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COMPARISON OF ISC2 DRY DEPOSITION ESTIMATES BASED ON CURRENT AND PROPOSED DEPOSITION ALGORITHMS

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PREFACE

The ability to accurately estimate deposition of particulate matter is of special concern in assessing environmental impacts from a variety of sources including Superfund sites, municipal waste incinerators, and surface coal mines. The limitations of the Industrial Source Complex (ISC2) model (version dated 92273) for use in such assessments are discussed elsewhere and are noted in the following. The deposition algorithm currently employed in ISC2 was developed for applications to large particles dominated by gravitational settling (i.e., particles greater than about 20 μm diameter). The current algorithm was not intended for use with small particles and, in fact, includes an assumption that particles less than 5.7 μm in diameter are totally reflected at the surface and, thus, experience no deposition. This is in conflict with recent observations.

In light of these limitations, a new deposition algorithm which will handle the full range of significant particle sizes (0.1 to 100 μm) is being considered for use in ISC2. A description of the new algorithm including comparisons with alternative methods for estimating deposition is provided in an April 1994 EPA report "Development and Testing of A Dry Deposition Algorithm (Revised)", EPA-454/R-94-015.

The new deposition algorithm has been tested within the framework of the ISC2 model and comparisons of deposition estimates using the old (current) and new deposition algorithms have been made for a range of source types and particulate emission scenarios. Similar comparisons have been made of particulate concentration estimates as affected by the old and new deposition algorithms. This report documents these analyses.

The Environmental Protection Agency must conduct a formal public review before the Agency can recommend the new deposition algorithm for use in regulatory analyses. Such a review will enable EPA to assess the potential consequences of replacing the old deposition algorithm in ISC2 with the new algorithm. This report is being released in accordance with this review process. The report is one of several reports on the ISC2 models that must be considered before any formal changes can be adopted.

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Comparison of ISC2 Dry Deposition Estimates Based on Current and Proposed Deposition Algorithms

1. INTRODUCTION

The Industrial Source Complex dispersion model [ISC2 (USEPA, 1992)] is a widely recommended refined model for use in assessments of air quality impacts from particulate sources and incorporates many features essential to the modeling of such sources. These include area and volume source algorithms, building wake algorithms, and a deposition algorithm based on Dumbauld et al. (1976) and Overcamp (1976). The latter was included in recently completed evaluations (USEPA, 1994) comparing the performance of several dry deposition algorithms and several plume depletion algorithms. As a result of these evaluations, EPA is considering replacing the current deposition algorithm in ISC2 (hereafter referred to as the "old" deposition algorithm) with the deposition algorithm now employed in the Acid Deposition and Oxidant Model [ADOM (Pleim et al., 1984)]. This algorithm will be referred to hereafter as the "new" deposition algorithm. In addition, EPA also proposes to incorporate a plume depletion algorithm in ISC2. The proposed plume depletion algorithm, a modified version of the source depletion technique (Horst, 1977), was selected following the evaluations in USEPA, 1994.

This report documents analyses to assess the potential consequences (i.e., differences in estimates of deposition and design concentrations) of replacing the old deposition algorithm in ISC2 with the new algorithm.

The old deposition algorithm in ISC2 simulates deposition as the movement of particles toward the surface by the combined processes of atmospheric turbulence and gravitational settling. The method was developed for applications to large particles dominated by gravitational settling; these are typically particles greater than 20 μm diameter. At the surface, a portion of the plume determined by a user-specified reflection coefficient[1] is reflected from the surface; the remainder is deposited, resulting in a reduction in concentration within the plume. It should be noted that for small particles, the ISC2 reflection coefficient was derived based on extrapolation of the gravitational settling-dominated data for larger particles (Dumbauld et al., 1976). The extrapolation led to the assumption that particles less than 5.7 μm in diameter are totally reflected

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[1] The empirical reflection coefficients recommended for use with ISC2 are based on experiments involving aircraft releases of two spray carriers (Duphar and No. 2 fuel oil) in which most of the particles (more than 99 percent) exceeded 20 μm diameter. Particles of this large size are nearly completely controlled by gravitational settling.

at the surface and thus experience no deposition. This is contrary to recent observations which indicate significant deposition velocities for these small particles.

The new deposition algorithm is intended to simulate processes important over the entire range of particle sizes. For example, the proposed algorithm includes effects due to inertial impaction and Brownian motion which control the deposition of small particles. These effects, which are dependent on meteorological and surface conditions, are not easily parameterized within the framework of a reflection coefficient algorithm such as used in the current ISC2.

The new deposition algorithm has been tested within the framework of the ISC2 models [ISCST2 (Short-Term) and ISCLT2 (Long-Term)] and comparisons of deposition estimates using the old and new deposition algorithms have been made for a range of source types and particulate emission scenarios. Similar comparisons have been made of particulate concentration estimates as affected by the old and new deposition algorithms. Documentation of these comparisons is provided in the following.

2. METHODOLOGY

2.1 Modeling Scenarios

2.1.1 Particle Size

In the development and testing of dry deposition algorithms it was noted that the important physical processes affecting dry deposition could be segregated by particle size (USEPA, 1994). These processes include gravitational settling, which is dominant for large particles (greater than 20 μm diameter), inertial impaction, which is dominant in the size range from 1.0 to 20 μm, and Brownian motion, which is important for small particles (less than about 0.1 μm). In the comparisons to be presented, seven particle size categories were employed to represent the important range of particle sizes. These were: 0.1, 1.0, 10, 20, 50, 80, and 100 μm diameter. The characteristic settling velocities (assuming spherical particles with a density of 1 g/cm^3) and reflection coefficients assigned to these particles for use in modeling based on the old deposition algorithm are given in Table 1. For use in modeling, each particle size category was treated as a separate source and assigned a mass fraction of 1.0.

Table 1 Particle diameter, gravitational settling velocity, and reflection coefficient used in modeling deposition

Particle Diameter (μm)	Settling Velocity (m/s)	Reflection Coefficient
0.10	0.00000	1.00
1.00	0.00003	1.00
10.0	0.003	0.87
20.0	0.012	0.76
50.0	0.074	0.55
80.0	0.190	0.27
100.	0.300	0.00

2.1.2 Meteorological Data

2.1.2.1 ISCST2

The meteorological data employed in the ISCST2 evaluations consisted of one year (1984) of hourly surface data and concurrent twice-daily mixing heights for the National Weather Service (NWS) station at Oklahoma City, Oklahoma. These data were processed using the EPA recommended Meteorological Processor for Regulatory Models [MPRM (USEPA, 1990)]. In addition to the standard set of meteorological variables required by Gaussian dispersion models (i.e., wind direction, wind speed, stability, temperature, and mixing height), the proposed new deposition algorithm also requires estimates of the Monin-Obukhov length and the surface friction velocity. These additional variables were calculated using software adapted from the meteorological preprocessor for the Hybrid Plume Dispersion Model (Hanna and Chang, 1991). To facilitate subsequent analyses, all hourly wind directions were set to a fixed value of 270 degrees (flow vector of 90 degrees).

2.1.2.2 ISCLT2

The same meteorological data (Oklahoma City hourly surface data for 1984) were also processed for use in ISCLT2. This processing was accomplished using the PCSTAR software which generates a joint frequency distribution of wind direction and wind speed by stability class. The Monin-Obukhov length and friction velocity required in the deposition algorithm are generated internally within ISCLT2. The algorithm for computing the friction velocity is based on Wang and Chen (1980) and is the same as was used for ISCST. The algorithm for computing the Monin-Obukhov length is based on Golder (1972).

2.1.3 Release Height

Both deposition and concentration are dependent on release height. The modeling performed for these evaluations, included a surface release, and three elevated releases, 35-m, 100-m, and 200-m. The source parameters associated with these four releases are given in Table 2.

Table 2 Source parameters employed in modeling

Stack Height (m)	Stack Diameter (m)	Exit Velocity (m/s)	Exit Temp. (K)	Buoyancy Flux (m^4/s^3)	Emission Rate (g/s)
0.1	1.0	0.1	293	---	1000
35	2.4	11.7	432	53	1000
100	4.6	18.8	416	288	1000
200	5.6	26.5	425	633	1000

2.1.4 Receptor Location

All receptors were assumed to be located in flat terrain and were assigned an elevation equal to the base elevation of the source. Receptor locations for use in ISCST and ISCLT are described in the following.

2.1.4.1 ISCST2

Receptors for use in ISCST2, were placed at intervals along the X axis beginning at 0.1 km from the source and extending to 50 km. A total of 35 receptors were employed in the modeling. This arrangement of receptors in combination with a fixed 90 degree flow vector facilitates the identification of the highest 1-hour results which, in this analysis, are independent of wind direction. The results obtained for longer averaging times (i.e., 3-hour, 24-hour, and annual) which are dependent on wind direction, will be conservative (higher) compared to results where the wind direction is allowed to vary.

2.1.4.2 ISCLT2

Screening analyses employing coarse polar grids were conducted to determine the distance to the maximum deposition using ISCLT2. Additional screening analyses were conducted using a refined polar grid employing 26 rings extending to 10 km. The screening showed that the highest deposition consistently occurred at receptors located along the 360 degree radial. Consequently, all subsequent analyses using ISCLT2 were conducted with receptors located on the 360 degree radial. These receptors were located at 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1.0, 1.2, 1.4, 1.6, 1.8, 2.0, 2.5, 3.0, 3.5, 4.0, 5.0, 6, 7, 8, 9, and 10 km.

2.2 Diagnostic Comparisons

In conducting the ISC2 analyses, it became apparent that a limited sensitivity study was needed to illustrate the sensitivity of the new and old algorithms to particle size, surface characteristics, meteorological conditions, release height, and source/receptor distance. Consequently, sensitivity analyses were constructed using 1-hour deposition and concentration estimates from ISCST2. These sensitivity analyses complement and extend the analyses in USEPA (1994).

2.3 Operational Comparisons

In a regulatory air quality analysis, ISC2 is used to estimate expected extreme (highest and second highest) concentrations for averaging times of interest, commonly, 1-hour, 3-hour, 24-hour and annual. Hence, a primary purpose of this analysis is to assess the operational consequences of the new algorithm by examining its effect on extreme value deposition and concentration estimates. This is accomplished by exercising ISCST2 and ISCLT2 in an operational mode and comparing the deposition and concentration estimates based on the old and new deposition algorithms. The performance measure used in the comparisons is patterned on the 'Fractional Bias' (Cox and Tikvart, 1990) and is defined here as the 'Fractional Difference' (FD):

$$FD = 2\,(NEW - OLD)/(NEW + OLD)$$

3. RESULTS

3.1 Diagnostic Comparisons

The results of the diagnostic comparison are presented first since they are essential to the understanding of the results of the operational comparisons. An initial pilot analysis was conducted for the 35-m release height to determine the maximum deposition as a function of particle size for all receptors and all meteorological conditions (i.e., unpaired in space and time), and to identify the meteorological conditions associated with these maxima.

Results (old and new deposition estimates as a function of downwind distance) for the 50 μm diameter particle are presented in Figure 1. The maximum deposition using the old algorithm occurs at 0.5 km under C stability with a wind speed of 15.4 m/s. By comparison, the maximum deposition using the new algorithm occurs at 3 km under F stability with a wind speed of 1.5 m/s. The same conditions (F stability and 1.5 m/s) were associated with a secondary maximum for the old algorithm which also occurs at 3 km downwind. The higher maximum with C stability for the old algorithm is a result of a combination of effects: first, with the higher wind speed (15.4 m/s versus 1.5 m/s) the plume rise from the 35-m stack is lower (19 meters versus 124 meters) and second, the plume disperses more rapidly in slightly unstable conditions (C stability) as compared to strongly stable conditions (F stability). Similar graphs for other particle sizes evaluated (10, 20, 50, 80, and 100 μm) are given in Appendix A.

The old ISC2 deposition algorithm employs a 'tilted-plume' approach for characterizing the gravitational descent of the plume as it disperses downwind. The degree of tilt is dependent on the ambient wind speed and the gravitational settling velocity. The latter, as shown in Table 1, is a function of particle size, density, etc. The old algorithm characterizes deposition at the surface through the use of an empirical reflection/absorption coefficient which is also a function of particle size. The effective deposition velocity, defined by the ratio of deposition flux and concentration, is dependent on plume tilt and the interaction of reflection terms with the underlying surface. The end result is that the effective deposition velocity in the old algorithm decreases with downwind distance.

The new deposition algorithm also employs a tilted plume approach for characterizing the gravitational descent of the plume. Deposition at the surface is computed as the product of a deposition velocity and the ground-level air concentration. However, in contrast to the old algorithm, the deposition velocity in the new algorithm is a function of surface conditions and meteorology, but is independent of distance from the source. These differences preclude summarization of the results of these comparisons in simple statements.

Table 3 and Figure 2 summarize the results of the above analyses for all particle sizes (maximum deposition estimates unpaired in space and time) for 1-hour averaging. For the smaller (0.1 and 1.0 μm - the old algorithm always results in no deposition for these particles) and larger (50, 80, and 100 μm) particle sizes, the new algorithm results in higher deposition estimates than the old algorithm. However, for intermediate particle sizes (10 and 20 μm) the new algorithm results in lower deposition estimates.

Table 3 Highest 1-hour average ISCST deposition flux estimates (g/m^2) based on the old and new algorithms for a 35-m release.

Particle Diameter (μm)	Maximum Deposition (g/m^2) OLD	Maximum Deposition (g/m^2) NEW	Distance to Max (m) OLD	Distance to Max (m) NEW
0.1	-	0.01 (*)	-	600
1.0	-	0.00 (*)	-	600
10	1.04 (*)	0.62 (*)	500	600
20	1.94 (*)	0.71 (*)	500	600
50	3.99 (*)	4.86 (**)	500	3000
80	20.8 (**)	32.7 (**)	1400	1200
100	69.9 (**)	75.9 (**)	900	800

Key to meteorological conditions noted () above:
(*) C stability at 15.4 m/s
(**) F stability at 1.54 m/s

Additional modeling using the meteorological conditions identified with the modeled extremes (see Table 4) was conducted to assess the sensitivity of the algorithms to meteorology. In the course of these analyses, two additional meteorological cases were included: the first, C stability at 3 m/s, was included to assess the sensitivity of the algorithms to wind speed; the second, E stability at 1.54 m/s, was included to aid in understanding the concentration results for a 200-m release of 100 μm particles. These latter two sensitivity analyses are discussed in Appendix B.

Table 4 Meteorological conditions used in sensitivity Analyses

P-G Stability Class	Wind Speed (m/s)	Temperature (K)	Mixing Height (m)	Friction Velocity (m/s)	M-O Length (m)
A	2.57	307	1536	0.29	-8
C	15.4	295	808	1.35	-839
C	3.00	295	808	0.30	-60
E	1.54	297	1368	0.07	10
F	1.54	306	2756	0.07	10

Figure 3 shows the results of the analyses of the Table 3 extremes. It should be noted that this figure is similar to Figure 2 except, in this case, the results are paired in time (i.e., the old and new estimates were based on the same meteorological conditions). As shown in Figure 3, the relative magnitude of the deposition estimates based on the new and old algorithms is dependent on the meteorology and, as indicated by the solid lines, the ratio (slope) appears to be a constant for particle sizes above about 20 μm in diameter for a given meteorological condition. In general, deposition estimates based on the old algorithm exceed the estimates based on the new algorithm for the unstable conditions, while the reverse is the case for stable conditions. The two cases for stability class C (3 m/s and 15 m/s) show the effect of wind speed on the deposition estimates. At the lower wind speed the estimates from the two algorithms are similar. At the higher wind speed, the deposition estimates based on the old algorithm exceed those based on the new algorithm.

