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Deposition Velocity Estimation with the GENII v2 Software

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Abstract

In 2010, the Department of Energy (DOE) Chief of Nuclear Safety and Office of Health, Safety and Security (HSS), with the support of industry experts in atmospheric sciences and accident dose consequences analysis, performed detailed analyses of the basis for the dry deposition velocity (DV) values used in the MACCS2 computer code. As a result of these analyses, DOE concluded that the historically used default DV values of 1 centimeter/second (cm/s) for unfiltered/unmitigated releases and 0.1 cm/s for filtered/mitigated releases may not be reasonably conservative for all DOE sites and accident scenarios.

HSS recently issued Safety Bulletin 2011-02, *Accident Analysis Parameter Update*, recommending the use of the newly developed default DV, 0.1 cm/s for an unmitigated/unfiltered release. Alternatively site specific DV values can be developed using GENII version 2 (GENII v2) computer code.

Key input parameters for calculating DV values include surface roughness, maximum wind speed for calm, particle size, particle density and meteorological data (wind speed and stability class). This paper will include reasonably conservative inputs, and a truncated parametric study.

In lieu of the highly-conservative recommended DV value (0.1cm/s) for unmitigated/unfiltered release, GENII v2 has been used to justify estimated 95th percentile DV values. Also presented here are atmospheric dilution factors (χ/Q values) calculated with the MACCS2 code using the DV values from GENII v2, χ/Q values calculated directly with GENII v2, and a discussion of these results compare with one another.

This paper will give an overview of the process of calculating DV with GENII v2 including a discussion of the sensitivity of input parameters.

Introduction

In the wake of HSS Safety Bulletin 2011-02 (Ref. 1) either a conservative dry deposition velocity (DV) value of 0.1 cm/s must be used or a site specific DV can be calculated with the GENII v2 software. Deposition velocity (DV) is reliant upon several factors and is computed in GENII v2 from the inverse sum of various resistances and the settling velocity for particles such that the total deposition velocity can be determined by Equation 1.

$$DV = [Ra + Rb + Rc + Ra Rb Vg]^{-1} + Vg \quad (1)$$

In Equation 1 the subscripts for the resistances R, represent the atmospheric layer (a), the quasi-laminar sublayer (b), and the canopy layer (c) which represents the bulk resistance of various surfaces. Gravitational settling, V_g is zero for gases and R_c is zero for particles. The resistance components depend upon meteorological conditions as well as the properties of the surface. Using these resistance factors, GENII v2 computes the DV (units of m/s). The DV is not output in GENII v2, but can be determined from other output parameter values.

GENII v2 uses the Gaussian plume model and meteorological data to calculate for a given release the time-integrated air concentration (χ , units of Bq-s/m³) near the ground, which is output by GENII v2. GENII v2 also calculates the ground deposition (ω , units of Bq/m²) from the product of the deposition velocity and the time-integrated air concentration near ground level. Since the ground deposition is also an output parameter, its output can be used together with the output of the time integrated concentration to calculate the DV calculation as shown in Equation 2.

$$DV = \omega_{ij}(t) / \chi_{ij}(1,t) \quad (2)$$

where:

$\omega_{ij}(t)$ = Total dry ground deposition at an i distance in the j direction at time t (Bq/m²)

$\chi_{ij}(1,t)$ = Time-integrated air concentration at a height of 1 m at an i distance in the j direction at time t (Bq-s/m³)

The purpose of this paper is three-fold:

- to give an overview of the process of calculating dry DV for a particulate release with GENII v2
- to provide a parametric study of three input parameters: stability class (SC), wind speed (WS), and surface roughness (SR)
- to provide a comparison between the results of atmospheric dilution factor (χ/Q) from GENII and MACCS2 for given meteorological input (χ/Q has units of s/m³ and is simply χ normalized by the release quantity, Q in units of Bq).

Methodology for Calculating χ/Q with GENII v2 and MACCS2

Create the GENII v2 Site Conceptual Model and Inputs

The GENIIV2 calculation for the site-specific deposition velocity makes use of three components that are represented by icons on the FRAMES workspace: Constituent [con1], User Defined [usr2], and Air [air3]. For complete guidelines for setting up the Site Conceptual Model, see the GENII Version 2 User's Guide (Ref. 2) and the GENII Version 2 Getting Started Guide (Ref. 3).

