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AIR

A Comparison of CALPUFF with ISC3

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DISCLAIMER

PREFACE

In this report a comparison is made of two different dispersion models, CALPUFF and ISC3. CALPUFF is a Lagrangian puff model which simulates continuous puffs of pollutants released into the ambient flow, whereas ISC3 is a Gaussian plume model that treats emissions from a source as a contiguous mass. CALPUFF may be configured to treat emissions as integrated *puffs* or as *slugs*. ISC3 is currently recommended for routine use in assessing source impacts involving transport distances of less than 50km. This report is being released to establish part of the basis for review of the consequences resulting from use of CALPUFF in routine dispersion modeling of air pollution impacts.

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1. Introduction

With the initial use of models such as CALPUFF for regulatory applications, there is the question of how the model will behave with respect to more widely used models like the Industrial Source Complex Short Term (ISC3ST) model, hereafter ISC3. Several sensitivity and comparison studies were designed and performed to determine how CALPUFF would behave when set to emulate ISC3. The results of those runs were analyzed and are discussed here.

This evaluation features a systematic, phased series of implementation modes. Section 3.1 involves simple screening modes in which conditions are extremely limited and controlled. Section 3.2 addresses the more general mode in which meteorological conditions are allowed to vary hourly. Section 4 provides a summary and conclusions from this investigation. References are listed in Section 5, followed by the appendices.

2. Technical Background

CALPUFF is a Lagrangian puff model. The model is programmed to simulate continuous puffs of pollutants being emitted from a source into the ambient wind flow. As the wind flow changes from hour to hour, the path each puff takes changes to the new wind flow direction. Puff diffusion is Gaussian and concentrations are based on the contributions of each puff as it passes over or near a receptor point. For these tests, CALPUFF was set to emit 99 puffs per hour (default). A sufficiently large number of puffs is necessary to adequately reproduce the plume solution at near-field receptors.

CALPUFF was originally designed for mesoscale applications and treated emissions as integrated puffs. As features were added to the model for handling local-scale applications, it was realized that use of the integrated puff approach was inefficient. A more efficient approach was developed to treat the emissions as a *slug*, in which the slug is stretched so as to better characterize local source impacts. The slug can be visualized as a group of overlapping circular puffs having very small separation distances. When run in the slug mode, the hourly averaged pollutant mass is spread evenly throughout the slug. For a given hour, if all of the hourly slug has not passed over a receptor, concentrations are reduced by the mass that has not passed over the receptor (Appendix E; Section 2.1 of Reference #2). Note that when run in a *slug* mode, once the slug's lateral dispersion (σ_y) approaches the length of the slug itself (as eventually happens with downwind distance), CALPUFF samples the pollutant mass as a *puff* to improve computational efficiency. At sufficient downwind distance, there becomes no benefit or advantage for the slug simulation.

In the comparison studies described in this report, CALPUFF was run in both the puff mode (emissions simulated as integrated puffs) and the slug mode (emissions simulated as slugs). When the distinction between puffs and slugs is important or significant, they will appear in italics (i.e., *slugs* or *puffs*; see Appendix E). In the generic sense, the use of "puffs" will be used to connote the characterization of a continuous release of a series of overlapping averaged puffs, in which the transport and dispersion of each puff is treated independently, based on local (time and space varying) meteorological conditions. Whereas, the use of "plume" will be used to connote the characterization of a continuous release, in which the release and sampling times are long compared with the travel time from source to receptor, and the meteorological conditions are steady state over the travel time.

3. Results

In this comparison, CALPUFF (Version 4.0, level *960612*) was compared with the latest version of ISC3 (dated *96113*). CALPUFF was run in a mode that enabled ISC3-type meteorological data as input, and therefore winds are horizontally homogeneous for each hour. ISC3 was implemented in the “Regulatory Default” mode and the input file for CALPUFF was configured so as to emulate this to the best extent possible (see Appendix A). Both surface and elevated sources were simulated for *rural* environments in flat terrain, free of obstacles.