3.2 Operational Comparisons

3.2.1 Deposition

3.2.1.1 ISCST2

Operationally, one is often interested in maximum deposition estimates, unpaired in space and time. These would be cumulative estimates; i.e., summed over some period of time (e.g., annual) and over all particle sizes. The latter would be a weighted sum based on the mass fraction of each particle size in the source term.

Deposition estimates were computed for four time periods (1-hour, 3-hour, 24-hour, and annual) for each of four release scenarios and each of seven particle size categories. The results are given in Table 5. Note that for each old/new pair of estimates, the corresponding Fractional Difference (FD) comparison statistic is also given. For example, the estimates for a 35-m release of 50 μm diameter particles over a 1-hour period are 3.99 g/m^2 using the old algorithm and 4.86 g/m^2 using the new algorithm. The FD comparison statistic in this case is computed as:

$$FD = 2(4.86 - 3.99)/(4.86 + 3.99) = 0.20$$

The resulting value, 0.20 in this example, indicates that the estimate based on the new algorithm increased (in this case by 22 percent) relative to the estimate based on the old algorithm. For use in interpreting the FD statistic, it should be noted that a value of -0.67 (+0.67) indicates that estimates based on the new algorithm decreased (increased) by a factor of 2 relative to estimates based on the old algorithm.

The FD values from Table 5 are presented graphically in Figures 4 (1-hour), 5 (3-hour), 6 (24-hour) and 7 (annual average). It should be noted, since the old algorithm assumes that particles less than 5.7 μm in diameter do not deposit, that the FD statistic for the first two particle size categories (0.1 and 1.0 μm) will always be 2.

For surface releases, the new algorithm results in higher deposition estimates for all except the 10 and 100 μm particle size categories for the 1-hour period, for all except the 100 μm particle size for the 3-hour period, and for all particle size categories for the 24-hour and annual periods. In general, the magnitude of the increase in the deposition estimate for a surface release increases as the time period of the deposition increases. Annual deposition estimates from a surface release (Figure 7), for example, are increased by more than a factor of 2 using the new algorithm as compared to the old algorithm.

For elevated releases, the new algorithm results in higher estimates for the smaller (0.1 and 1.0 μm) and larger (80 and 100 μm) particle sizes. The increase in the deposition estimates for 80 and 100 μm particles is generally less than a factor of two.

For intermediate particle sizes (10 and 20 μm), deposition estimates using the new algorithm are decreased relative to the corresponding estimates based on the old algorithm. The decrease generally exceeds a factor of 2 for 100-m and 200-m releases.

Results vary for elevated releases of 50 μm particles; for example, deposition estimates for a 35-m release increase (generally by less than a factor of 2), whereas estimates for 100-m and 200-m releases may increase (annual) or decrease (1-hour and 3-hour) depending on the averaging period.

3.2.1.2 ISCLT2

Annual deposition estimates were also computed using ISCLT2. These results are presented in Table 6. For a surface release, annual deposition estimates based on the new algorithm exceed estimates based on the old algorithm for all particle sizes. The FD statistic for the surface release ranges from 1.5 to 2.0. For elevated releases, deposition estimates based on the new algorithm may be higher or lower than estimates based on the old algorithm, depending on particle size and release height.

3.2.2 Concentration

Ambient concentrations are reduced by the deposition of particulate matter and, as such, model estimates of ambient concentrations depend on the algorithms employed to model deposition processes.

In the case of the old algorithm, the fractional reduction in concentration is equal to one half of the fraction deposited (i.e., one minus the reflection coefficient). Thus, concentrations of 100 μm particles, which experience no reflection, are reduced by factor of 2. It should be noted that the treatment of the gravational settling in the old deposition algorithm results in a 'bouncing plume'. As such, concentration estimates using the old deposition algorithm are invalid beyond the point of plume touch down. The latter is a function of particle size (settling velocity), release height, and wind speed. Because of uncertainties resulting from the bouncing plume, most past applications of ISC2 for estimating concentrations of particulate matter have normally been made with the deposition algorithm turned off.

In the case of the new algorithm, the reduction in concentration is estimated using a modified source depletion technique based on Horst (1977). With this technique, the source term (emission rate) is adjusted (decreased) to simulate the increased pollutant removal with distance. In addition to these changes, the new algorithm incorporates necessary changes to eliminate the bouncing plume.

3.2.2.1 ISCST2

As was done for deposition, corresponding concentration results for 1-hour, 3-hour, 24-hour, and annual averaging are presented in Table 7. The FD values from Table 7 are presented graphically in Figures 8 (1-hour), 9 (3-hour), 10 (24-hour) and 11 (annual average).

For particles up to 20 μm in diameter, the differences in concentration estimates are not significant (less than 10 percent).

For surface releases of larger particles, the concentration estimates using the new algorithm are consistently lower than the corresponding estimates using the old algorithm. The decrease in this case ranges between a factor of 1.5 and 2 (50 to 100 percent decrease).

For elevated releases of larger particles, the results are mixed. For 50 μm particles, the concentration estimates using the new algorithm are lower than the corresponding estimates using the old algorithm. However, for elevated releases of the largest particle size category (100 μm), the concentration estimates using the new algorithm are increased relative to the corresponding estimates using the old algorithm. The increase approaches a factor of 2 for 100-m and 200-m release heights (for short-term averaging periods). For annual averaging, the increase approaches a factor of 1.5. This apparent contradiction with the deposition results (deposition estimates based on the new algorithm also exceed the estimates based on the old algorithm for elevated releases of large particles) is a direct result of a combination of inherent differences in the two algorithms. These differences, which are manifest in the modeling of elevated releases of large particles, are discussed in Appendix B.

The above results are for ISCST2 run with the deposition (old and new) and plume depletion (new only) options activated (turned-on). The concentration estimates from the 'old' and 'new' versions of ISCST2 are identical when deposition is not turned-on.

3.2.2.2 ISCLT2

Annual concentration estimates were also computed using ISCLT2. These results are presented in Table 8. For a surface release, annual concentration estimates using the new algorithm are less than the corresponding estimates using the old algorithm for all particle sizes. The FD statistic for the surface release ranges from zero (no change) to -0.2 (a decrease of 20 percent).

For elevated releases, with the exception of 100 μm size particles, the differences are generally not significant. For 100 μm particles, concentration estimates using the new algorithm are higher by 30 to 40 percent.

4. Summary and Conclusions

The proposed algorithm was expected to provide deposition estimations similar to the old algorithm for particles 20 μm in diameter and larger, and to provide more realistic (higher) deposition estimates for particles less than 20 μm in diameter.

4.1 Deposition

For surface releases, this comparison shows that the new algorithm results in higher deposition estimates for all particle size categories for the 24-hour and annual periods. The annual deposition estimates are increased by more than a factor of 2 using the new method.

For elevated releases, the new algorithm results in higher estimates for the smaller (0.1 and 1.0 μm) and larger (80 and 100 μm) particle sizes. The increase in the deposition estimates for 80 and 100 μm particles is generally less than a factor of two. For intermediate particle sizes (10 and 20 μm), deposition estimates using the new algorithm are decreased relative to the corresponding estimates based on the old algorithm. The decrease generally exceeds a factor of 2 for 100-m and 200-m releases.

The ratio of the deposition estimates based on the new and old algorithms is dependent on the meteorology and appears to be a constant for particle sizes above about 20 μm for a given meteorological condition. In general, deposition estimates based on the old algorithm exceed the estimates based on the new algorithm for the unstable conditions, while the reverse is the case for stable conditions (e.g., see Figure 3).

4.2 Concentration

For a surface release of large particles (50, 80, and 100μm), estimated concentrations using the new algorithm are decreased relative to the corresponding estimates using the new algorithm. The decrease ranges between a factor of 1.5 and 2 (50 to 100 percent decrease). For small and intermediate particles (0.1, 1, 10, and 20 μm), the differences are not significant (less then 10 percent).

For elevated releases of larger particles the results are mixed. However, in all cases, the differences for these larger particles do not exceed a factor of 2. As was the case for surface releases, the differences for small and intermediate size particles are not significant (less than 10 percent).

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TABLE 5

Comparison of ISCST deposition flux estimates based on the old and new algorithms for selected averaging times, release heights, and particle diameters as indicated.

Fractional Difference: FD = 2 (NEW - OLD) / (NEW + OLD)

1-HOUR EXTREMES (g/m^2)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
10	352	230	-0.4	1.04	0.62	-0.5	0.43	0.06	-1.5	0.27	0.01	-1.9
20	418	727	0.5	1.94	0.71	-0.9	0.79	0.07	-1.7	0.49	0.02	-1.8
50	1096	2299	0.7	3.99	4.86	0.2	1.48	0.52	-1.0	0.93	0.15	-1.4
80	1906	1987	0.0	20.83	32.67	0.4	2.39	3.63	0.4	1.51	1.43	-0.1
100	1296	1156	-0.1	69.86	75.88	0.1	7.75	14.05	0.6	2.48	4.41	0.6

3-HOUR EXTREMES (g/m^2)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
10	357	549	0.4	2.19	1.40	-0.4	0.59	0.14	-1.2	0.34	0.03	-1.7
20	647	1799	0.9	4.10	1.64	-0.9	1.10	0.16	-1.5	0.63	0.04	-1.8
50	3125	6464	0.7	8.55	14.20	0.5	2.21	1.46	-0.4	1.23	0.34	-1.1
80	5338	5533	0.0	59.99	92.35	0.4	6.51	10.49	0.5	2.17	4.18	0.6
100	3388	2913	-0.2	198.90	211.25	0.1	21.99	38.80	0.6	5.52	10.94	0.7

24-HOUR EXTREMES (g/m^2)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
10	990	2626	0.9	6.24	6.07	0.0	0.95	0.42	-0.8	0.43	0.08	-1.4
20	2267	5957	0.9	12.00	7.99	-0.4	1.77	0.61	-1.0	0.76	0.13	-1.4
50	11659	27498	0.8	29.50	41.95	0.3	3.44	4.07	0.2	1.45	0.89	-0.5
80	14414	19622	0.3	172.50	254.91	0.4	17.15	25.74	0.4	3.80	8.18	0.7
100	12256	14292	0.2	563.50	583.65	0.0	56.73	78.85	0.3	13.44	21.68	0.5

ANNUAL EXTREMES (g/m^2)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
10	111539	503090	1.3	855.00	530.00	-0.5	62.00	40.40	-0.4	19.00	8.60	-0.8
20	243405	1318515	1 4	1677.00	1107.00	-0.4	120.00	92.50	-0.3	35.00	20.50	-0.5
50	955851	4041833	1.2	4838.00	6697.00	0.3	343.00	695.00	0.7	80.00	159.00	0.7
80	1258514	3773714	1.0	26225.00	36422.00	0.3	2625.00	3928.00	0.4	583.00	989.00	0.5
100	905441	2679361	1.0	81102.00	83232.00	0.0	8589.00	9344.00	0.1	1990.00	2548.00	0.2

TABLE 6

Comparison of ISCLT annual deposition flux estimates based on the old and new algorithms for release heights and particle diameters as indicated.
Fractional Difference: FD = 2 (NEW - OLD) / (NEW + OLD)

Diameter (microns)	Surface Release OLD	Surface Release NEW	Surface Release FD	35-Meter Release OLD	35-Meter Release NEW	35-Meter Release FD
0.1	0	2831	2.0	0	2	2.0
1	0	1093	2.0	0	1	2.0
10	1199	67358	1.9	96	67	-0.4
20	3202	117317	1.9	187	103	-0.6
50	12376	239284	1.8	505	412	-0.2
80	21440	235098	1.7	1794	2182	0.2
100	28738	194290	1.5	5483	5136	-0.1

Diameter (microns)	100-Meter Release OLD	100-Meter Release NEW	100-Meter Release FD	200-Meter Release OLD	200-Meter Release NEW	200-Meter Release FD
0.1	0	0	2.0	0	0.0	2.0
1	0	0	2.0	0	0.0	2.0
10	9	5	-0.6	3	1.0	-1.0
20	17	8	-0.7	6	1.8	-1.1
50	41	37	-0.1	13	7.5	-0.5
80	149	210	0.3	34	51.6	0.4
100	488	511	0.0	114	135.0	0.2

TABLE 7

Comparison of ISCST concentration estimates based on the old and new algorithms for selected averaging times, release heights, and particle diameters as indicated.

Fractional Difference: FD = 2 (NEW - OLD) / (NEW + OLD)

1-HOUR EXTREMES (micro-g/m^3)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
0.1	21711142	21608136	0.00	2836	2824	0.00	897	894	0.00	439	437	-0.01
1	21712652	21625196	0.00	2836	2832	0.00	897	895	0.00	439	438	0.00
10	20370922	20260306	-0.01	2658	2839	0.07	836	895	0.07	410	438	0.07
20	18579514	16512426	-0.12	3403	3414	0.00	787	865	0.09	386	424	0.09
50	14046924	8455137	-0.50	20355	17875	-0.13	2208	1931	-0.13	648	563	-0.14
80	5646102	2841743	-0.66	48452	47026	-0.03	5386	5235	-0.03	1626	2063	0.24
100	1504833	1032195	-0.37	59623	69928	0.16	6895	12947	0.61	2230	4072	0.58

3-HOUR EXTREMES (micro-g/m^3)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
0.1	17028218	16957118	0.00	2490	2484	0.00	486	484	0.00	186	185	0.00
1	17029042	16972472	0.00	2491	2488	0.00	486	485	0.00	186	185	0.00
10	15960174	16089264	0.01	2353	2491	0.06	454	484	0.06	174	186	0.07
20	14728003	13625220	-0.08	3278	3270	0.00	429	472	0.10	165	179	0.08
50	13971580	7921412	-0.55	19687	17414	-0.12	2119	1797	-0.16	525	416	-0.23
80	5475584	2639824	-0.70	45792	44300	-0.03	5122	5034	-0.02	1242	2008	0.47
100	1407853	875861	-0.47	57704	64895	0.12	6734	11918	0.56	1675	3362	0.67

24-HOUR EXTREMES (micro-g/m^3)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
			Sfc.			35-m			100-m			200-m
0.1	6225974	6197444	0.00	1777	1770	0.00	151	149	-0.01	56	55	-0.01
1	6226221	6205344	0.00	1778	1775	0.00	151	150	0.00	56	55	-0.01
10	5832943	5893759	0.01	1687	1521	-0.10	142	150	0.06	51	55	0.08
20	5392277	4966362	-0.08	1661	1621	-0.02	148	141	-0.05	48	51	0.06
50	6232613	4292841	-0.37	7885	7277	-0.08	832	705	-0.17	182	142	-0.24
80	2300707	1241776	-0.60	18098	17401	-0.04	1832	1756	-0.04	388	559	0.36
100	836814	530638	-0.45	22210	25557	0.14	2319	3453	0.39	509	950	0.60