For each of these components, the user selects among available database or model options. The deposition velocity calculations make use of the following selections for database and models for the three components as shown in the second column of Table 1. The third

column in Table 1 shows the input parameter requirements for each selected database or model and the value used for each parameter in the DV calculations. After each individual input page for a module is filled out, the user must go to “file” on the menu bar and select “Save and Exit” or all inputs will be lost and an error message will be shown on the GUI.

Table 1. GENII Database and Models Used in Deposition Velocity Calculations

Component	Database or Model	Input Parameters
Constituent [con1]	I. GENII Radionuclide Database Selection	A. Constituents of Concern [Pu-238, Pu-239 or mixture]
User_Defined [usr2]	II. AFF Air Module	A. Release <ol style="list-style-type: none"> 1. Type (point or area) [point source] 2. Exit area of source [zero] 3. Exit height of source [zero] 4. Height of adjacent structure [zero] 5. Exit velocity of source [zero] 6. Exit temperature of source [20°C] 7. Ambient air temperature [20°C] 8. Constituent [Pu-238, Pu-239] {after Flux Types entered} 9. Release Duration [yr – start = 0 and end = 1] 10. Release Rate [1 Bq/yr for both timeframes]* B. Flux Types (Particle Characteristics) <ol style="list-style-type: none"> 1. Particle radius [0.5 or 1.5] 2. Particle density [1 gm/cc] C. Release Multiplier (Options Tab) [not used]
Air [air3]	III. GENII V.2 Air Module – Acute 95 th Percentile	A. Model - Radial Grid Definition <ol style="list-style-type: none"> 1. Number of Sectors (16 or 36) [16 sectors] 2. Distances (for 10 locations) [100 m to 3,000 m] B. Model - Parameters <ol style="list-style-type: none"> 1. Sigma Parameterization [Pasquill-Gifford(NRC)] 2. Calm wind distribution [not used] C. Model - Default Parameters <ol style="list-style-type: none"> 1. Minimum wind speed during plume rise [not used] 2. Sigma for semi-infinite cloud shine [not used] 3. Transfer resistance for iodine [10 s/m; not used] 4. Transfer resistance for particles [100 s/m] 5. Maximum wind speed for calm [0.5 m/s] ** D. Model – Meteorological Files [path and file name] E. Source Information <ol style="list-style-type: none"> 1. Plume rise option [not used] 2. Enhanced dispersion option [not used]

* With a 1 Bq release, the output of χ represents the χ/Q value.

** Recommended by EPA (Ref. 4) and consistent with MACCS minimum wind speed.

Reference 5 details the selection of each component database or model and the associated input data specifications including justifications. All input specifications are consistent with the methodology that is outlined in Reference 6 which documents the analysis for the Los Alamos National Laboratory (LANL) site performed by the GENII v2 code developer.

Key Input Parameters:

The DV and χ/Q calculations are a function of several site-specific parameters, which include the local meteorology (wind speeds and stabilities), maximum wind speed for “calm” conditions, local surface roughness, and particle size and density.

Surface Roughness

The surface roughness length is a measure of the amount of mechanical mixing introduced by the surface roughness elements over a region of transport. Roughness elements include, but are not limited to, human built structures, vegetation, and other surface features. As a general rule, z_0 is approximately 0.1 times the average height of roughness elements located on the transport region of interest. Very flat surfaces have relatively constant wind speed-elevation profiles and small values of z_0 . Surfaces with tall obstacles have parabolic wind speed-elevation profiles and large values of z_0 . The EPA AERSURFACE software is a tool that is available to determine surface roughness length for a region up to 5 km in radius using input of land cover data from the U.S. Geological Survey.

Maximum wind speed for “calm”

Unrealistically high estimates can be obtained under calm conditions. For site-specific monitoring, the EPA recommends for using a wind speed of 0.5 m/s for a “calm” wind (Ref. 4). In general, if the starting threshold wind speed for the anemometer readings is ≤ 0.5 m/s, the maximum wind speed for “calm” should be 0.5 m/s. With this specification, 0.5 m/s is the minimum wind speed used in the atmospheric transport and dispersion calculations. The 0.5 m/s threshold value is consistent with the MACCS2 code. MACCS2 substitutes a value of 0.5 m/s for the wind speed whenever it reads a wind speed value of less than 0.5 m/s from the meteorological data file.

