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11.10 SENSITIVTY OF THE INDUSTRIAL SOURCE COMPLEX MODEL TO INPUT PARAMETERS

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1. INTRODUCTION

In recognition of the need for a state-of-the-science model for estimating pollutant concentrations, as well as dry and wet deposition of these pollutants, the U.S. Environmental Protection Agency (USEPA) released a new version of the Industrial Source Complex-Short Term model (ISCST2) (USEPA, 1992). This new version, ISCST3, integrates the algorithms for modeling simple terrain found in ISCST2 and the algorithms found in the COMPLEX I model, a USEPA screening-level model for complex terrain applications. In addition, the model includes a newly developed algorithm for modeling dry deposition of particulates, algorithms for modeling wet deposition, and a new algorithm for modeling area sources. The model is described in an updated user's guide (USEPA, 1995).

In this paper we examine the sensitivity of predicted concentrations, dry deposition fluxes and wet deposition fluxes to input parameters related to deposition of particles. We consider the effects of dry and wet plume depletion, the shape of the particle size distribution, the resolution of the particle size distribution, the particle density, scavenging coefficients, and the use of gridded terrain data. The results reported here should be considered preliminary until the analysis can be repeated using alternate data sets.

2. TEST PARAMETERS

A test data set was created for use in the sensitivity analysis. A single stack, emitting particulate matter, with a height of 100 m was used for all of the tests except the terrain grid tests. A shorter stack was used for those tests to insure high pollutant impact on the terrain. A source-centered, gridded-polar receptor network was used for all the sensitivity tests. Thirty-six radials, from 10° to 360° every 10°, were used, with receptors defined along each radial at distances from 0.1 to 20 km. The receptors were defined on flat terrain for most of the sensitivity tests, except the terrain grid tests. Gridded terrain elevation data, described in section 3.6, were used for the terrain sensitivity tests. One year of hourly meteorological data was used for all tests.

3. RESULTS

In this section we describe the results of the individual sensitivity tests and speculate as to the reasons for these results. We chose to examine the highest 25 values of concentration, dry deposition flux, and wet deposition flux unpaired in space or time since these are of concern in many regulatory applications. All cases except those described in section 3.1 were run including the effects of plume depletion due to dry and wet deposition.

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TABLE 1

Diameter(μm)	0.32	0.55	0.7	0.9	1.55	3.4	5.56	8.37	12.66	17.61
Mass Frac.	0.13	0.04	0.07	0.05	0.13	0.06	0.06	0.18	0.23	0.05
Scav. Coeff.*	1.4	0.88	0.6	0.56	1.32	2.44	3.41	4.74	7.05	10.22
Diameter(μm)	0.32	1.38	4.61	8.37	15.53					
Mass Frac.	0.13	0.29	0.12	0.18	0.28					
Scav. Coeff.*	1.4	1.13	2.99	4.74	8.82					
Diameter(μm)	1.26	6.78	15.53							
Mass Frac.	0.42	0.3	0.28							
Scav. Coeff.*	0.98	3.98	8.82							

* - the scavenging coefficients should be multiplied by 10^{-4}

3.1 Depletion

Depletion accounts for the mass lost from the plume due to deposition. To test the effects of plume depletion on the resulting maximum concentration and deposition fluxes, ISCST3 was run using an example particle size distribution with dry depletion only, wet depletion only, and no depletion. Maximum concentrations were lowered due to the dry depletion and were unaffected by the use of the wet depletion option. Since wet deposition fluxes were generally high for the test cases used, it makes sense that maximum concentrations would occur when the wet deposition flux and, therefore, the wet depletion is minimal. Figure 1 shows the effect of dry and wet depletion on the maximum dry deposition fluxes. Both dry and wet depletion have an effect due to the reduced mass, however the dry depletion appears to have more of an effect than wet depletion because the receptors with maximum dry deposition flux do not necessarily correspond to the receptors with maximum wet deposition flux. The use of dry depletion has little effect on the maximum predicted wet deposition flux since the highest wet deposition fluxes generally occur close to the source, where ground level concentrations and dry deposition fluxes are lower.