ANNUAL EXTREMES (micro-g/m^3)

Diameter	Surface			35-meter			100-meter			200-meter		
(microns)	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD	OLD	NEW	FD
0.1	2259888	2252064	0.00	1020	1015	0.00	85	84	-0.01	18	18	-0.01
1	2260180	2256171	0.00	1020	1019	0.00	85	84	0.00	18	18	0.00
10	2138979	2174798	0.02	985	956	-0.03	82	78	-0.05	17	17	-0.05
20	2081605	2028710	-0.03	1025	1017	-0.01	89	88	-0.01	19	19	-0.02
50	1971727	1534105	-0.25	2421	2497	0.03	266	256	-0.04	63	58	-0.08
80	886039	594997	-0.39	5207	5829	0.11	587	627	0.07	143	157	0.10
100	342726	274974	-0.22	6485	8699	0.29	756	975	0.25	185	266	0.36

TABLE 8

Comparison of ISCLT annual concentration estimates as affected by the old and new deposition algorithms for release heights and particle diameters as indicated.
Fractional Difference: FD = 2 (NEW - OLD) / (NEW + OLD)

Diameter (microns)	Surface Release OLD	Surface Release NEW	Surface Release FD	35-Meter Release OLD	35-Meter Release NEW	35-Meter Release FD
0.1	194905	193914	0.0	88	88	0.0
1	194905	194452	0.0	88	88	0.0
10	182408	177153	0.0	84	78	-0.1
20	170238	156715	-0.1	84	83	0.0
50	103686	83371	-0.2	128	137	0.1
80	45320	35293	-0.2	286	336	0.2
100	23616	19240	-0.2	376	521	0.3

Diameter (microns)	100-Meter Release OLD	100-Meter Release NEW	100-Meter Release FD	200-Meter Release OLD	200-Meter Release NEW	200-Meter Release FD
0.1	7.0	6.9	0.0	1.9	1.8	-0.1
1	7.0	6.9	0.0	1.9	1.9	0.0
10	6.6	6.1	-0.1	1.7	1.6	-0.1
20	6.6	6.5	0.0	1.7	1.7	0.0
50	12.0	12.4	0.0	2.7	2.4	-0.1
80	28.9	32.2	0.1	7.1	7.8	0.1
100	38.3	51.7	0.3	9.4	13.6	0.4

FIGURE 1

Comparison of highest 1-hour ISCST deposition estimates based on old and new algorithms for a 35-meter release for 50 micron diameter particles.

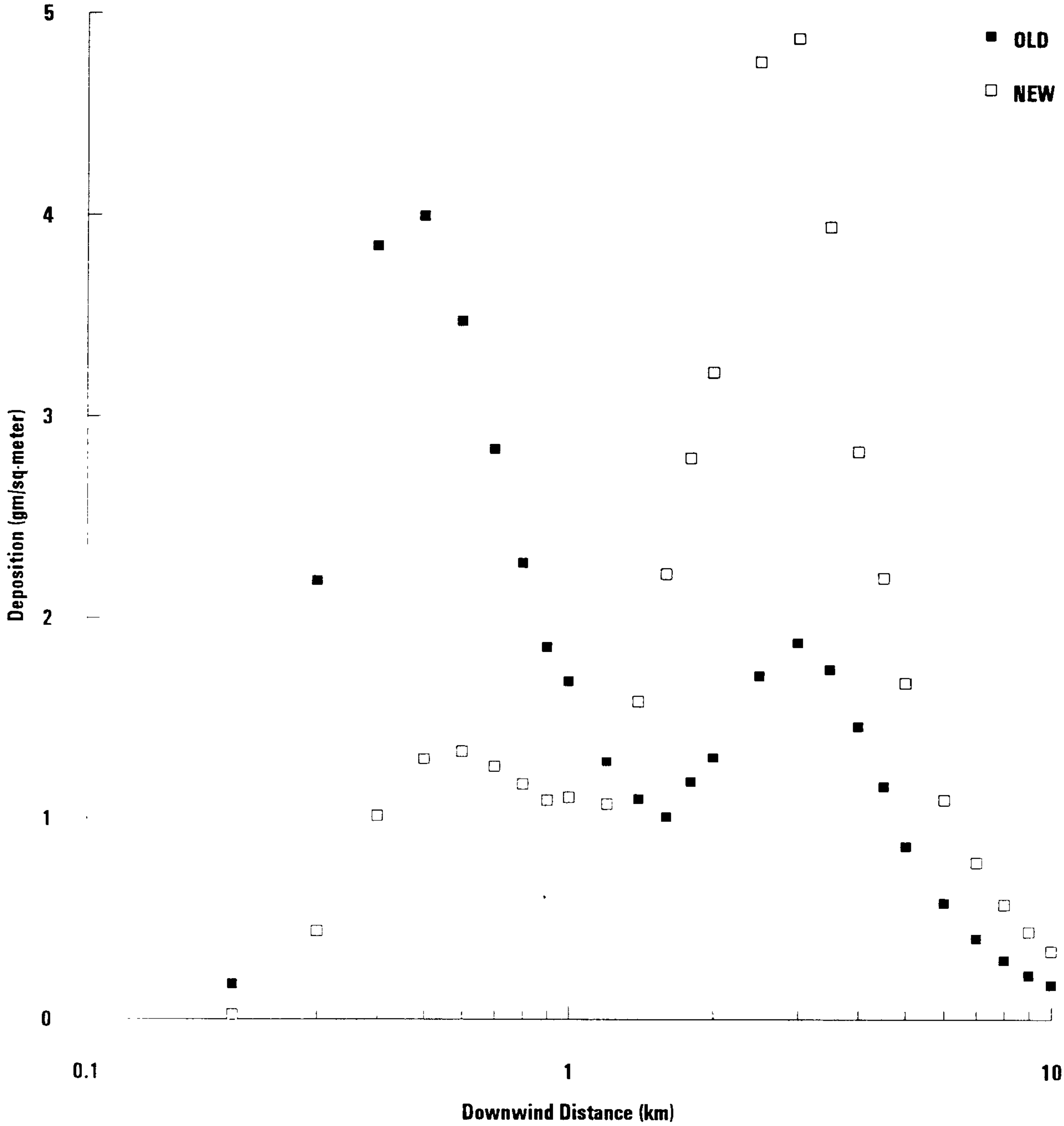


FIGURE 2

Comparison of highest 1-hour ISCST deposition estimates (g/m^2) based on the old and new algorithms for a 35-meter release for particle diameters (microns) as indicated:

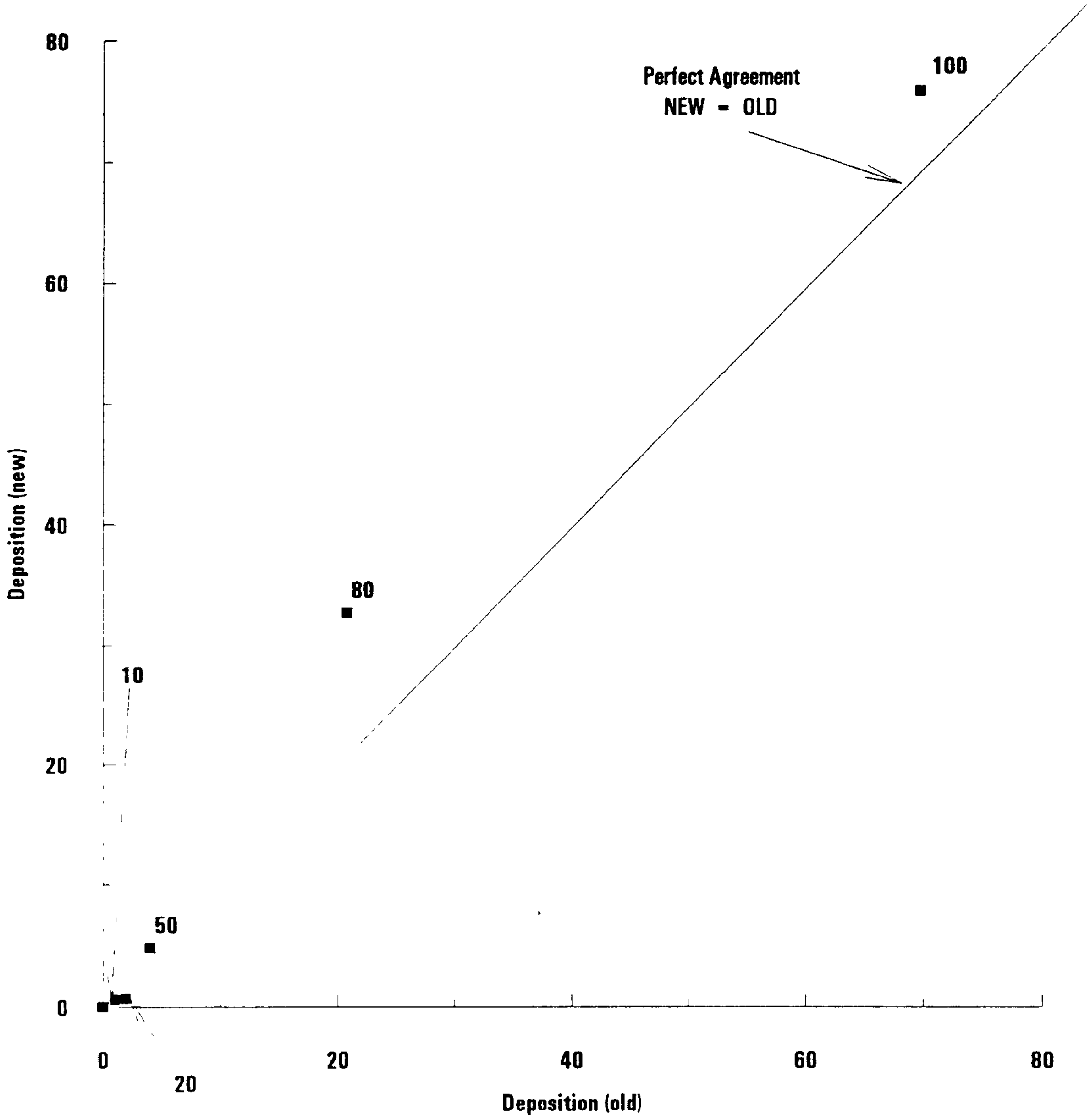


FIGURE 3

Comparison of ISCSTdeposition estimates (g/m^2) based on the old and new algorithms for selected extreme meteorological conditions and particle diameters (microns) as indicated, for a 35-meter release

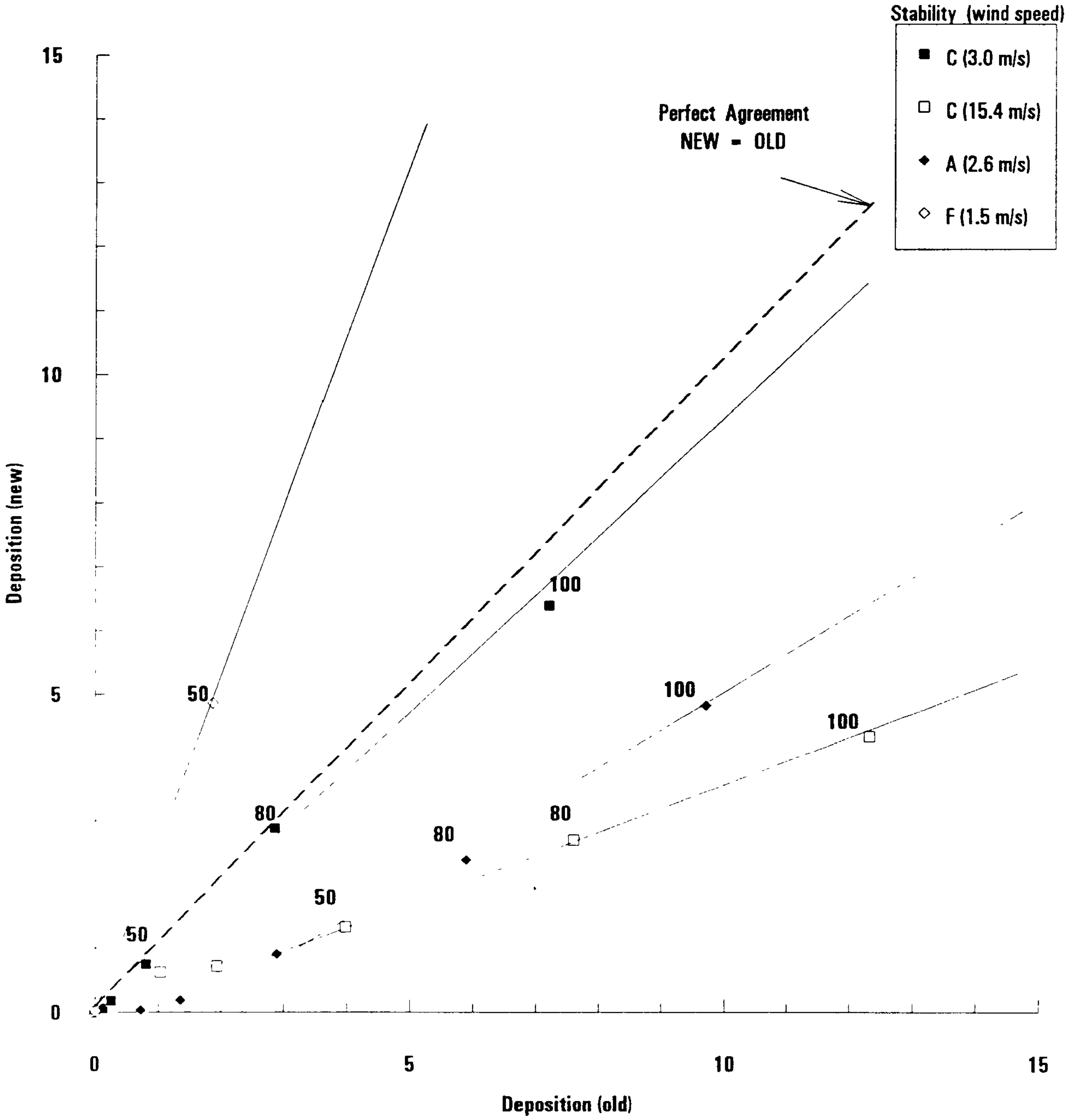


FIGURE 4

Fractional difference (FD) of highest 1-hour ISCST deposition estimates based on old and new algorithms for particle sizes and release heights as indicated
FD = 2 (NEW - OLD) / (NEW + OLD)