Particle Size Determination

A particle distribution with a 1 micrometers (μm) aerodynamic equivalent diameter (AED) size and unit density is conservatively assumed as a lower bound. This has the effect of minimizing the deposition velocity and making it relatively uniform regionally (no early fallout of large particles). To fit within the 2-4 μm range specified in the HSS Safety Bulletin (Ref. 1) a 3 μm particle size with unit density (i.e., 3 μm AED) can also be selected. A 0.3 μm diameter PuO_2 particle (density = 11.46 g/cc) is approximately 1 μm AED and a 0.9 μm diameter PuO_2 particle is approximately 3 μm AED. The DV is relatively insensitive to particle size in the 1 to 3 μm AED size range. The DV results performed for WIPP show differences of approximately 2% between the DV calculated with 3 μm AED and the DV calculated with 1 μm AED.

Methodology for Creating meteorological input file for GENII v2

The calculations documented in this paper use hourly GENII v2 meteorological files. More information on the different types of GENII v2 meteorological files can be found in Reference. 2.

The first line of a GENII meteorological file consists of 2 numbers [surface roughness length (m) and wind speed reference height (m)] separated by a comma. For a surface roughness of 10 cm, and a wind speed reference height of 10m, the first line would be: 0.10, 10.0

All other lines consist of 12 numbers separated by a space or a comma (it doesn't matter which) and include: year, month, day, hour, stability class (SC), flow vector [degrees], wind speed (WS) [m/s], dry bulb T [K], mixing height [m], precipitation type, precipitation rate [mm/h], and weighting factor

The second line corresponds to the first hour of the year and may look like:

2000 1 1 1 4 45.0 3.1 100.00300.0 0 0.00 1.0

Additional information on GENII meteorological files is provided in Reference 6 which documents the analysis for the Los Alamos National Laboratory (LANL) site performed by the GENII v2 code developer

Performing Model Runs for the GENIIV2

Once all the parameters are entered into GENII v2 (i.e., the stoplights for the User Defined" and the "Air" icon are yellow), the model can be run. To run GENII v2, one just simply selects the icon at the beginning of an exposure pathway (i.e., "User Defined" icon) and selects the "Run Model". This is done for all modules in the flow pathway for the Site Conceptual Model. Upon running the module, the "Print/View User Input" and "Print/View User Output" options are activated and the stop light should turn green to indicate that the model has been successfully run. This process is repeated for each icon in the flow pattern of the Site Conceptual Model until all the stoplights are green.

Determining the Deposition Velocity from the Output Data

To view the results, go the "Air" icon, right click the icon, and select the "View/Print Module Output" from the drop down menu. Select the "ATO Text View". This entire data set can be copied and pasted into an EXCEL worksheet for further calculations. Of interest for the DV calculation are the "Air Exposure" and the "Total Deposition-Dry" outputs.

The deposition velocity (m/s) determined by dividing the amount of material deposited on the ground (ω) in Bq/m² or Ci/m² by the time integrated air exposure (χ) in Bq-s/m³ or Ci-s/m³. The average, minimum, and maximum deposition velocity for each distance across all the radials is determined and the total average, minimum and maximum deposition velocity is determined from all the resultant data.

Inputs and Assumptions

Table 2 gives the input for the sensitivity study for deposition velocity inputs.

Table 2: Parametric Values

Input #	Parameter (units)	Value
1	Wind Speed (m/s)	0.5, 1.0, 2.0
2	Stability Class	D (neutrally stable), E (slightly stable), F (moderately stable)
3	Surface Roughness Length (m)	0.1, 0.4, 0.7, 1.0

The parametric values given in input 3 will be used for the parametric study of deposition velocity with GENII v2. For the comparison of MACCS2 and GENII v2 χ/Q values, surface roughness of 10 cm was used.

Input 4: The meteorological file used for the comparison between MACCS2 and GENII v2 χ/Q output is given in Ref. 7.

Meteorology

The wind speeds, stability classes, and surface roughness lengths given in Table 1 were used to create 36 meteorological files (each with constant wind speed and stability class values for all hours of the year) that were used for the parametric study of deposition velocity with GENII v2.