3.2 Mass Fraction

The deposition velocity calculated by the dry deposition algorithm and the scavenging coefficient specified by the user for use in the wet deposition algorithm are a function of particle diameter, so the distribution of the mass at a particular particle size is an important input to the model. We selected three particle size distributions (Set 1, Set 2, Set 3) for use in this test that are typical of different control strategies that might be used with a municipal waste combustor. These distributions are plotted in Figure 2. The same scavenging coefficients were used for each distribution. Figure 3 shows the effect of using these different distributions on the maximum predicted dry deposition flux. We see that there is a greater difference in the dry deposition flux between using set 1 versus set 2 compared to set 2 versus set 3. This is likely due to the peak in the set 1 distribution at 10 μm which would result in high deposition, whereas there is less of a difference in the shape of distributions 2 and 3. As expected, the maximum concentrations are lower for the sets with higher dry deposition. The wet deposition flux is less sensitive to the distribution used than is the dry deposition flux. This is because the relative differences between scavenging coefficients for different size categories is less than the differences between dry deposition velocities.

3.3 Particulate size resolution

The resolution (number) of particle size categories was varied from 10 to five to three, with a corresponding variation in the mass fraction and scavenging coefficients. The 10 size categories correspond to set 1 in the mass fraction tests described above. The 10 categories were combined to form five categories. Diameters from combined categories were used to calculate a mass mean diameter for the new category. Scavenging coefficients were calculated using a formula described in section 3.4 below. The five categories were similarly combined to form the three categories. The size categories and corresponding mass fractions and scavenging coefficients used are shown in Table 1.

TABLE 2

Diameter(μm)	0.32	0.55	0.7	0.9	1.55	3.4	5.56	8.37	12.66	17.61
Base case	1.4	0.88	0.6	0.56	1.32	2.44	3.41	4.74	7.05	10.22
Base case + σ	0.85	0.54	0.37	0.34	0.8	0.28	0.18	0.12	0.11	0.27
Base case - σ	2.31	1.46	0.99	0.92	2.17	4.02	5.63	7.82	11.63	16.85

The results show that changing the number of categories has little effect on concentration. Figure 4 shows the comparison of maximum dry deposition fluxes for the three sets of size categories. Coarser resolution results in an increase in the predicted dry deposition flux. As a result of combining categories, the distribution becomes skewed toward larger particles, which likely causes the estimated dry deposition flux to increase. The trend for wet deposition is not as clear. The maximum wet deposition flux is greatest for the case with 5 categories, while the wet deposition estimates for the case with 3 categories fall between those of the 10 category case and the 5 category case. This may have occurred because the distribution for the case with 3 categories is heavily weighted at a diameter of about 1 μm which corresponds to a very low scavenging coefficient.

3.4 Particle density

Density was varied to simulate different particulate materials. Four densities were modeled: 1.0, 1.5, 2.0 and 5.0 g cm^{-3}. The first three densities are more representative of combustion materials from a facility that burns traditional fossil fuels, while the fourth density is more representative of metals that may be emitted as a result of burning waste-derived fuels. The results for dry deposition are shown in Figure 5. As expected, an increase in particle density results in an increase in the maximum dry deposition flux. The increased density likely promotes gravitational settling, a component of dry deposition. Due to the effects of plume depletion, the increased deposition results in decreased maximum concentrations. Density variations showed no effect on the maximum predicted wet deposition flux since maximum wet deposition usually occurs close to the source where ground level concentration and dry deposition are minimal.

3.5 Scavenging coefficients

Three sets of scavenging coefficients were modeled. The first set of coefficients is based on a particle size distribution used in previous sections. The following formula, developed by Crouch (1993) based on the work of Jindal and Heinhold (1991), was used to obtain the scavenging coefficient, α, for each particle size category for liquid precipitation scavenging:

$$\ln\alpha = \frac{A}{(z + z_0)^2 + \lambda} + B + Cz(z + z_1)^2 + \mu$$

where A= 0.0523, B = -8.569, C = 0.214, z_0 = 0.0786, z_1 = 1.288, λ = 0.0419, and z = $\log_{10}$ (d), where d is the particle diameter in microns. μ is a random variable with a normal distribution with a mean of 0 and variance, σ^2, of 0.242 (i.e., $N(0,\sigma^2)$).

The coefficients then are obtained from $e^{\ln(\alpha)}$. The second and third sets were obtained from the first using $\ln(\alpha) \pm \sigma$, where σ is the standard deviation and equal to the square root of σ^2 above. The resulting scavenging coefficients for liquid precipitation are given in Table 2.

The effect on the maximum wet deposition fluxes is shown in Figure 6. As expected, increasing the scavenging coefficients increases the predicted wet deposition flux. Varying the coefficients has no effect on the maximum concentrations and dry deposition fluxes since the maximum values for wet deposition occur close to the source where concentration and dry deposition will be minimal.