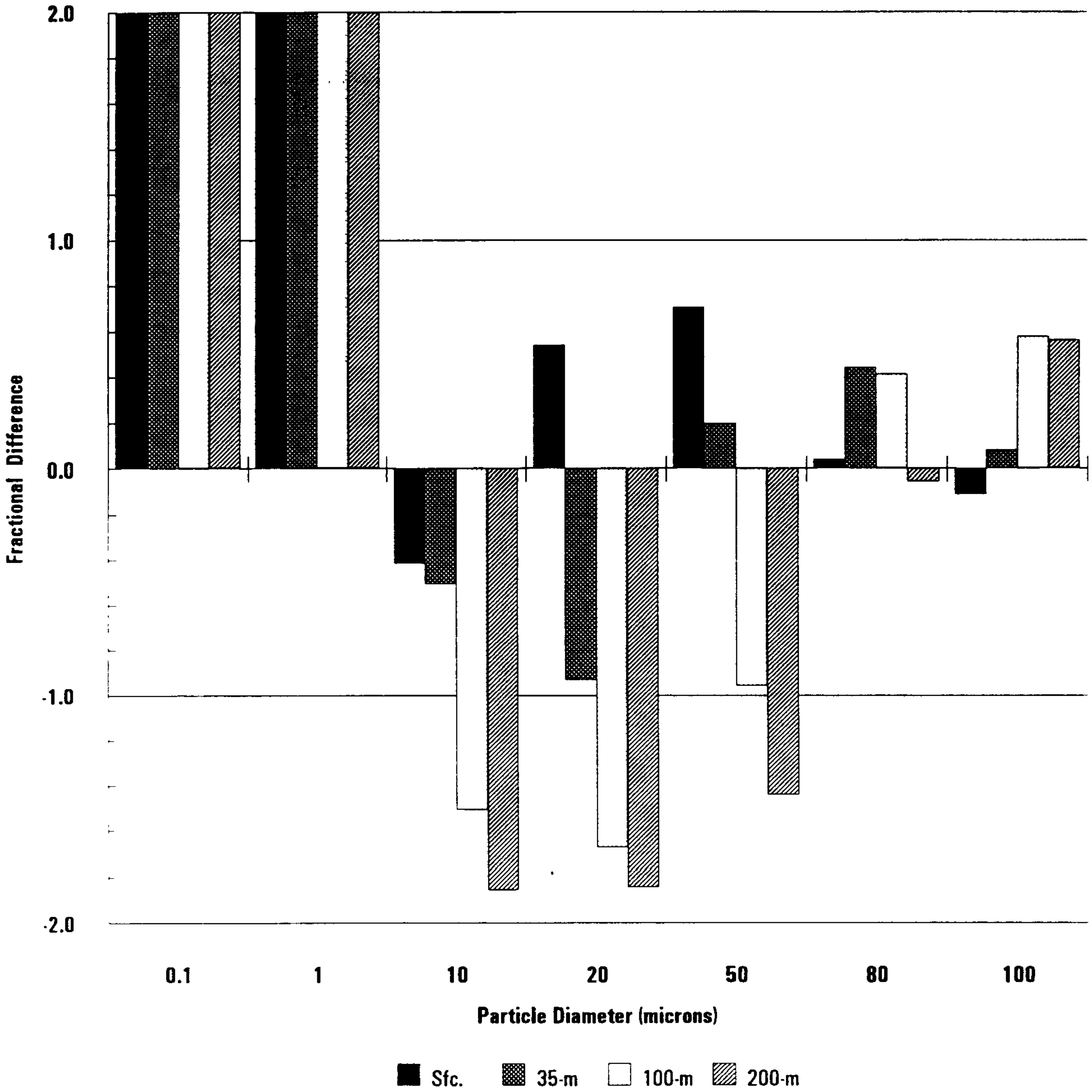


FIGURE 5

Fractional difference (FD) of highest 3-hour ISCST deposition estimates based on old and new algorithms for particle sizes and release heights as indicated
FD = 2 (NEW - OLD) / (NEW + OLD)

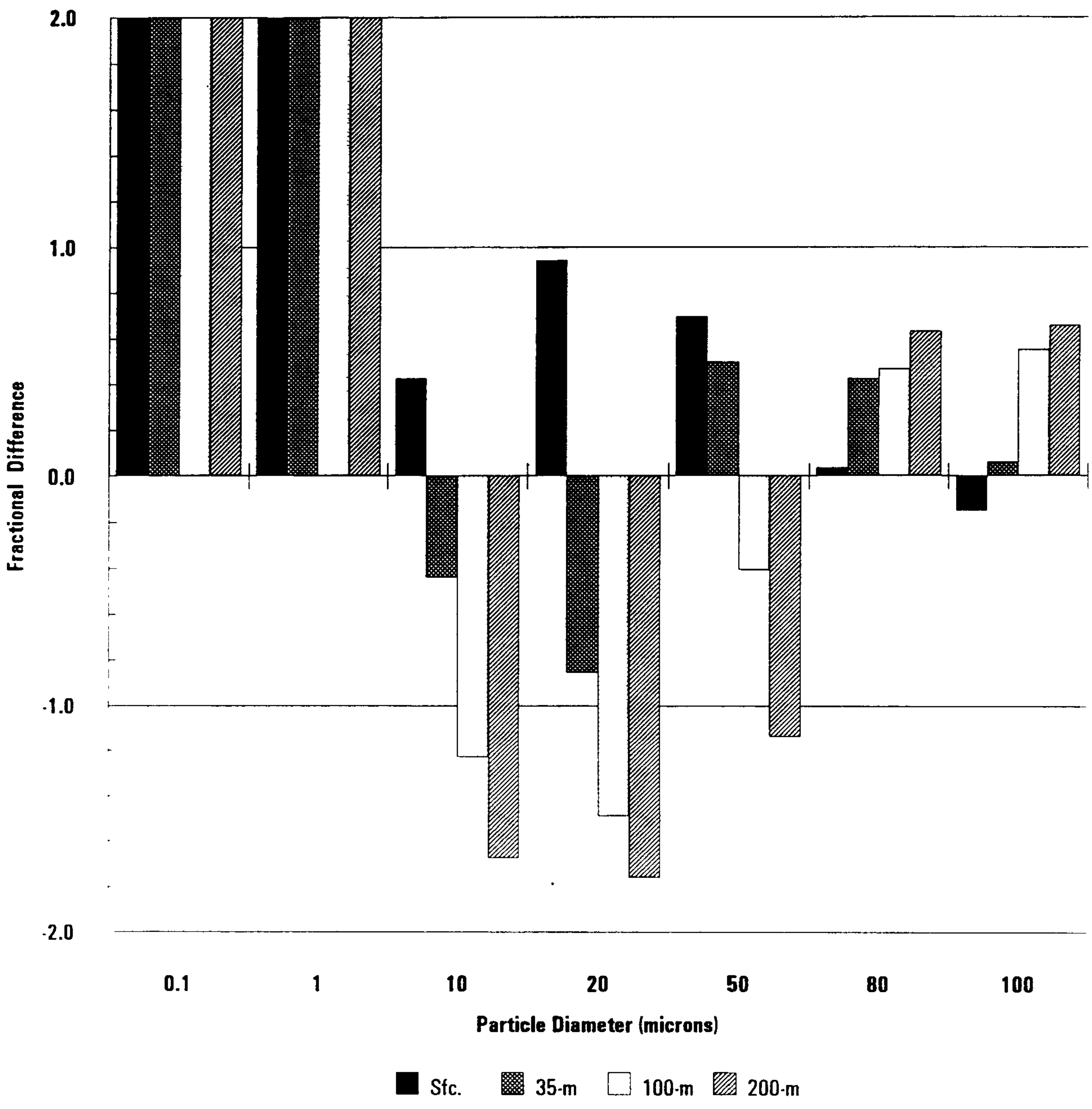


FIGURE 6

Fractional difference (FD) of highest 24-hour ISCST deposition estimates based on old and new algorithms for particle sizes and release heights as indicated
FD = 2 (NEW - OLD) / (NEW + OLD)

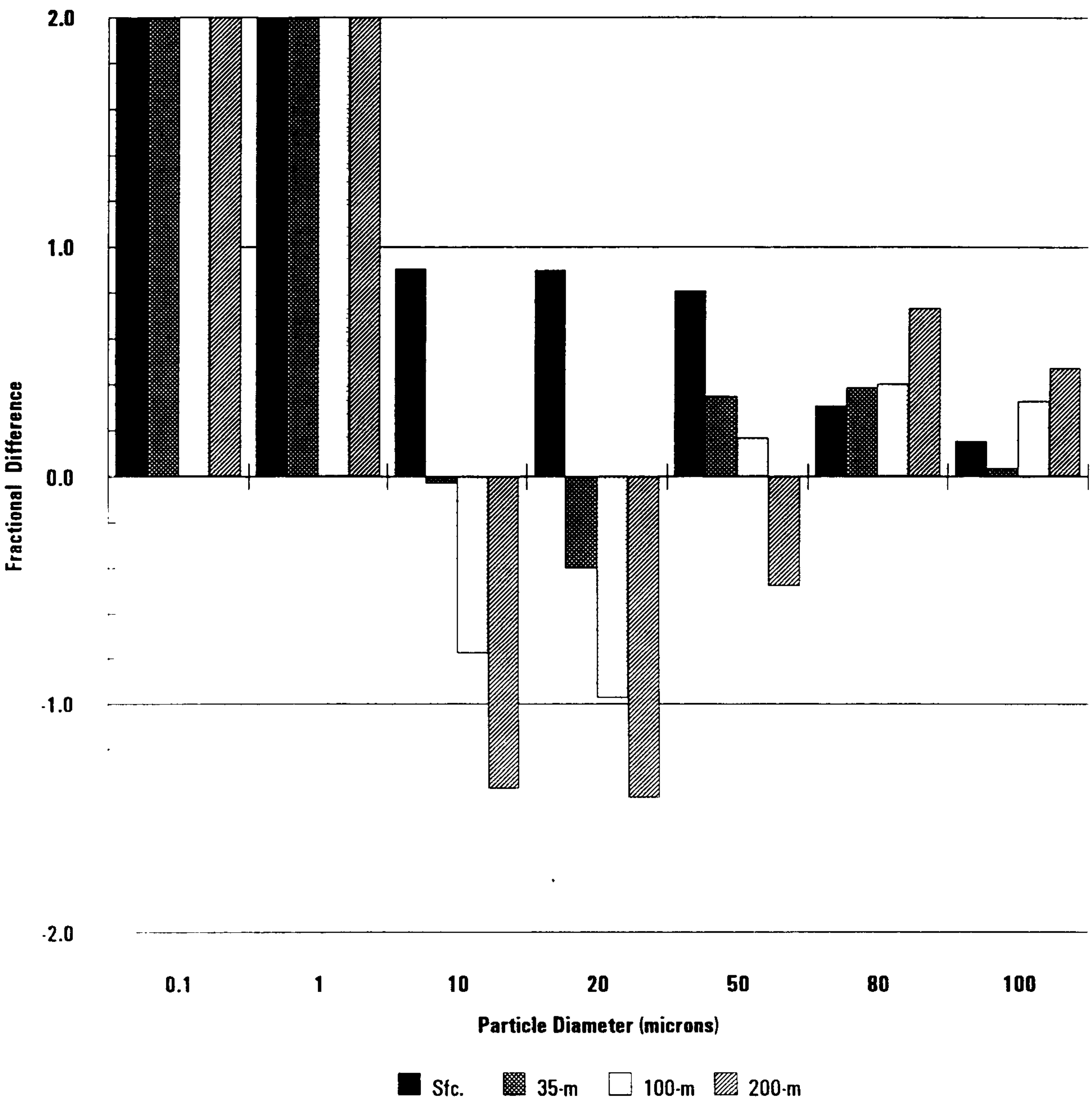


FIGURE 7

Fractional difference (FD) of highest annual ISCST deposition estimates based on old and new algorithms for particle sizes and release heights as indicated
FD = 2 (NEW - OLD) / (NEW + OLD)

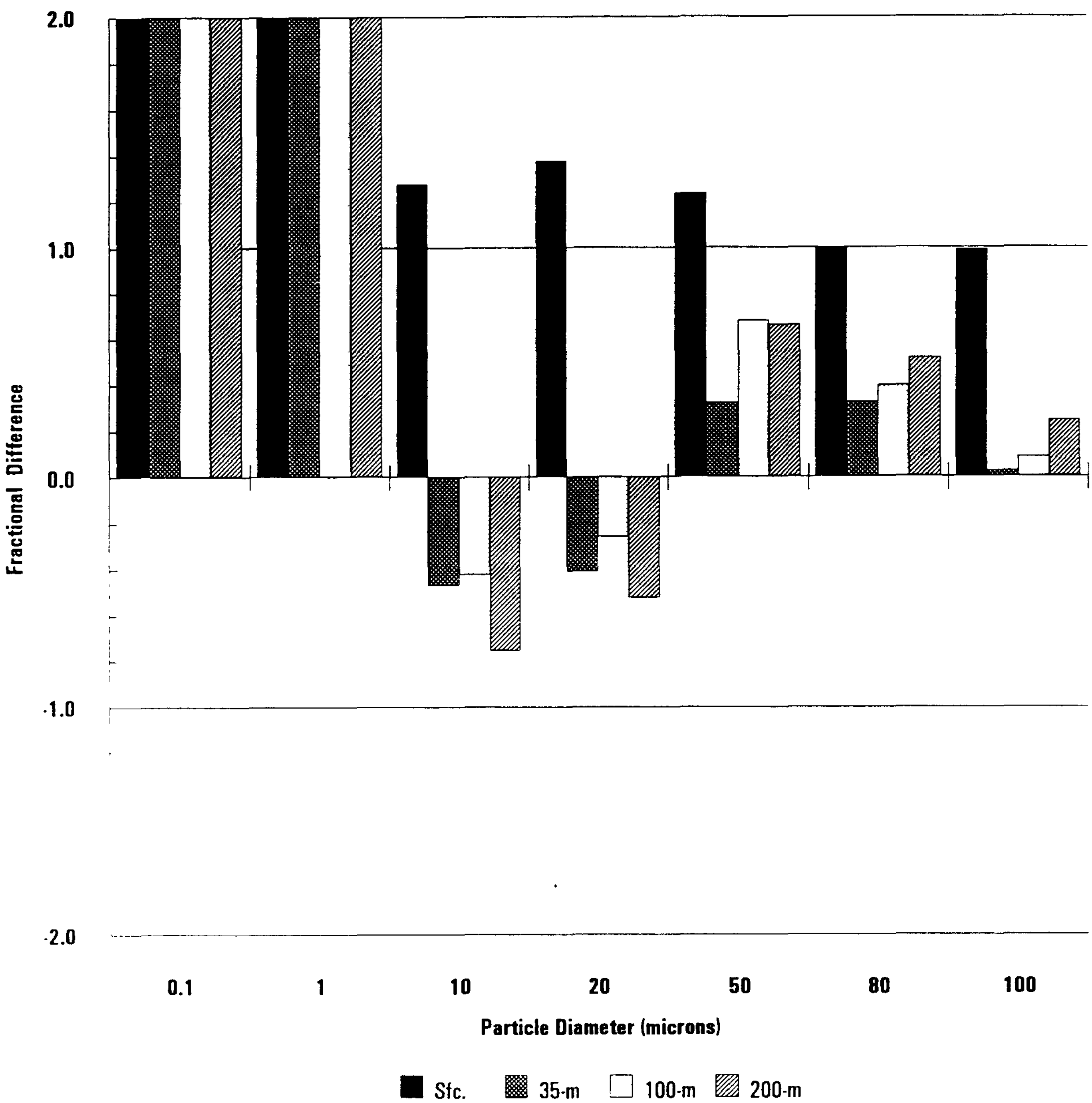


FIGURE 8

Fractional Difference (FD) of highest 1-hour ISCST concentration estimates considering effects of old and new deposition algorithms for particle diameters and release heights as indicated
FD = 2 (NEW - OLD) /(NEW + OLD)