For the comparison of MACCS2 and GENII v2 χ/Q , the MACCS2 meteorological file given in Input 4 will be used. Reference 5 describes how to create a GENII v2 meteorological file from a MACCS2 meteorological file.

Determining the χ/Q from the Output Data with GENII v2

χ/Q is simply the time integrated air exposure information per unit quantity of material released. With 1 Bq/yr assumed for the release rate for the DV calculation, the χ/Q can be determined directly from the information provided in the GENII v2 output. The average, minimum, and maximum χ/Q for each distance across all the radials is determined.

Determining the χ/Q from the Output Data with MACCS

The DV value evaluated using GENII v2 may be entered in MACCS2 in place of the default 0.1 cm/s as recommended in Reference 1. Under the new HSS recommendations, the χ/Q values calculated by MACCS2 are reasonably conservative and defensible provided the DV value is 0.1 cm/s for unfiltered/unmitigated release or calculated using GENII v2.

Results of Analysis

Deposition Velocity Input Sensitivity

The results of the parametric study, comparing the effects of wind speed, stability class and surface roughness on deposition velocity are demonstrated graphically in Figure 1. DV increases with respect to wind speed and surface roughness. To a lesser extent, DV increases slightly as stability increase.

The minimum DV in the parametric study (0.0996 cm/s) was calculated from wind speed of 0.5 m/s, surface roughness of 10 cm, and stability class F which represents moderately stable conditions. The maximum DV in the parametric study (0.747 cm/s) was calculated from wind speed of 2.0 m/s, surface roughness of 100 cm, and stability class D which represents neutrally stable conditions.

Under constant wind speed conditions, deposition velocity does not vary with respect to distance from the source. DV varies minimally by distance when hourly meteorological data is evaluated. In Figure 2, the meteorological data in Reference 7 was used to plot DV with respect to distance from the source for each of the surface roughness values considered in the parametric study.