3.1 Steady State (screening) Meteorological Conditions

In this approach to the comparison, meteorological conditions were held constant (as in SCREEN3) so as to express true model differences, i.e., without the bias of a varying (temporally and spatially) meteorological regime. Meteorological data sets were synthesized with fixed meteorological conditions (Pasquill-Gifford stability category, wind speed, and mixing height) and were of duration estimated to be sufficient to advect CALPUFF's puffs to the edge of domain (generally 24 - 48 hours). (Of course, ISC3's steady state plume reaches the edge of the domain instantaneously.) For Pasquill-Gifford (P-G) stability category *A*, 5 wind speeds were used, for *B*, there were 9 wind speeds, for *C*, 11 wind speeds, for *D*, 13 wind speeds, for *E*, 9 wind speeds, and for *F*, 7 wind speeds. A matrix describing the basis for the 54 meteorological conditions used is provided in Appendix B.

The elevated point sources were 35m, 100m and 200m, respectively. Surface releases were simulated with a 2m point source, a 500m X 500m area source, and a typical volume source. Characteristics for each source type are described in Appendix C. Sources were placed at the center of a 2 X 2 grid cell domain, with grid spacing set to 150km. While effects within the first 50km are of most interest and significance, straight-line receptors were located with decreasing density out to 100km (Appendix D). The 62 receptors were placed along a radial aligned at 360°, coincident with the bearing used for transport winds.

Unique model runs were made for each combination of source type and meteorological condition (i.e., Pasquill-Gifford stability category, wind speed, and mixing height). Each model was configured to output the highest hourly average concentration for SO_2 (no deposition or chemical transformation).

3.1.1 Residual Analysis

For each pair of model runs (CALPUFF and ISC3), a signed residual (R_i, $\chi_{CALPUFF}$ - χ_{ISC3}, µgm^{-3}) was computed at each of the 62 receptors. From the 62 residuals, a mean ($\bar{R}$, µgm^{-3}), standard deviation (σ_R, µgm^{-3}), and sum of residuals squared ($\Sigma\ R_i^2$) were computed. The statistic $\bar{R}$ provides an indication (sign) of bias along the receptor radial. The statistic σ_R provides general indication of the variance along the receptor radial. Because many of the absolute residuals were quite small, $\Sigma\ R_i^2$ provides a relatively robust indicator of accord along the receptor radial.

Another robust statistic was envisioned in which the absolute residual at each receptor was related to, say, ISC3's predicted concentration value at that receptor. Because of the mathematical problem posed by zero values (can't divide by zero), the statistic $\%R_i$ (*% residual*) was defined in terms of the *maximum* concentration predicted by ISC3 for each run:

$$\%R_i = \left(\frac{R_i}{\chi_{ISC3max}}\right) 100$$

The *mean % residual* follows as:

$$\overline{\%R} = \frac{\Sigma\ \%R_i}{62}$$

As with $\bar{R}$, the statistic $\overline{\%R}$ provides an indication (sign) of bias along the receptor radial.

Another statistic of interest was the Fractional Bias (FB):

$$FB_i = \frac{R_i}{\dfrac{\chi_{CALPUFF} + \chi_{ISC3}}{2}}$$

Having by definition a distribution from -2 to +2, a value of zero indicates no bias between $\chi_{CALPUFF}$ and χ_{ISC3}.

One problem that arises with the FB statistic is when the mean paired concentration is very close to zero: the FB statistic can be artificially inflated to a value close to ±2. Since cases in which the mean is close to zero are of little interest in this comparison, a filter was applied:

$$If \quad \left(\frac{\chi_{CALPUFF} + \chi_{ISC3}}{2}\right) < 0.001\mu gm^{-3}, \quad then \ FB_i = 0.0$$

For each run pair (i.e., CALPUFF versus ISC3), a mean fractional bias was computed as:

$$\overline{FB} = \frac{\Sigma FB_i}{62} \qquad \text{(62 receptors)}$$

As with $\overline{R}$ and $\overline{\%R}$, $\overline{FB}$ provides an indication (sign) of bias along the receptor radial. While a value of zero would be ideal for $\overline{FB}$, the following was established as a "goal":

$$-0.10 \le \overline{FB} \le 0.10$$

Specific instances for which this goal was not met were noted.