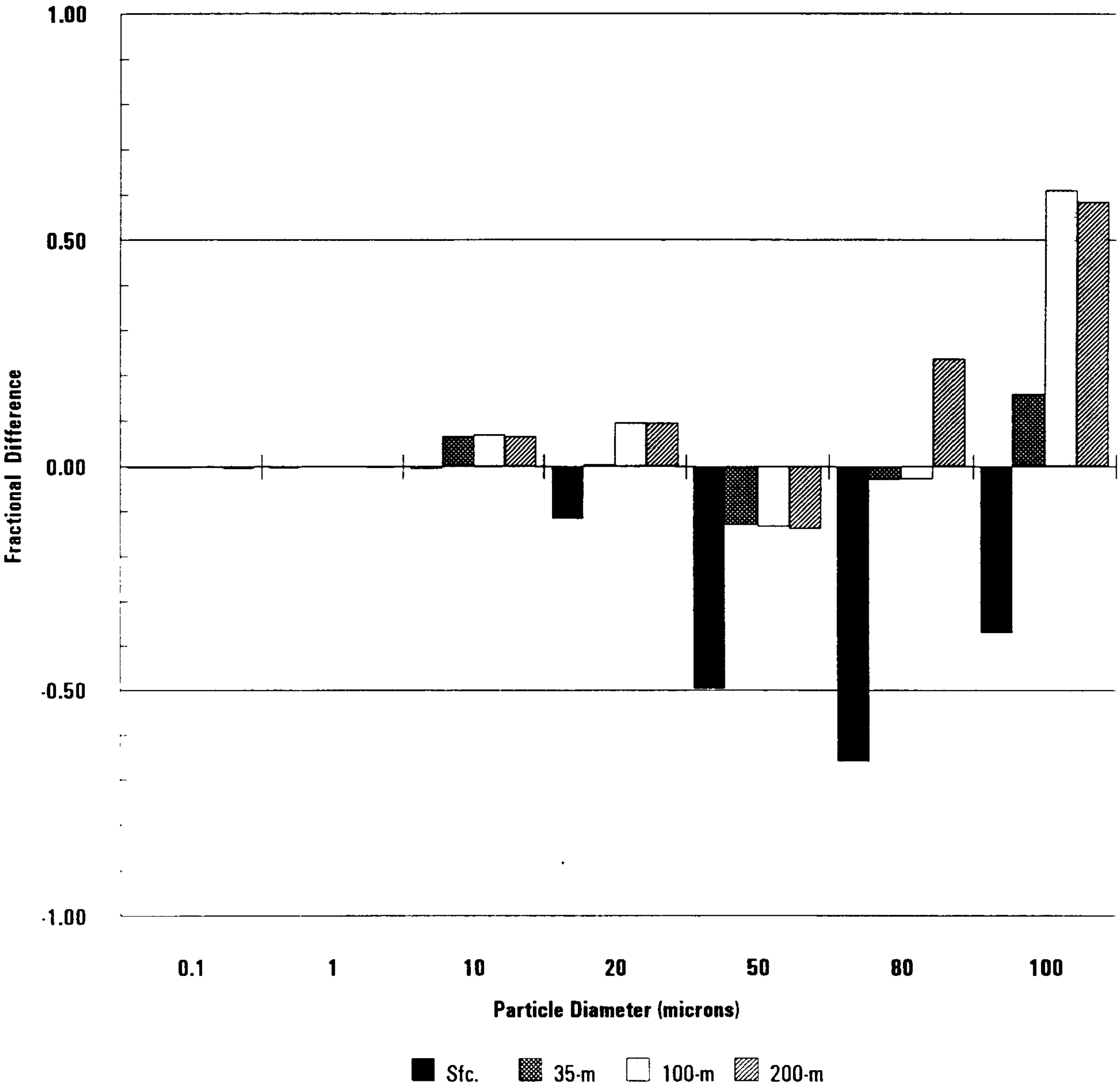


FIGURE 9

Fractional Difference (FD) of highest 3-hour ISCST concentration estimates considering effects of old and new deposition algorithms for particle diameters and release heights as indicated

FD = 2 (NEW - OLD) /(NEW + OLD)

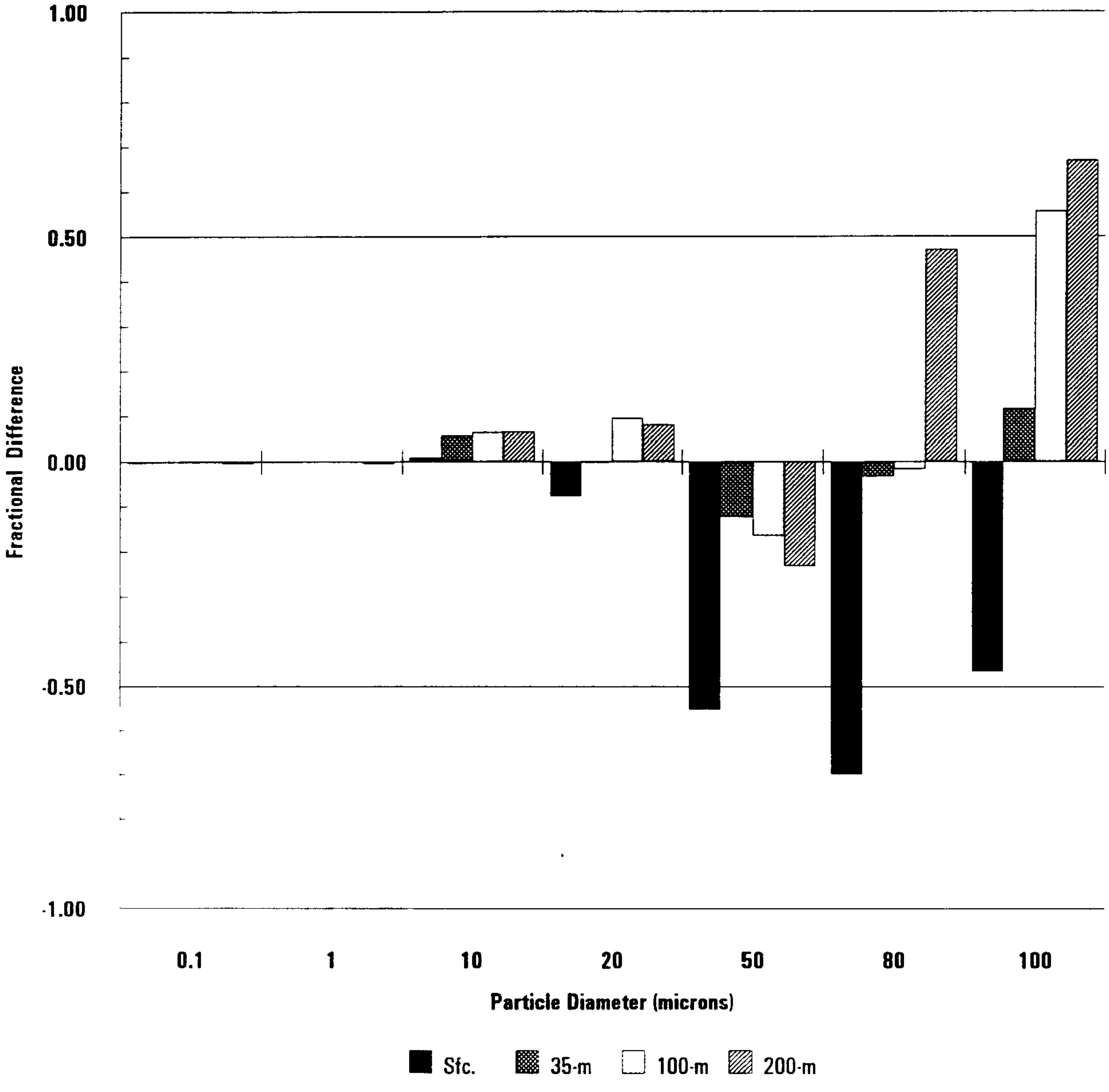


FIGURE 10

Fractional Difference (FD) of highest 24-hour ISCST concentration estimates considering effects of old and new deposition algorithms for particle diameters and release heights as indicated

FD = 2 (NEW - OLD) /(NEW + OLD)

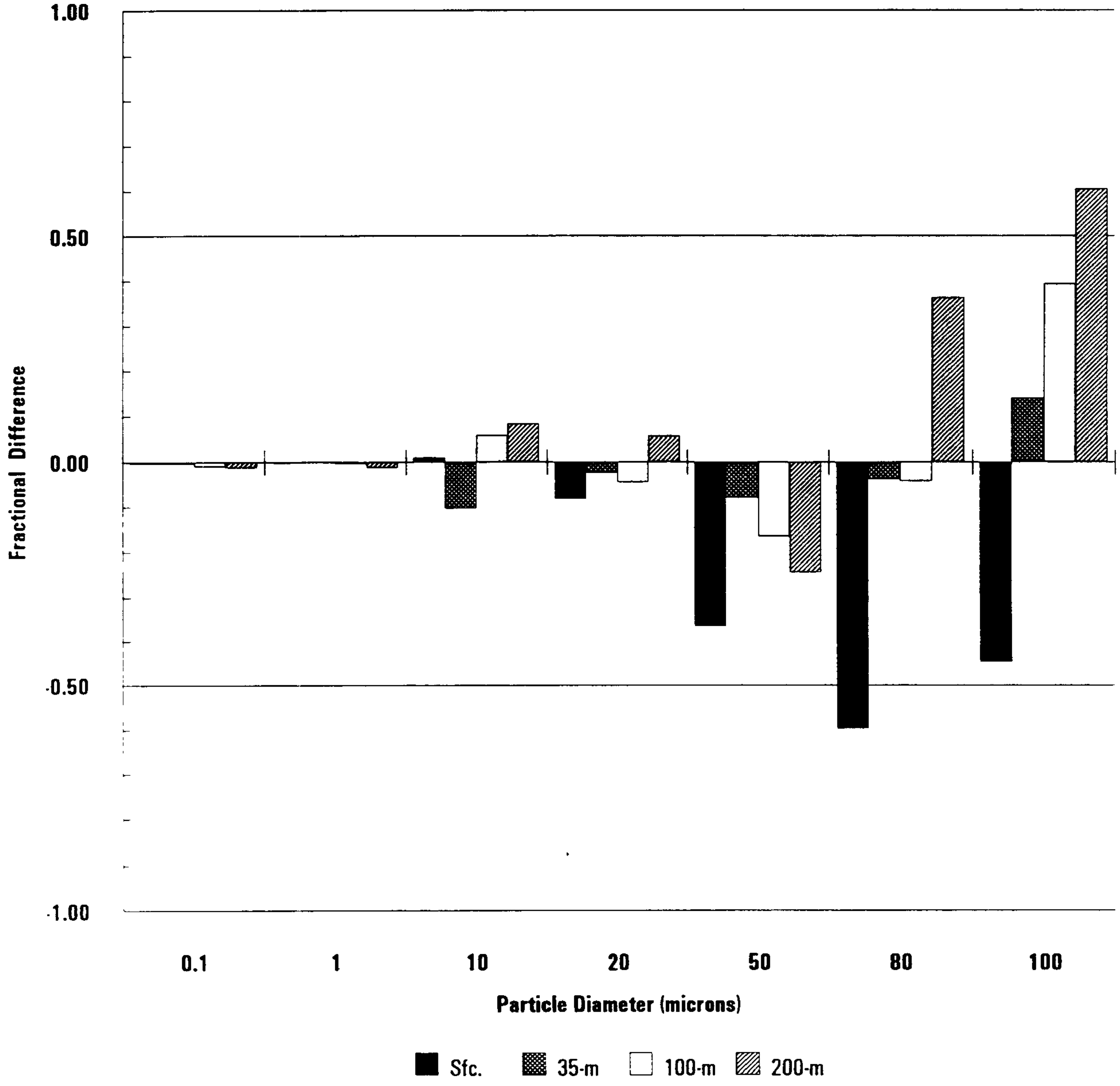
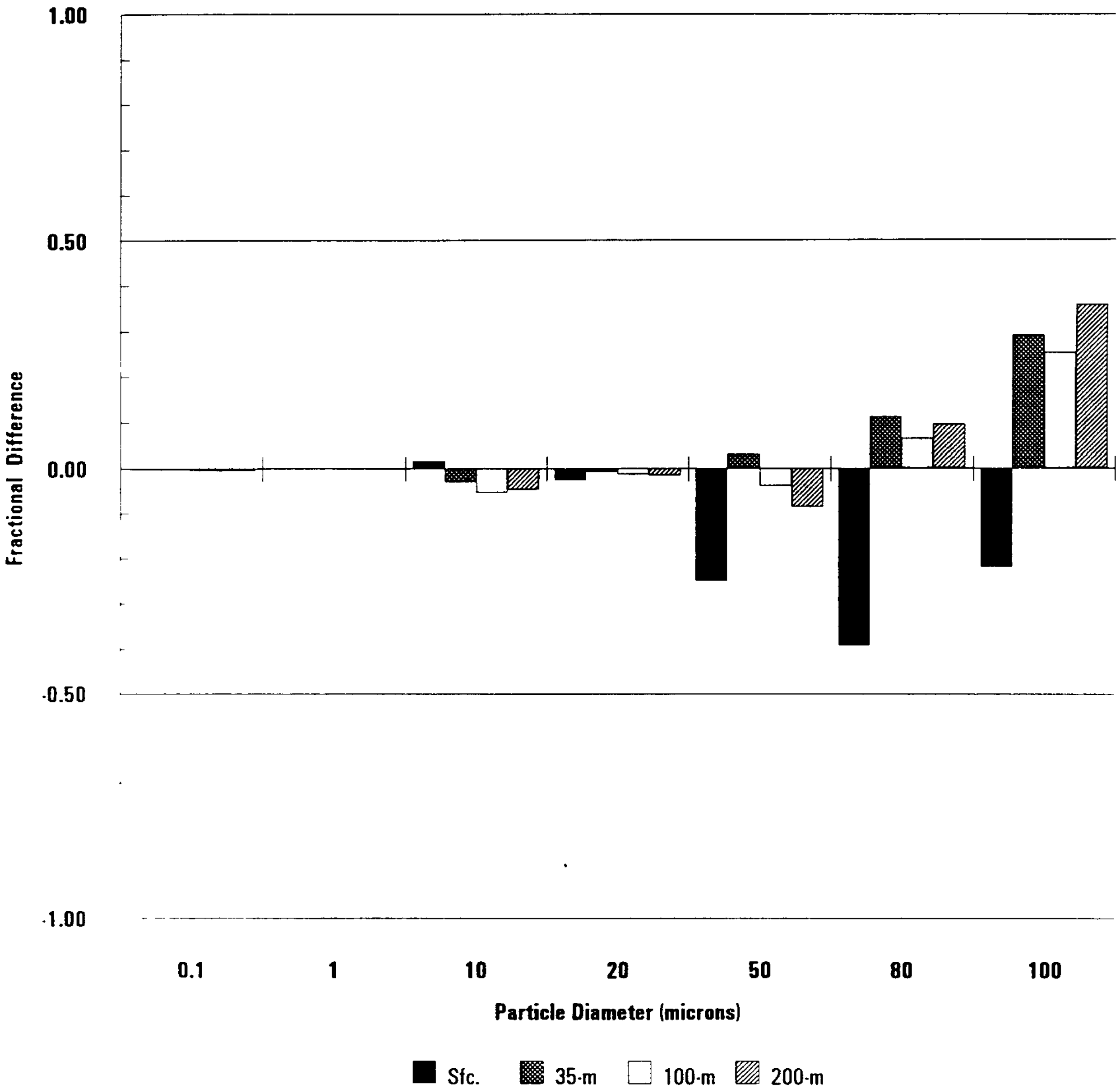


FIGURE 11

Fractional Difference (FD) of highest annual-hour ISCST concentration estimates considering effects of old and new deposition algorithms for particle diameters and release heights as indicated

FD = 2 (NEW - OLD) /(NEW + OLD)



APPENDIX A

Comparison of Highest 1-hour ISCST Deposition Estimates Based on the Old and New Algorithms for a 35-m Release

APPENDIX A

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FIGURE A-1

Comparison of highest 1-hour ISCST deposition estimates based on old and new algorithms for a 35-meter release for 10 micron diameter particles.