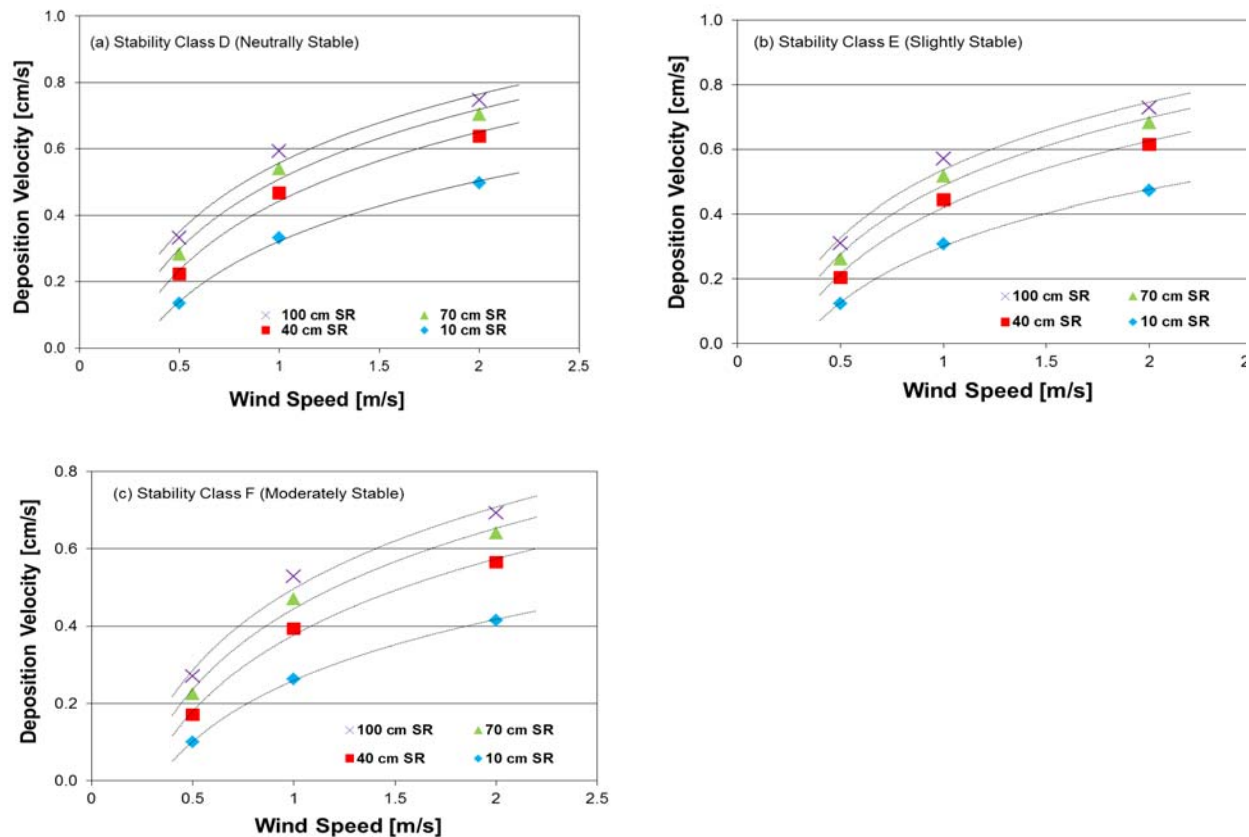


Figure 1. Deposition Velocity Input Sensitivity Study

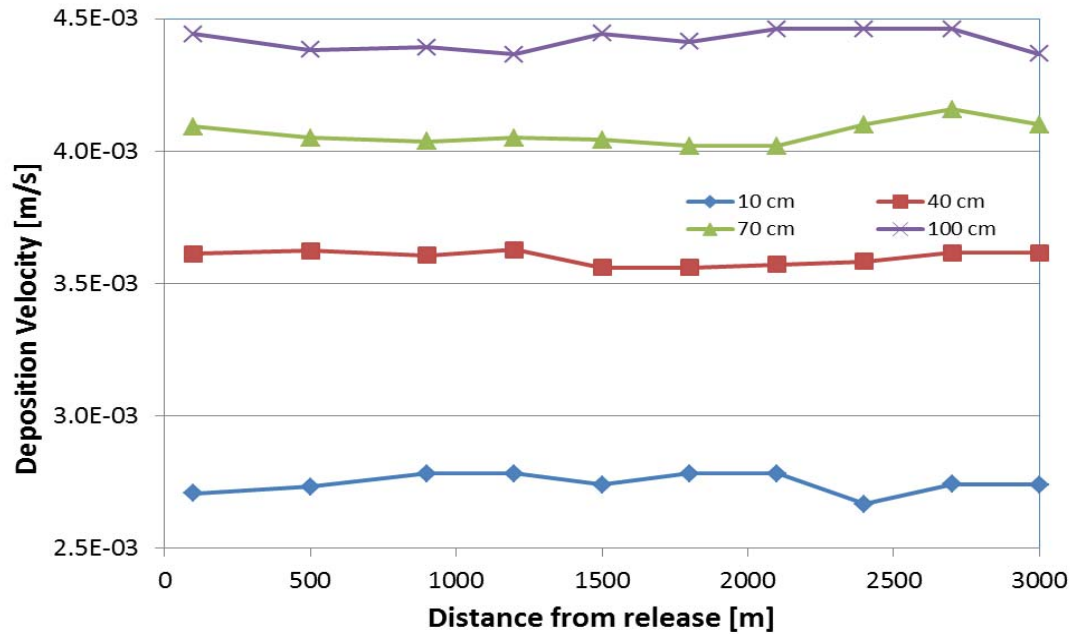


Figure 2: Sensitivity of DV with respect to surface roughness

The minimum wind speed for calm conditions is an input for modeling with GENII v2 which was not included in the parametric study. Hourly wind speeds included in the meteorological input below the minimum are increased to the minimum. The impact of minimum wind speed for calm is dependent on the fraction of calm hours in the meteorological data. However, the impact of this input on DV will be less profound than that of constant wind speed as demonstrated in Figure 1.

A minimum wind speed for calm of 0.5 m/s was used to calculate the results demonstrated in Figure 2.

Figure 3 shows the analogous χ/Q values for each surface roughness length as calculated using GENII v2. While the deposition velocity varies greatly, χ/Q seems to vary little with respect to surface roughness.