There are some caveats to the interpretation of FB. Its behavior is closely related to its structure. Its value is influenced not only by the absolute difference of the paired concentrations, but by their relative magnitude as well. Thus, modest R_i's related to "large" $\overline{\chi}$'s (e.g., from a low level release) yield modest FB_i's (and a modest $\overline{FB}$). Such a scenario can include a fairly large variance (σ_R = 56 µgm^{-3}) and mean residual (e.g., $\overline{R} = -32 \ \mu gm^{-3}$) along the receptor radial but still result in a fairly low $\overline{FB}$ (e.g., $\overline{FB}$ = -0.06). Conversely, modest R_i's related to "small" $\overline{\chi}$'s (e.g., from an elevated release) may yield substantial FB_i's. Such a scenario can include a modest variance (σ_R = 0.5 µgm^{-3}) and mean residual (e.g., $\overline{R} = 0.3 \ \mu gm^{-3}$) along the receptor radial but still result in a sizeable $\overline{FB}$ (e.g., $\overline{FB}$ = 0.35). While a useful indicator of correspondence between two quantities, the FB must be interpreted in the context of other comparison statistics.

At the conclusion of the runs, a performance matrix was created and aggregate statistics were compiled. For basic residual analysis, the value, run (distinct combination of source type, wind speed, P-G category, mixing height) and receptor for $R_{i(min)}$ and $R_{i(max)}$ were noted. Likewise, across all runs, the value and run for $\overline{\%R}_{min}$ and $\overline{\%R}_{max}$ were noted, as were the value and run for $\overline{R}_{min}$ and $\overline{R}_{max}$. Across all runs, the value and run for $\sigma_{R(min)}$ and $\sigma_{R(max)}$ were also noted.

Finally, for the FB statistic, the value, run and receptor for $FB_{i(min)}$ and $FB_{i(max)}$ were noted. Across all runs, the value and run for $\overline{FB}_{min}$ and $\overline{FB}_{max}$ were noted. The values and cases in which $\overline{FB}$ did not meet the "10% goal" were also noted.

3.1.2 Point Sources (surface and elevated)[1]

3000m mixing height

To model the four point sources, CALPUFF had to be run 216 times while ISC3 was run 54 times.[2] As indicated in Appendix A, CALPUFF was run in the *slug* mode to emulate ISC3's Gaussian plume simulation.[3] The results indicated good accord (Appendix F). For all cases, $|\overline{FB}| \le 0.10$ ($\overline{FB}_{max} = 0.02$). The *maximum* residual was 25.0 μgm^{-3} (0.13% of the concentration mean at the incident receptor), while the *minimum* residual was -8.0 μgm^{-3} (0.03% of the concentration mean at the incident receptor). Mean residuals for any run were less than one μgm^{-3}, and total range for σ_R was 0.0 - 3.2 μgm^{-3}. Overall, perhaps the most practical performance parameter was $\overline{\%R}$, which indicates accord well within one percent across all release heights, meteorological conditions and receptors (the value for $\overline{\%R}_{min}$ was -0.04% and $\overline{\%R}_{max}$ was 0.13%). A qualitative inspection of residuals as they appear along the receptor array indicated no distinct pattern of bias for any case. Across all runs, a slight negative bias (CALPUFF relative to ISC3) is apparent for the 2m source, and the greatest variance is associated with the 2m source, especially for P-G category *A*.