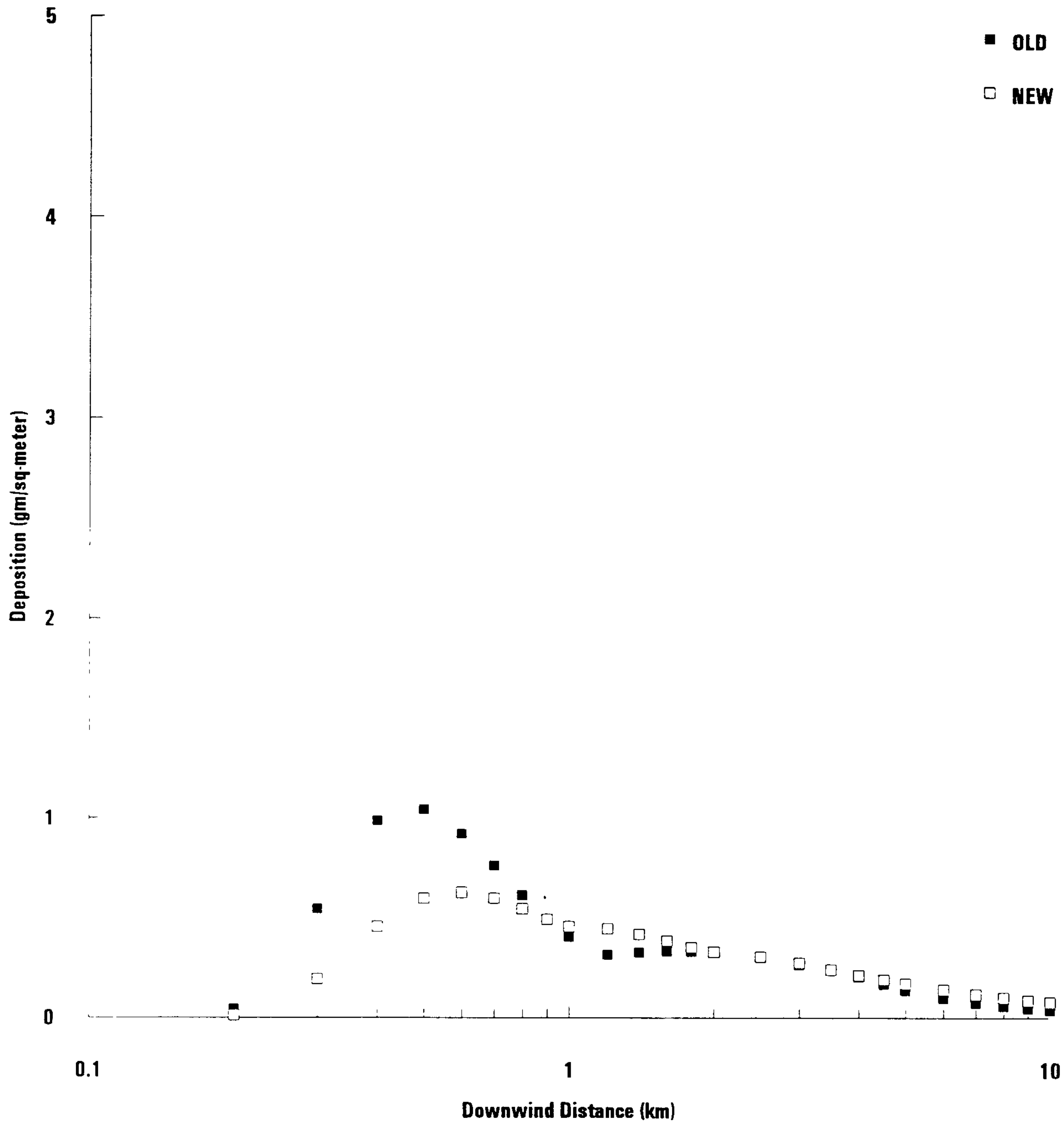


FIGURE A - 2

Comparison of highest 1-hour ISCST deposition estimates based on old and new algorithms for a 35-meter release for 20 micron diameter particles.

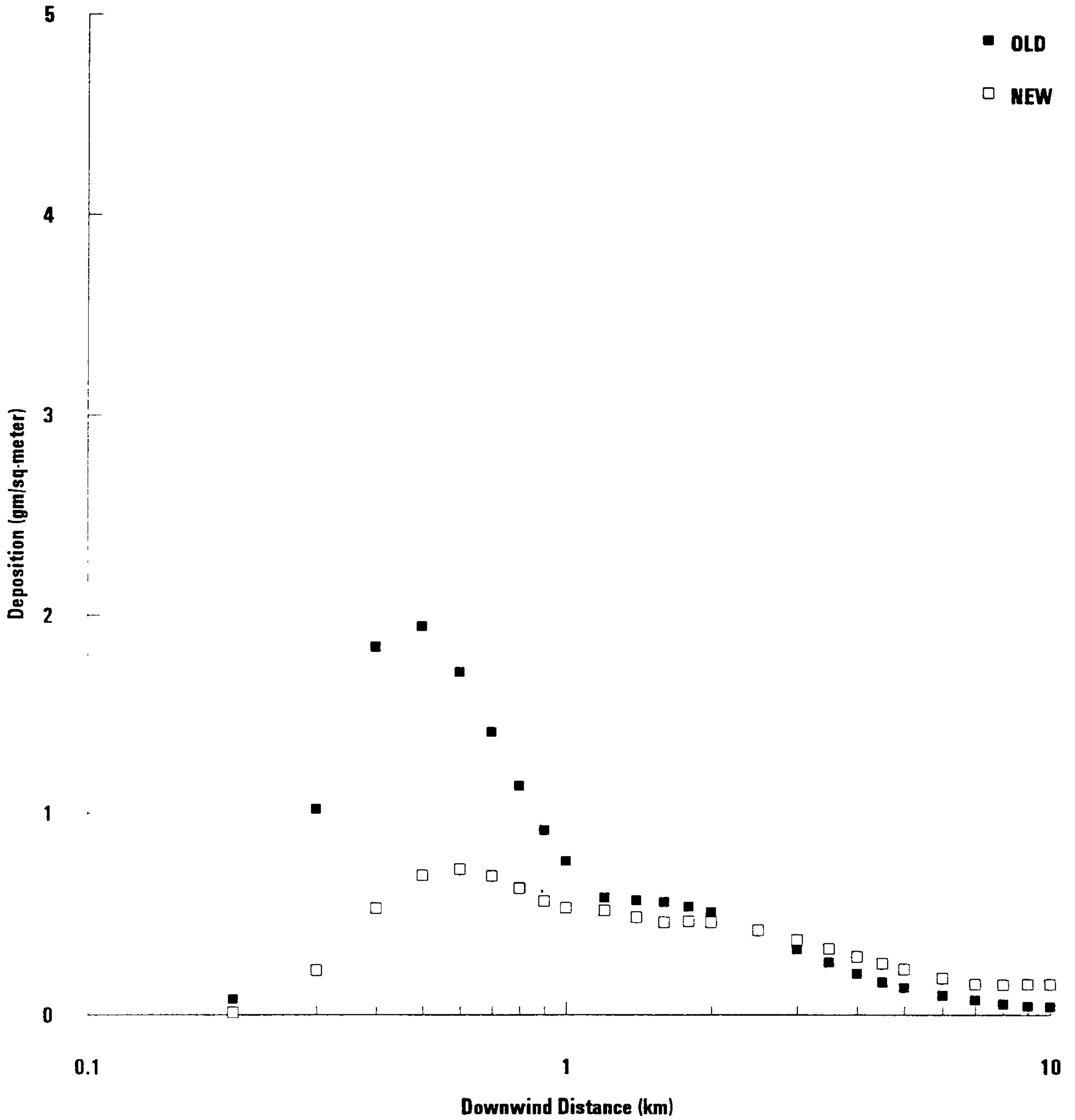


FIGURE A-3

Comparison of highest 1-hour ISCST deposition estimates based on old and new algorithms for a 35-meter release for 50 micron diameter particles.

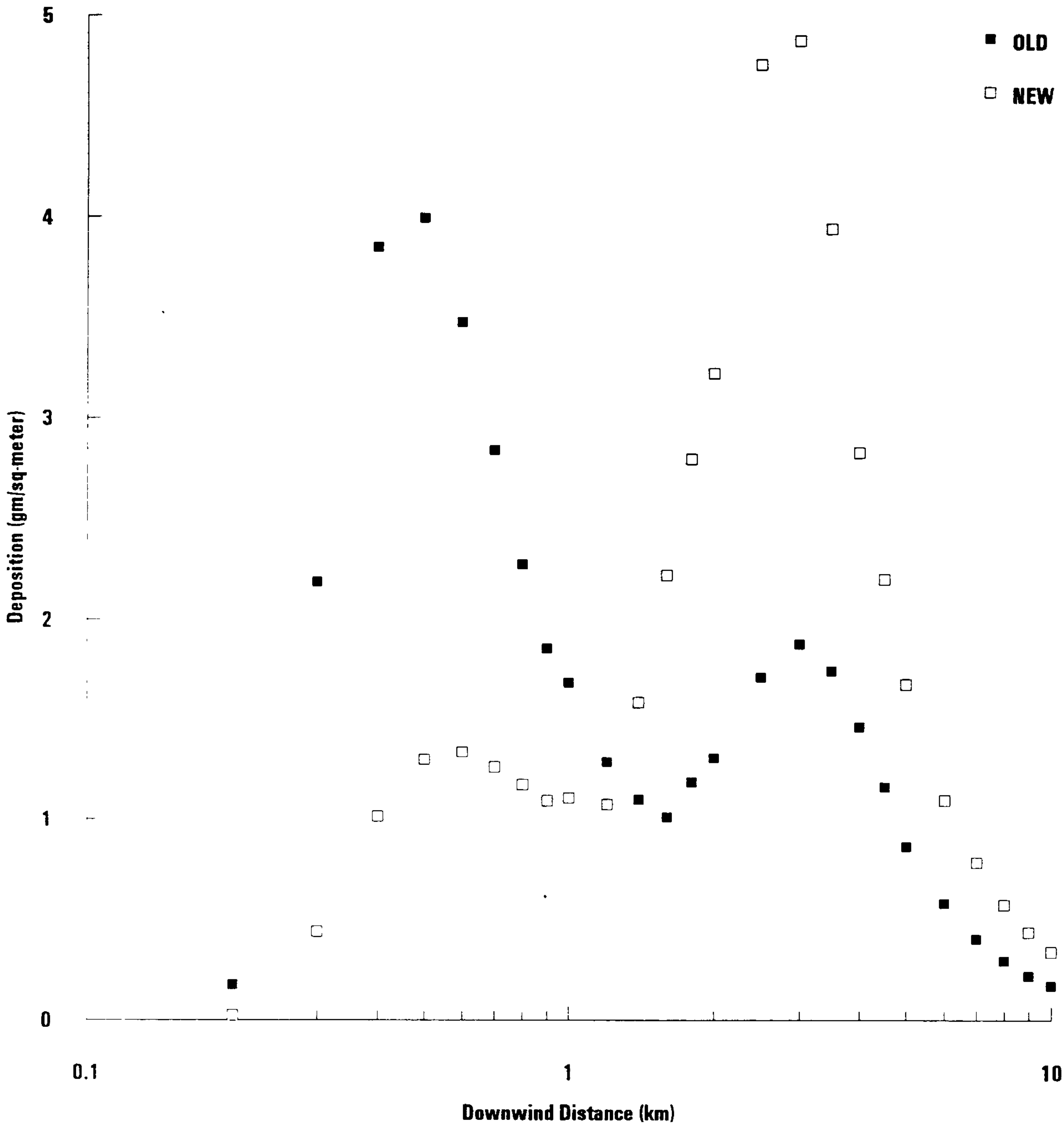


FIGURE A-4

Comparison of highest 1-hour ISCST deposition estimates based on old and new algorithms for a 35-meter release for 80 micron diameter particles.

