HotSpot has a significant effect in reducing the TEDE results by about a factor of two. These lower TEDE results are consistent with Equation 1, which shows that the χ/Q value (and thus the TEDE) are inversely proportional to the wind speed. Excellent agreement is shown between HotSpot and MACCS2 results that are based on the Briggs open country dispersion coefficients (Figure 5). A few other observations are apparent with respect to the sensitivity cases as shown in Figure 5 that highlight different behaviors than those observed with the ground-level releases.

- Different cases produce the maximum results depending upon the location. In contrast, for the ground level release cases, relative results between the cases over the range distances tested follow more orderly trends. A likely contributing factor is related to the atmospheric stability represented by the plotted points. For the ground-level cases, the 95th results plotted are expected to all correspond to stable atmospheric conditions (e.g. E or F stability category). In contrast for an elevated release, more unstable atmospheric stability conditions lead to higher ground-level concentrations close to the source. Unstable atmospheric conditions provide greater amount of dispersion (plume spread) to support higher ground-level concentrations near the source. Further from the source, the more stable atmospheric conditions lead to higher ground-level concentrations similar to the ground level release cases.

- The 100 cm surface roughness length case (MACCS2 with Tadmor-Gur dispersion coefficients) produced the maximum results in the approximate range of 600 m to 1600 m. In contrast, this case produced the minimum results for all distances for the ground-level releases.

- At distances greater than 2000 m, the Briggs dispersion cases (MACCS2 and HotSpot) produce the maximum results showing the same trend as observed with the ground-level cases. At the 5000 m location, the absolute values of the stack results are close to those of the ground-level results.

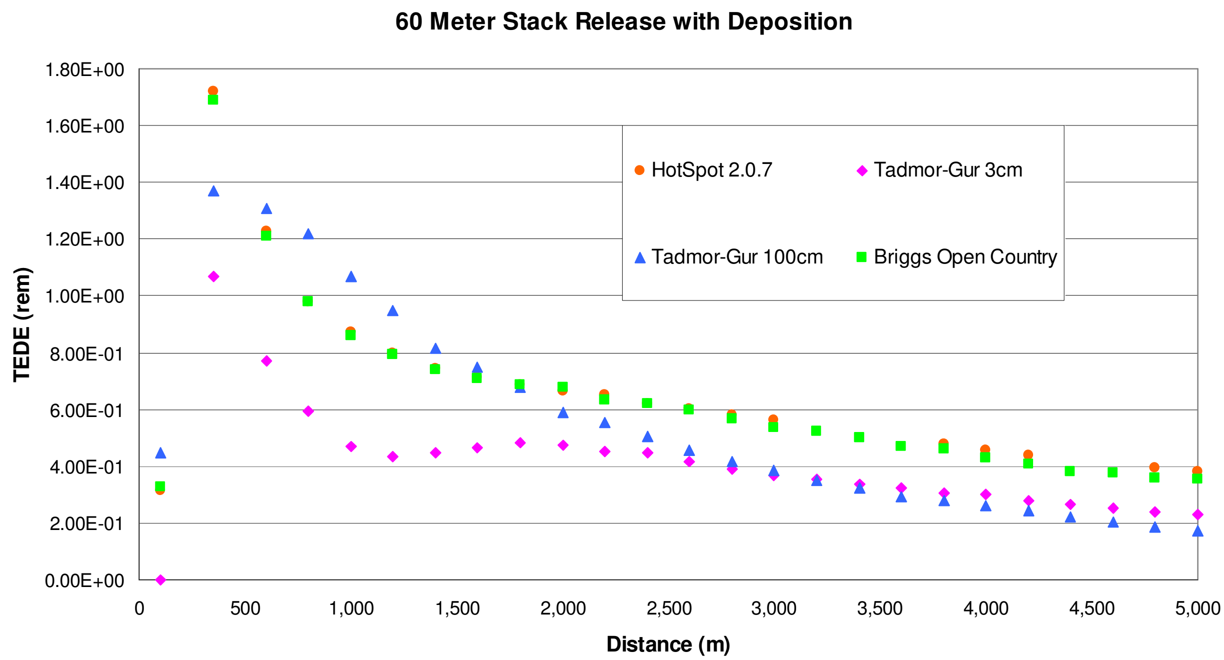

Figure 5 TEDE Results for Stack Release.