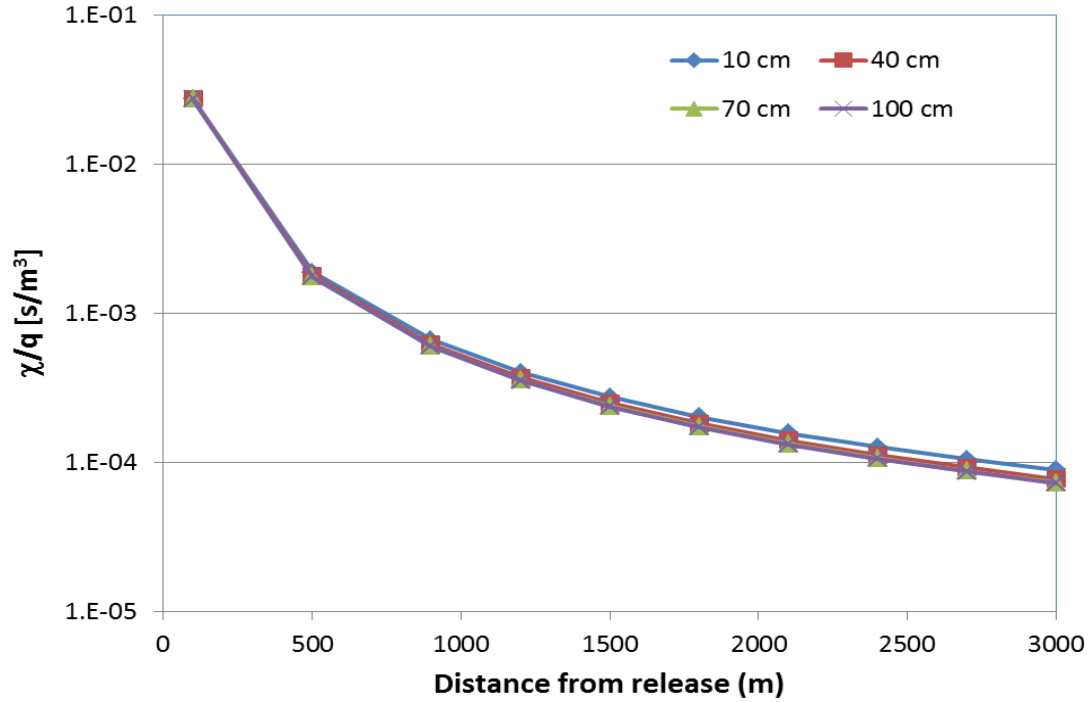


Figure 3: Sensitivity of χ/Q with respect to surface roughness

MACCS2 possesses the ability to calculate the overall 95th percentile χ/Q which is needed for DOE EM engineering calculations (Ref. 8). Currently, GENII v2 does not possess the capability to calculate an overall 95th percentile χ/Q . Instead it calculates the 95th percentile for each of the 16 sectors. Figure 4 shows 95th percentile χ/Q values (with deposition) for MACCS2 with GENII average and maximum sector 95th percentile χ/Q values. Meteorological data from Reference 7 was used as specified in Input 4. The MACCS2 calculations use deposition velocities calculated by GENII for the same meteorological data. As shown in Table 3, the average 95th sector GENII values are 2.2-2.9 times higher than the 95th percentile MACCS2 values, and the maximum 95th sector GENII values are 2.62-3.42 times higher than the 95th percentile MACCS2 values.