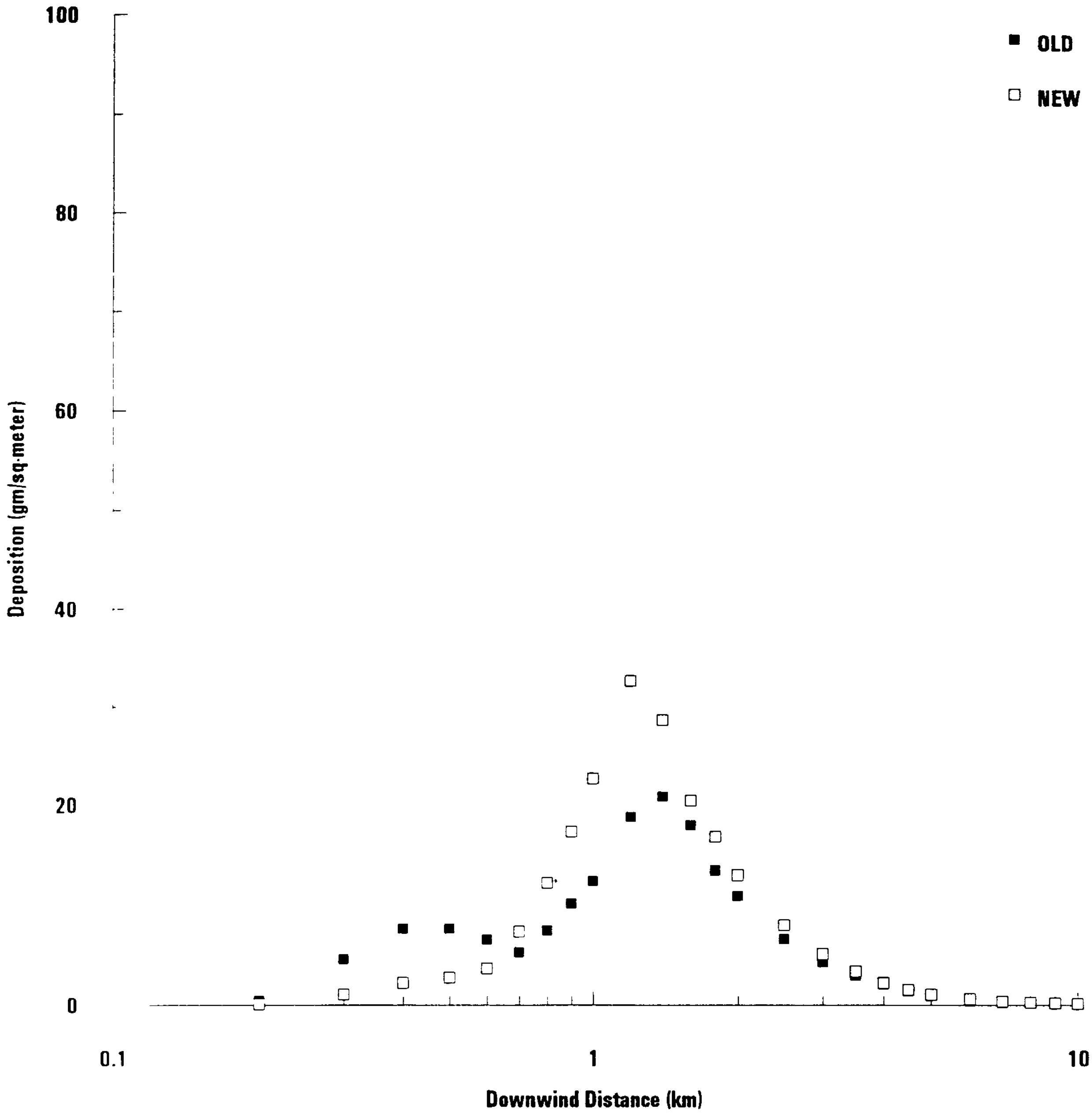
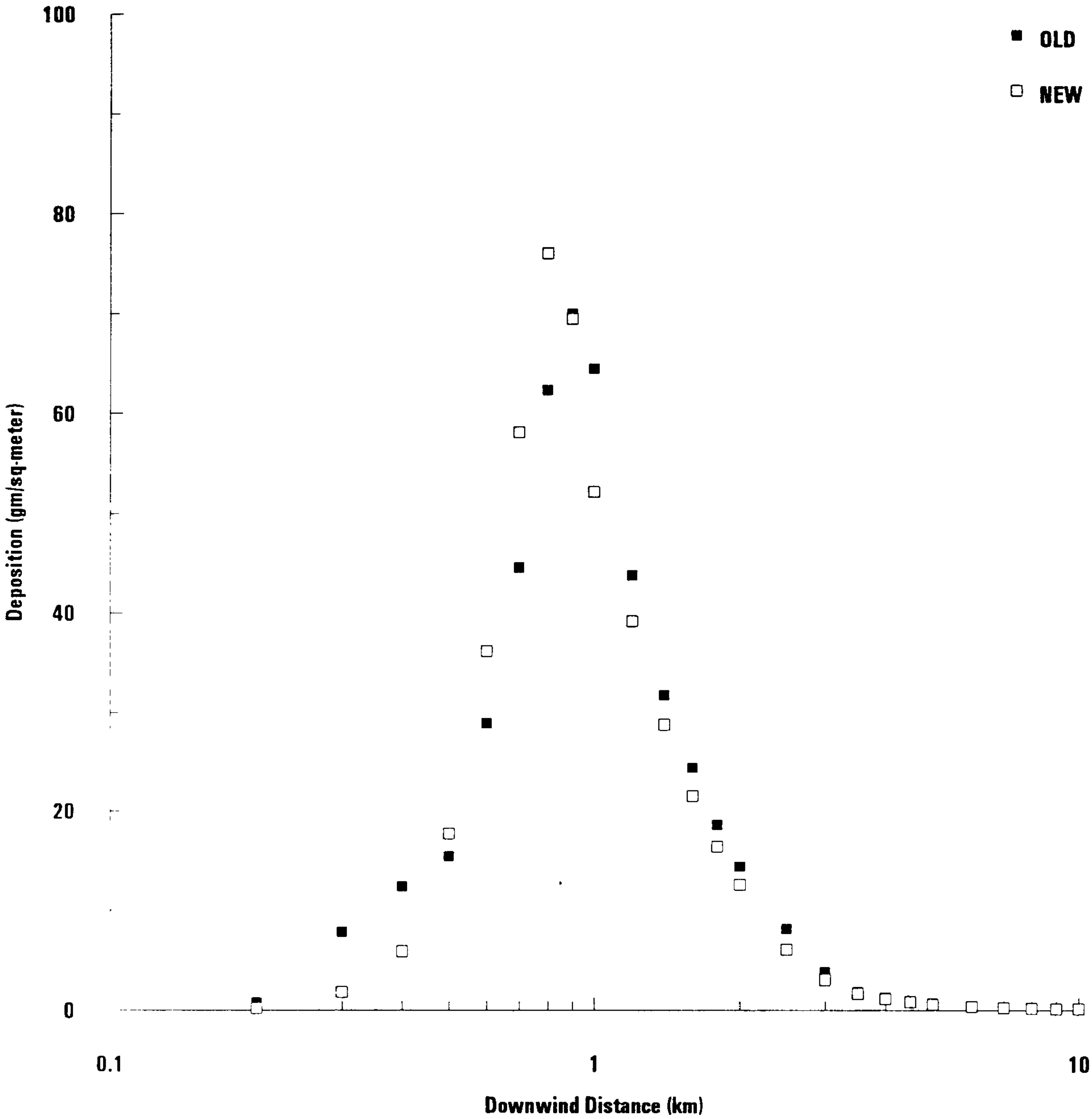


FIGURE A-5

Comparison of highest 1-hour ISCST deposition estimates based on old and new algorithms for a 35-meter release for 100 micron diameter particles.



APPENDIX B

Comparison of Highest 1-Hour Concentration Estimates as Affected by the Old and New Deposition Algorithms for Elevated Releases

APPENDIX B

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B-1 Comparison of ISCST concentration estimates as affected by the old deposition algorithm for C stability with a 3 m/s wind speed for a 35-m release for particle diameters as indicated. . . . B-5

B-2 Comparison of ISCST concentration estimates as affected by the old deposition algorithm for C stability with a 15 m/s wind speed for a 35-m release for particle diameters as indicated. . . . B-6

B-3 Comparison of ISCST concentration estimates as affected by the new deposition algorithm for C stability with a 3 m/s wind speed for a 35-m release for particle diameters as indicated. . . . B-7

B-4 Comparison of ISCST concentration estimates as affected by the new deposition algorithm for C stability with a 15 m/s wind speed for a 35-m release for particle diameters as indicated. . . . B-8

B-5 Comparison of ISCST concentration estimates as affected by the old and new deposition algorithms for E stability with a 1.5 m/s wind speed for a 200-m release for 100 μm diameter particles. . . . B-9

The results presented in Appendix B reflect diagnostic analyses of selected extreme 1-hour concentration events for elevated releases.

Figures B-1 through B-4 show results for a 35-m release for C stability with a 3 m/s wind speed [Figure B-1 (old) and Figure B-3 (new)] and with a 15 m/s wind speed [Figure B-2 (old) and Figure B-4 (new).

Effect of Wind Speed on Concentration

For the 3 m/s wind speed, the maximum concentration increases, and the distance to the maximum decreases with increasing particle size. This is the case for both the old (Figure B-1) and new (Figure B-3) algorithms. These results reflect the influence of gravitational settling and its affect on plume tilt. Gravitational settling of a 100 μm particle (0.3 m/s) is significant relative to a 3 m/s wind speed. Under these conditions, an elevated plume of 100 μm particles descends more steeply and intersects the surface closer to the source than a plume composed of smaller particles.

By comparison, gravitational settling and plume tilt are not as significant with a 15 m/s wind speed. In this case, concentrations with the old deposition algorithm (Figure B-2) actually decrease with increasing particle size (note that deposition increases with particle size). With the new algorithm (Figure B-4), concentrations appear to increase with particle size (at least to a downwind distance of 1 km.) - this reversal may possibly be due to the affect on deposition of a higher friction velocity.

Effects of Deposition on Concentration

Concentration estimates were also computed with the deposition option turned off. These estimates are shown by the solid curves in Figures B-1 and B-3 for the 3 m/s wind speed, and by the solid curves in Figures B-2 and B-4 for the 15 m/s wind speed.

For both old (Figures B-1 and B-2) and new (Figures B-3 and B-4) algorithms, the no deposition curve coincides with the concentration estimates for the 1 μm particle size category. This is as expected for the old algorithm since it considers effects due to gravitational settling only and assigns a reflection coefficient of 1.0 (no deposition) to this size category. For the new algorithm, the 1 μm particle size does not have a noticeable effect on concentration estimates. For larger particles, the maximum concentration increases with particle size.

Results for a 200-m Release of 100 μm Particles

Figure B-5 shows the estimated concentrations for a 200-m release of 100 μm particles for the extreme 1-hour meteorological conditions associated with this case (E stability at 1.5 m/s). Concentration estimates as affected by the new deposition algorithm are shown for two cases (with and without plume depletion). It is seen that the effects of plume depletion become significant at downwind distances beyond the location of the maximum (about 5 km). The results show that the concentration estimates as affected by the new deposition algorithm are about a factor of 2 greater than the corresponding estimates for the old algorithm.

FIGURE B - 1

Comparison of ISCST concentration estimates as affected by the old deposition algorithm for C stability with a 3 m/s wind speed for a 35-m release for particle diameters as indicated

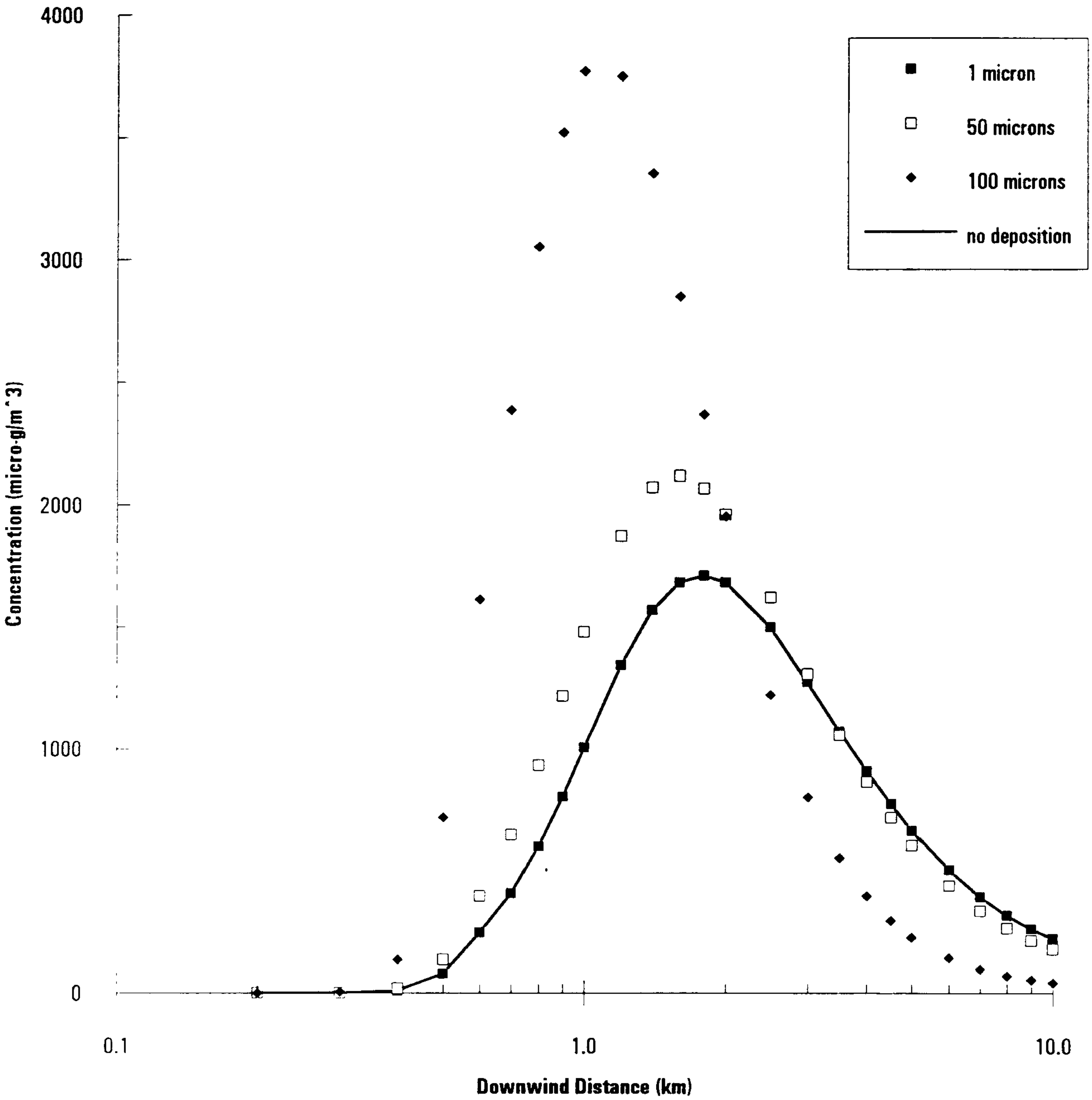


FIGURE B - 2

Comparison of ISCST concentration estimates as affected by the old deposition algorithm for C stability with a 15 m/s wind speed for a 35-m release for particle diameters as indicated