3.6 Effect of terrain grid

In this series of tests, the effect of the use of a terrain grid was examined. The terrain grid is used only in the calculation of the plume depletion due to dry deposition where an integration of the material deposited along the plume path is performed. A 10 km by 10 km Cartesian gridded terrain network, with terrain elevation specified every 100 m in the north-south and east-west directions, was defined for ISCST3. An elevation was assigned to each receptor in the polar grid. The ISCST3 model was run both with and without this terrain grid. In the absence of a terrain grid, the model represents the effect of terrain by linearly interpolating between the source elevation and receptor elevation.

The use of a terrain grid has no effect on the maximum predicted wet deposition. It does, however affect the concentration and dry deposition. Maximum concentration estimates decreased by up to 4% and the maximum dry deposition flux decreased by as much as 7% when the terrain grid was used. These results likely depend on the terrain being considered.

4. CONCLUSIONS

We have reported the results of initial sensitivity testing of the ISCST3 model to input parameters controlling deposition. While these results are not comprehensive, they provide useful information to model users in selecting model inputs. For the model sensitivities explored, the predicted maximum concentrations and deposition fluxes responded in a manner that is supported by the technical basis of the model. Further tests should be done with other test conditions to affirm our results.

5. REFERENCES

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DISCLAIMER

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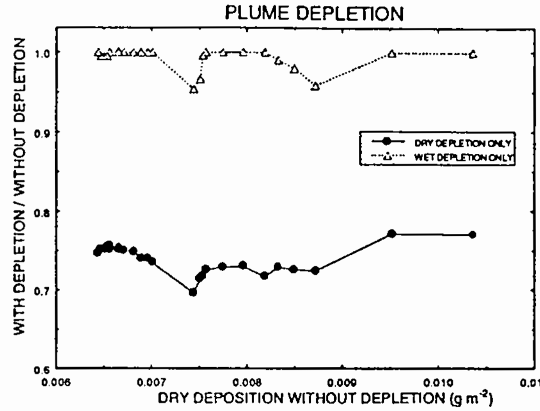

Figure 1. Comparison of the predicted maximum dry deposition flux for ISCST3 model run where depletion was not considered with cases where dry or wet depletion was considered.

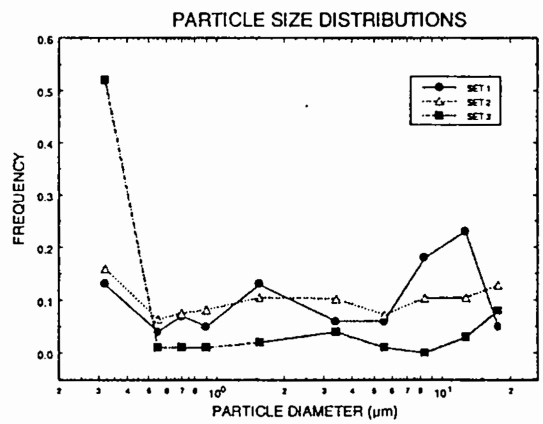

Figure 2. Plot of the three particle size distributions used in the sensitivity analysis.

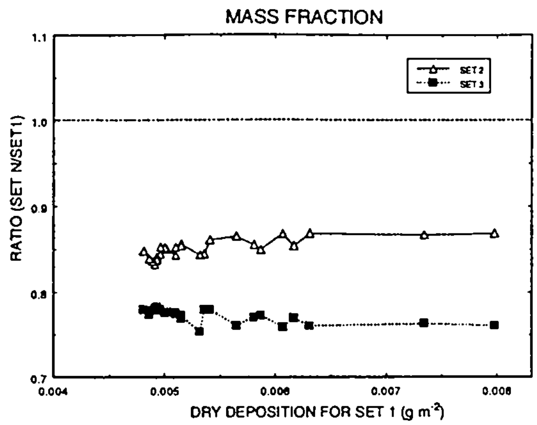

Figure 3. Comparison of maximum dry deposition flux predicted by ISCST3 for the three different distributions of the mass fraction.

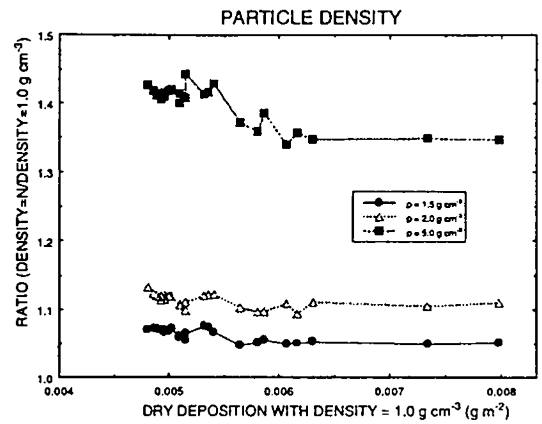

Figure 5. Comparison of maximum dry deposition flux predicted by ISCST3 for 4 different particle densities.