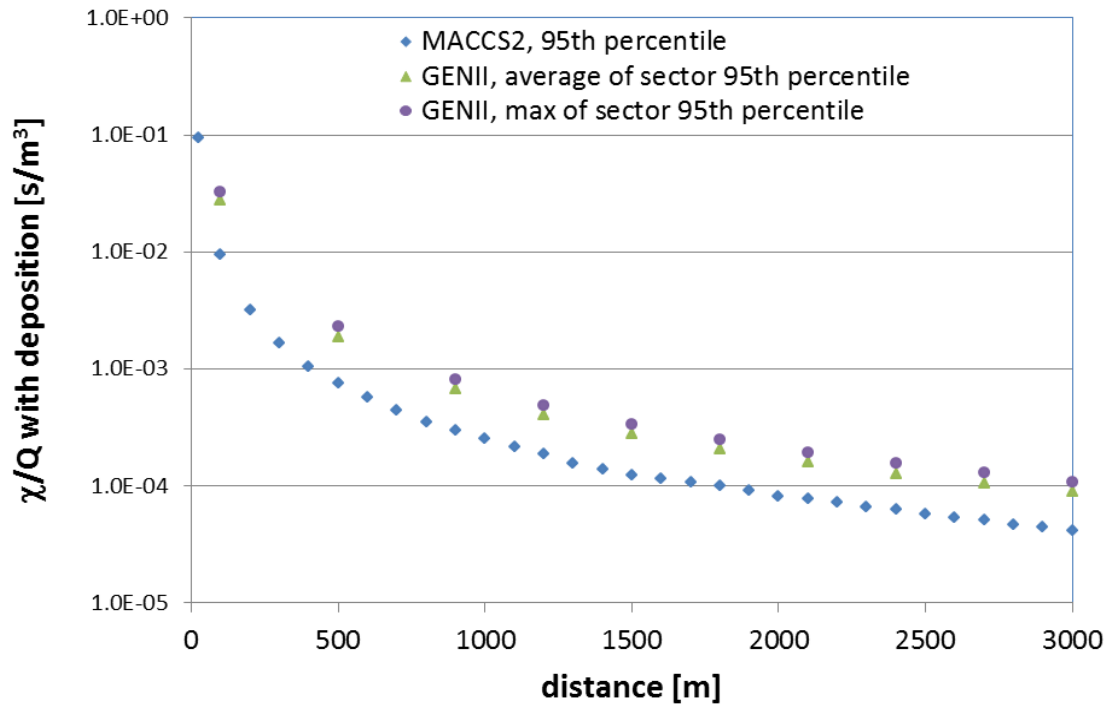


Figure 4: χ/Q comparison between GENII and MACCS2 X/Qs with deposition (SR=10cm)

The MACCS2 results are based on the same approach used in a technically reviewed engineering calculation. The approach is consistent with (1) the HSS Safety Bulletin in 2011 on deposition velocity input and (2) the methodology and input guidance given in the DOE-sponsored MACCS2 Computer Code Application Guidance for Documented Safety Analysis that accompanied MACCS2 inclusion into the DOE Central Registry as toolbox software in 2004 (Ref. 9). DOE DSA application guidance does not exist for GENII v2, and the authors have not used GENII v2 for DSA applications. Therefore, the GENII v2 results should be considered preliminary. For this paper, the authors attempted to make input specifications for GENII v2 that most closely matched those used in the MACCS2 calculations.

Table 3: Ratio of GENII values to MACCS2 values

distance [m]	For GENII average sector 95 th percentile χ/Q	For GENII maximum sector 95 th percentile χ/Q	distance [m]	For GENII average sector 95 th percentile χ/Q	For GENII maximum sector 95 th percentile χ/Q
100	2.89	3.42	1800	2.03	2.47
500	2.47	3.00	2100	2.04	2.48
900	2.22	2.70	2400	2.02	2.45
1200	2.15	2.62	2700	2.06	2.49
1500	2.21	2.69	3000	2.17	2.62

Conclusion

This paper provides an overview of the process of calculating dry DV for a particulate release with GENII v2. Table 1 shows input requirements and parameters values selected for the DV calculations.

The DV results of the parametric study ranged from 0.1 cm/s to 0.75 cm/s. These values are based on a range of surface roughness lengths (10 cm to 100 cm) representative of most DOE sites and on a range of meteorological conditions that likely reflect 95th percentile conditions for the sites.

Using GENII v2, deposition value is sensitive to surface roughness length as shown in Figure 1 and Figure 2. Values of χ/Q calculated by GENII v2 do not appear to demonstrate the same level of sensitivity to surface roughness length as shown in Figure 3.

MACCS2 calculates the overall 95th percentile χ/Q values and GENII v2 calculates sector specific 95th percentile χ/Q values. As shown in Table 3, the average 95th sector GENII χ/Q values are 2.2-2.9 times higher than the 95th percentile MACCS2 χ/Q values, and the maximum 95th sector GENII χ/Q values are 2.62-3.42 times higher than the 95th percentile MACCS2 χ/Q values.

The GENII χ/Q results and comparisons with MACCS2 should be considered preliminary as GENII calculations were performed solely for this paper without formal technical review. The variance of the GENII χ/Q results with respect to MACCS2 needs further investigation.

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