500m mixing height

The array of runs was redone (again, using *slugs*) with mixing height reduced to 500m to assess CALPUFF's response to reflection and to evaluate whether reflection is handled equivalently. The results were quite good. In 43 cases, the plume centerline computed by ISC3 exceeded the mixing height and set ground level concentrations to zero. CALPUFF treated the same cases equivalently. For the remaining 173 cases, $|\overline{FB}| \le 0.10$ ($\overline{FB}_{max} = 0.02$). The comparison statistics bear a striking resemblance to those for Z_i = 3000m. Mean residuals for

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[1]Certain runs may be referenced, e.g., D20H100 or B1p5H2. Under this nomenclature, the first signifies a 100m source running under *D* stability with 20 ms^{-1} winds. The second would be a 2m source running under *B* stability with 1.5 ms^{-1} winds.

[2]Each source was modeled 54 times for each of two mixing heights. In the current version of CALPUFF, it is impossible to isolate impacts from more than one source per run. ISC3, however, may be configured to simulate multiple sources during a single run and isolate impacts individually.

[3]For a description of integrated *puff* and *slug* formulations, see Sections 2.1.1 and 2.1.2 of the CALPUFF User's Guide (Reference #2) and Appendix E of this report.

any run were also less than one μgm^{-3}, and $\overline{\%R}$ indicates accord to well within one percent across all release heights, meteorological conditions and receptors (the value for $\overline{\%R}_{min}$ was 0.0% and $\overline{\%R}_{max}$ was 0.08%). A qualitative inspection of residuals as they appear along the receptor array also indicated no distinct pattern of bias for any case. As with the 3000m Z_i case, a slight negative bias is apparent for the 2m source, and the greatest variance is associated with the 2m source, especially for P-G category *A*.

3.1.3 Area Source

The area source was modeled with emissions simulated as *slugs*. While a significant difference would be expected between the behavior of *puffs* and *slugs*, *slugs* are considered to treat the area source more closely to the way of ISC3. This is because the "line-source" integrator, similar to that used in ISC3 to model area sources, is only implemented when emissions are simulated as *slugs*. *Puffs* use the effective σ_y treatment for area sources. If there are receptors within or very near an area source, the *slug* treatment is a better representation. If receptors are farther away, the *puff* treatment is reasonable, and less time-consuming. Mixing height was fixed at 3000m. These runs were done both for $\sigma_{z(init)} = 0$ and for $\sigma_{z(init)} = 2.5$m (specification of non-zero $\sigma_{z(init)}$ is optional in both models). The best accord was seen for the set in which $\sigma_{z(init)} = 0$ (Appendix G). For about one fifth of the cases, $|\overline{FB}| > 0.10$ ($\overline{FB}_{min} = -0.16$). The *maximum* residual was 561 μgm^{-3} (2.2% of the concentration mean at the incident receptor), while the *minimum* residual was -1537 μgm^{-3} (33% of the concentration mean at the incident receptor). Mean residuals and mean standard deviations among runs ranged over three orders of magnitude. Analysis of the residuals and fractional biases indicate a definite trend toward negative bias (CALPUFF relative to ISC3), and best accord for any P-G category was seen for the *higher wind speeds*. Also, within any P-G category, the variance falls off with higher wind speed. The parameter $\overline{\%R}$ indicates accord within two percent across meteorological conditions and receptors (the value for $\overline{\%R}_{min}$ was -1.5% and $\overline{\%R}_{max}$ was -0.07%) and again, the tendency toward negative bias is indicated. A qualitative inspection of residuals as they appear along the receptor array indicated no distinct pattern of bias for any case.

3.1.4 Volume Source

The volume source was modeled with emissions simulated as *slugs*. Because ISC3 does not compute concentrations for receptors within $2.15\sigma_y$ of the source (it's actually $2.15\sigma_y$ + 1m), no residuals were analyzed for receptors closer than 200m.

There is a fundamental feature of the way in which ISCST3 treats virtual sources (such as the volume source in question) that is at odds with the way in which CALPUFF treats such sources. The phenomenon is described and illustrated in Appendix H. A modified version of ISCST3 was created to ensure conformity in the treatment of virtual sources by both models. Once this modification was made, the accord between CALPUFF and ISC3 was quite good (Appendix I).