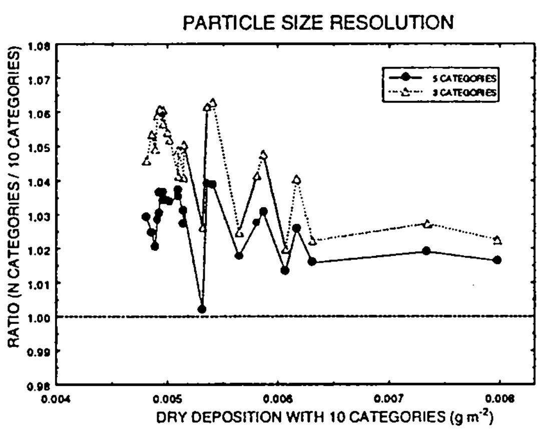

Figure 4. Comparison of the maximum dry deposition flux predicted by ISCST3 for the original 10 category particle size distribution and the 5 and 3 category distributions.

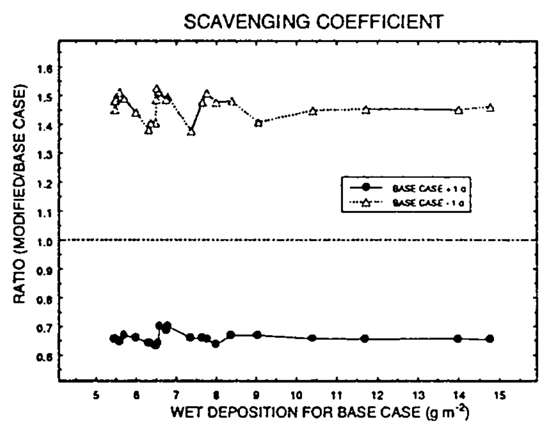

Figure 6. Comparison of the maximum wet deposition flux predicted by ISCST3 for the base case scavenging coefficients and variations ($\pm\sigma$) of the base case.

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16. ABSTRACT

In recognition of the need for a state-of-the-science model for estimating concentrations and dry and wet deposition of air pollutants, the U.S. Environmental Protection Agency has developed an improved modeling technique. The newest version of the Industrial Source Complex model (ISC3) integrates dry deposition, wet deposition, and complex terrain algorithms into the Industrial Source Complex - Short Term (ISCST2) model as well as a new area source algorithm and algorithms for modeling open-pit source types. The dry deposition algorithm couples a deposition velocity calculated from a resistance model with a modified source depletion algorithm. The wet deposition algorithm is a simple scavenging coefficient approach. Complex terrain algorithms from the COMPLEX I model were used. The new area source algorithm is a numerical integration approach. The method for modeling open-pit sources was derived from a fluid modeling study. The additional capabilities provided in ISC3 make the model an important tool for modeling for ambient air quality standards and for performing multi-pathway risk assessments that require concentration and deposition estimates as their starting point.

To better understand these new algorithms, particularly the deposition algorithms, we examined the sensitivity of the model results to various input parameters. The predicted dry deposition flux depends on the specification of the particle size distribution since this affects the calculated deposition velocity. We varied both the shape of the size distribution and the resolution of the distribution. The dry deposition algorithm also includes a depletion algorithm which integrates the mass-loss along the plume path. The terrain elevations along the plume path can be interpolated between the source and receptor elevations or can be specified explicitly using a terrain grid. We examined the effect of the use of the terrain grid as well as the resolution of the grid on the calculated depletion. The wet deposition flux depends on the scavenging coefficient which is specified as a function of particle size for a unit precipitation rate. For a given particle size distribution, we varied the scavenging coefficients from a base value to one standard deviation higher and lower than that value. Three point sources were run using one year of National Weather Service meteorology. The parameters listed above were varied independently and the concentration and deposition values were compared for 1-h, 3-h, 24-h and annual averaging times. Of the parameters tested, the modeled results are most sensitive to the specification of the scavenging coefficient, followed by the shape of the particle size distribution and the resolution of the particle size distribution. the sensitivity to terrain specification depended highly on the receptors examined.

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