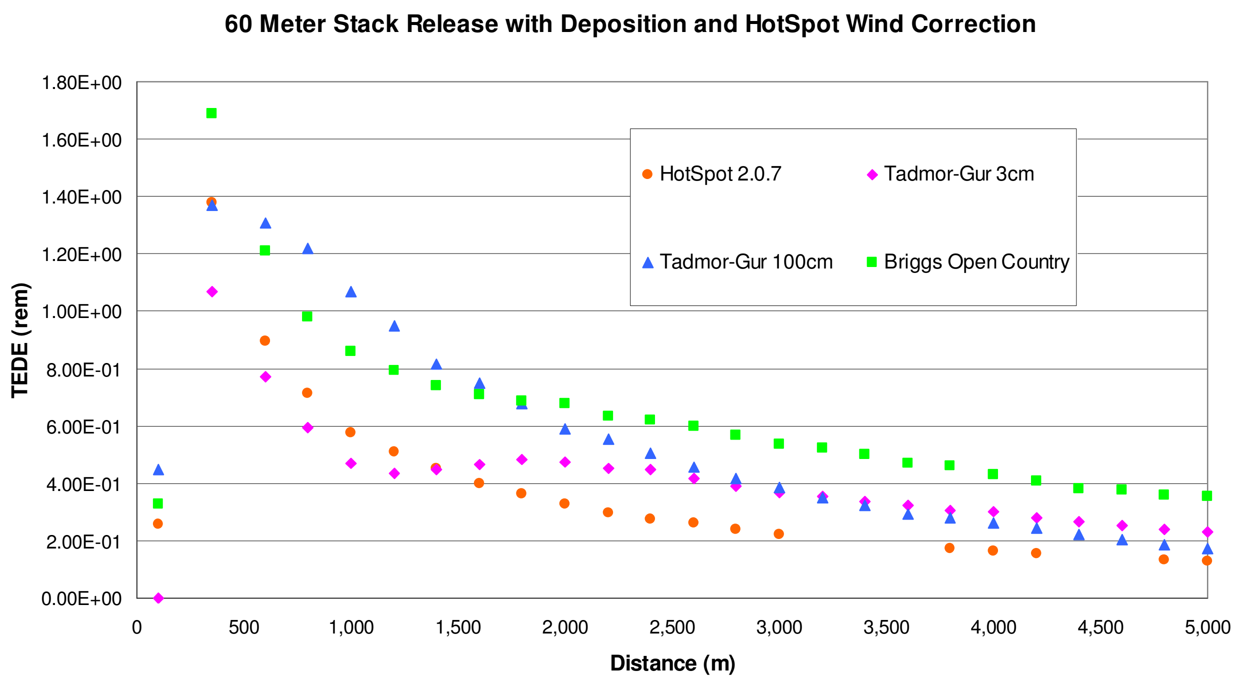

Figure 6 TEDE Results for Stack Release with HotSpot Wind Speed Correction.

Discussion of Result Differences

While there is generally excellent agreement between HotSpot and MACCS2 results with the Briggs open country dispersion coefficients, there are some differences. Figure 7 provides a graphical representation of the differences between the MACCS2 and HotSpot results. Equation 3 defines the percent difference that is plotted in Figure 7.

$$\text{Percent difference} = 100\% \times (TEDE_{MACCS2} - TEDE_{HotSpot})/TEDE_{MACCS2} \qquad \text{Eq. (3)}$$

Thus, negative values in Figure 7 represent lower results with MACCS2 in comparison with the HotSpot results.

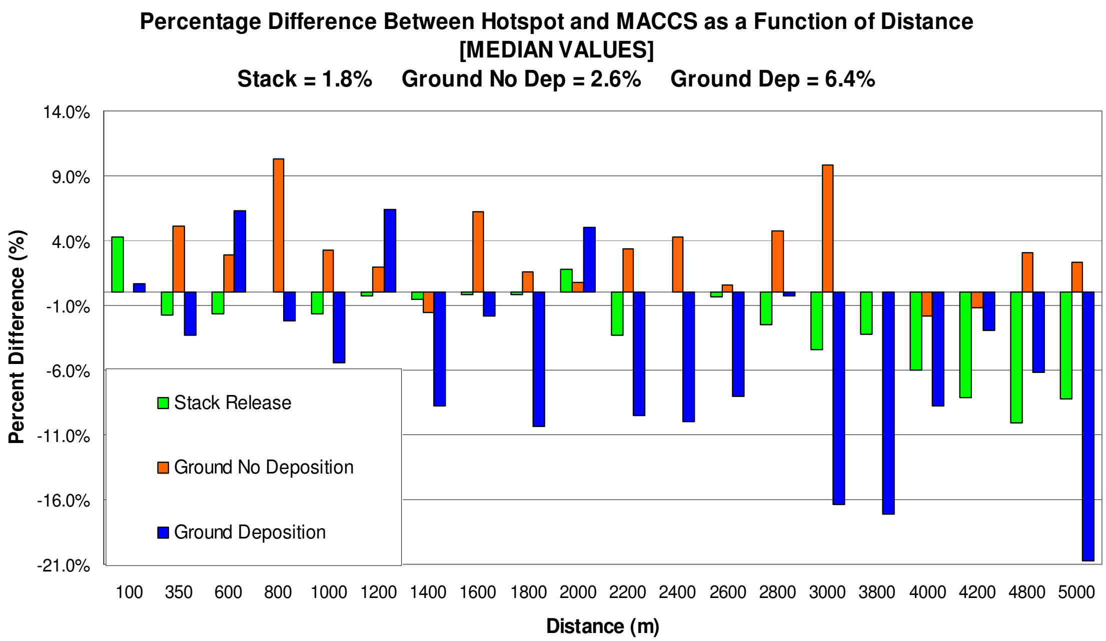

Figure 7 Difference Analysis.

Three sources have been identified as possible contributors to differences observed in Figure 7.

- Plume Transport and Dispersion Algorithm
  - HotSpot uses constant meteorological conditions throughout the entire period of plume travel.
  - With MACCS2 after each hour of plume transport time, meteorological conditions of the next hour are used in the transport and dispersion calculations until the plume reaches the final location of interest.

- Calculation Algorithm
  - Direct calculation for locations of interest.
  - MACCS2 provides output that is "representative of the entire length of the spatial element."[2] Inner and outer boundaries of the grid elements are defined in an input file such that the locations of interest are at the midpoint of these elements. In addition, the

output results are determined from interpolation of complementary probability distribution functions. The MACCS2 user's guide (p. 2-20) states that interpolation errors of 10% or more are possible.[2]

- Plume Deposition/Depletion Model
  - HotSpot uses model described in *Meteorology and Atomic Energy*.[1, 18]
  - MACCS2 uses model developed by Chamberlin.[2, 19]

Concluding Remarks

The favorable benchmarking of HotSpot (Version 2.07) results against those from MACCS2 (Version 1.13.1) provides confidence in using HotSpot results for accident analyses supporting DSAs. A beneficial unique feature of HotSpot is that it allows up to five years of meteorological data to be involved in the statistical analysis.

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