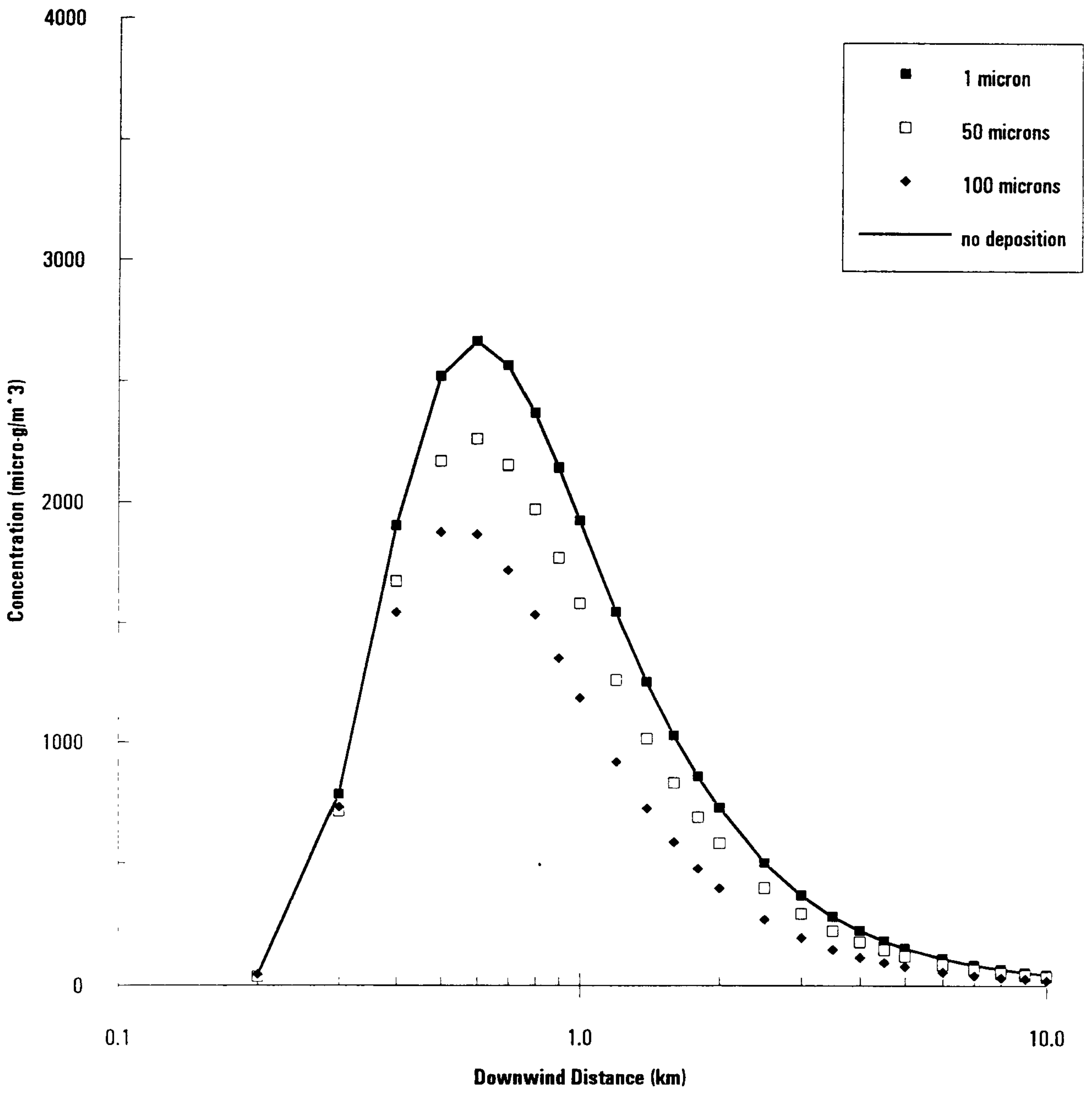


FIGURE B - 3

Comparison of ISCST concentration estimates as affected by the new deposition algorithm for C stability with a 3 m/s wind speed for a 35-m release for particle diameters as indicated

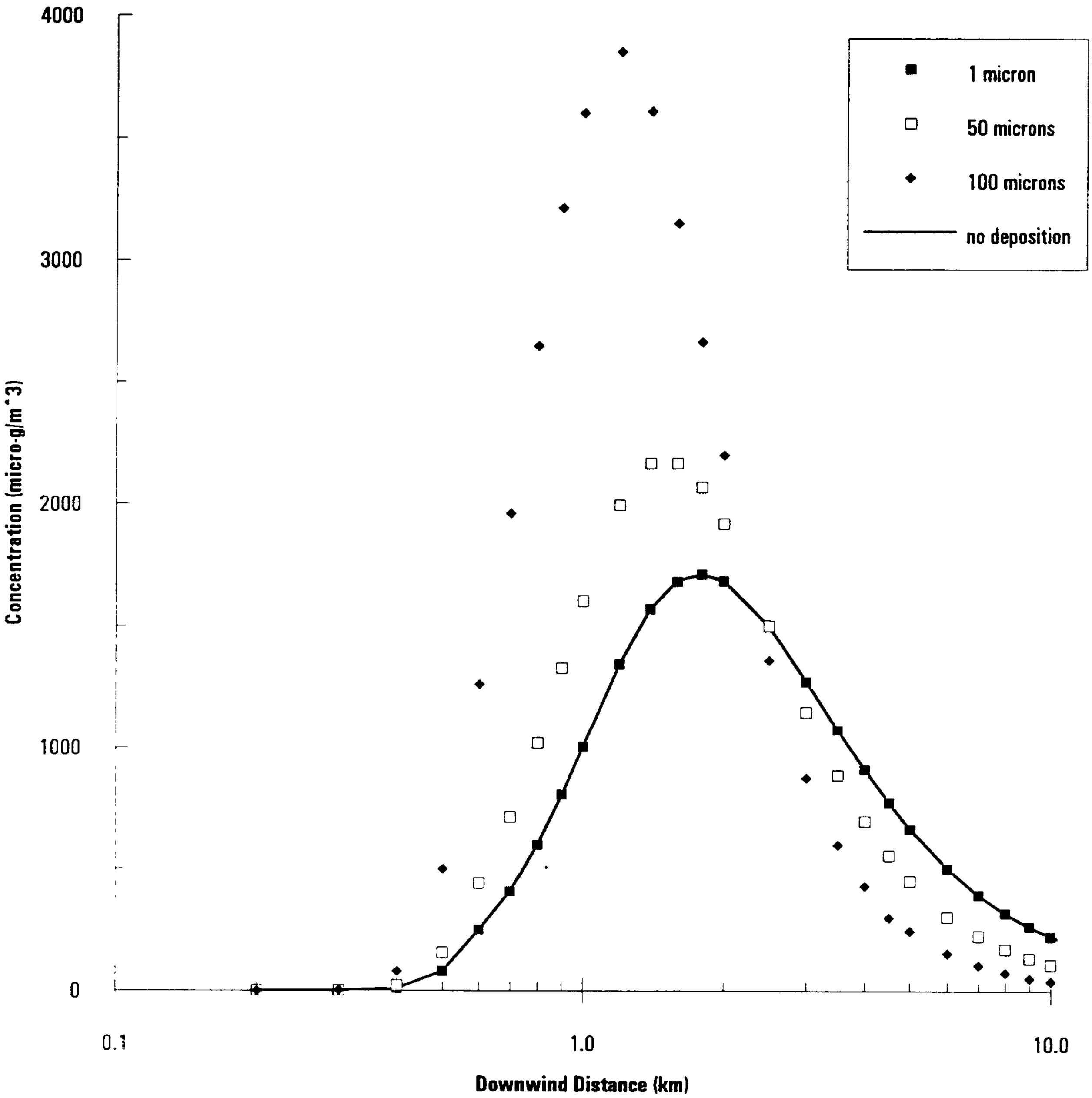


FIGURE B - 4

Comparison of ISCST concentration estimates as affected by the new deposition algorithm for C stability with a 15 m/s wind speed for a 35-m release for particle diameters as indicated

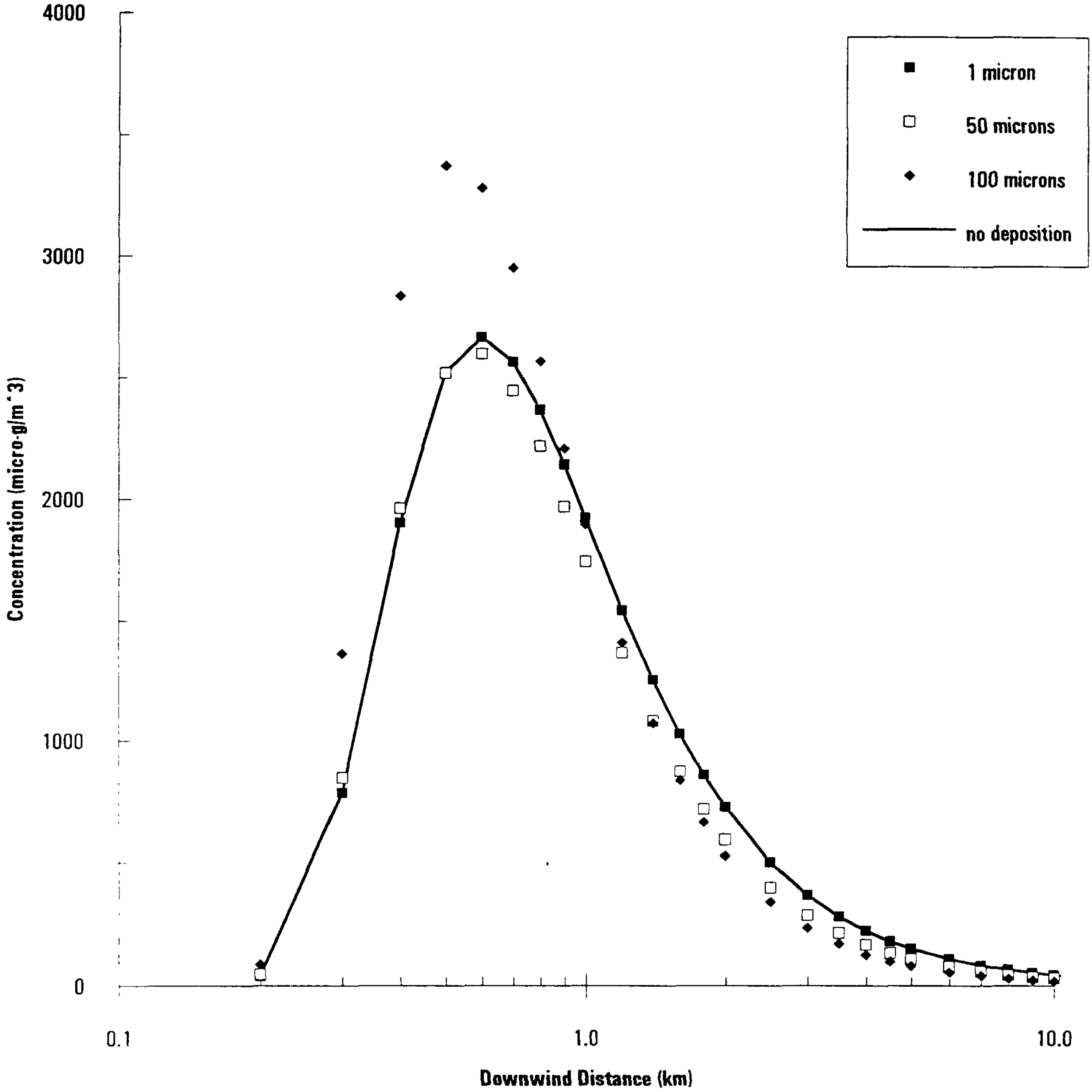
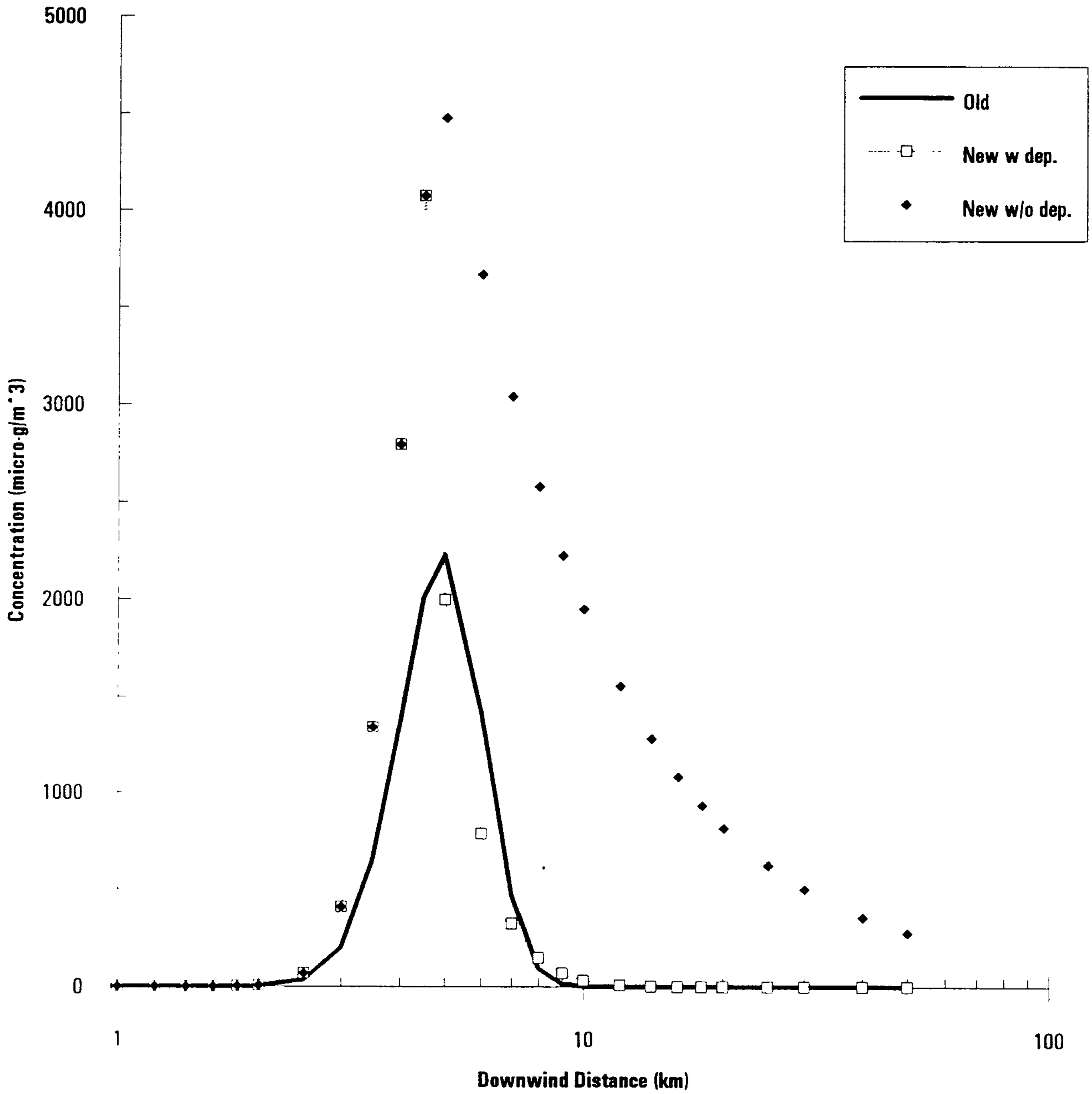


FIGURE B-5

Comparison of ISCST concentration estimates for a 200-m release of 100 micron particles as affected by the old and new deposition algorithms.
Meteorological Conditions: Stability E at 1.5 m/s



TECHNICAL REPORT DATA

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15 SUPPLEMENTARY NOTES

16 ABSTRACT

The ability to accurately estimate deposition of particulate matter is of special concern in assessing environmental impacts from a variety of sources including Superfund sites, municipal waste incinerators, and surface coal mines. The current deposition algorithm in ISC2 simulates deposition as the movement of particles toward the surface by the combined processes of atmospheric turbulence and gravitational settling. The method was developed for applications to large particles dominated by gravitational settling; these are typically particles greater than 20 μm diameter. The current algorithm was not intended for use with particles smaller than about 20 μm which are often of concern in air toxics assessments. In light of this limitation, a new deposition algorithm is being considered for use in ISC2. The proposed algorithm is intended to simulate processes important over the entire range of significant particle sizes (0.1 to 100 μm). The proposed algorithm employs a deposition velocity based on a resistance model. In this approach, deposition flux is calculated as the product of the near-surface air concentration and the deposition velocity. The latter is computed as the inverse sum of the aerodynamic layer and deposition layer resistances, plus gravitational settling. The new deposition algorithm has been tested within the framework of the ISC2 model and comparisons of deposition estimates using the old (current) and new deposition algorithms have been made for a range of source types and particulate emission scenarios. Similar comparisons have been made of particulate concentration estimates as affected by the old and new deposition algorithms.

17 KEY WORDS AND DOCUMENT ANALYSIS

a DESCRIPTORS	b IDENTIFIERS/OPEN ENDED TERMS	c COSATI Field/Group
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