For all cases $|\overline{FB}| = 0.0$. The *maximum* residual was 0.15 μgm^{-3} (0.1% of the concentration mean at the incident receptor), while the *minimum* residual was -0.92 μgm^{-3} (0.4% of the concentration mean at the incident receptor). Mean residuals for any run ranged from -0.2 μgm^{-3} to 0.0 μgm^{-3}, and total range for σ_R was 0.0 - 0.22 μgm^{-3}. The parameter $\overline{\%R}$ indicates accord well within a tenth of one percent across all meteorological conditions and receptors (the value for $\overline{\%R}_{min}$ was -0.07% and $\overline{\%R}_{max}$ was 0.01%). A slight tendency for negative bias was apparent for the stable P-G categories. As seen for the area source, for any of the stable P-G categories, variance falls off with higher wind speed. A qualitative inspection of residuals as they appear along the receptor array indicated slightly more bias for receptors in the near field of the source.

3.2 Variable Meteorological Conditions

3.2.1 Scenarios for Sensitivity Study

For the sensitivity study comparing CALPUFF and ISC3, meteorological conditions were allowed to vary hourly. The first test scenario was devised to see what effects variable meteorology would have on hourly averaged concentrations. One annual period of hourly averaged meteorological data was selected from each of three climatically different regions of the United States. The concentrations between CALPUFF (emissions simulated as a continuous series of puffs) and ISC3 (emission release simulated as a continuous plume) were compared in time and space. The comparisons were examined to try to find the underlying cause of significant differences. The second scenario was a rerun of the first case with some modifications. The averaging times were extended to 3-, 24-hour and annual periods. Maximum concentrations were compared for individual receptor rings at 15 downwind distances. The suite of four point sources described in Appendix C was used in these comparisons.

The meteorological data consist of hourly values of wind speed and direction, ambient temperature, stability class, and mixing heights. The three sites selected were: 1991 Boise, Idaho; 1990 Medford, Oregon; and 1964 Pittsburgh, Pennsylvania.

The Boise data set was selected because of the very directional nature of it winds (see 1991 Boise wind rose, Appendix J). Over 33% of the winds have a northwesterly component and over 33% of the winds have a southeasterly component with the majority of those winds having speeds greater than 2 ms^{-1}. With such persistence in wind direction, the puffs simulated by CALPUFF would be expected to be transported to the most distant receptors.

The Medford data set was selected because of the high number of calm wind situations (see 1990 Medford wind rose, Appendix J). In 1990, Medford Oregon recorded a value of 22.5% of calm winds. This compares to the average of 6.5% for the other two sets of data. Since CALPUFF processes calm winds and ISC3 "zeros" concentrations during calm wind events, there is good reason to expect differences to be seen in the simulated patterns of surface concentration values estimated by the two models.

The 1964 Pittsburgh data set was selected because it has been used as a standard test set for a number of years and because of its fairly well distributed wind directions and wind speeds (see 1964 Pittsburgh wind rose, Appendix J). Although there is a bias in the wind direction toward the southwest, this set was included because many data sets show a similar bias for a particular wind direction and also have a low number of calm winds.

The receptor placement consisted of 15 rings of 36 receptors each for a total of 540 receptors. The rings were spaced at distances of 0.5, 1, 2, 3, 5, 10, 15, 20, 30, 50, 100, 150, 200, 250, and 300km from the source. On each ring, the receptors were spaced every 10° starting at 360°.

3.2.2 Preliminary Studies

Three preliminary studies were done prior to the sensitivity study. In the first preliminary study, CALPUFF and ISC3 were run to create a plot of concentration curves under steady state conditions for centerline and laterally placed receptors. If there were differences in the way dispersion coefficients were calculated between the two models, that would become apparent in plots of concentration distributions. In the second preliminary study, the *puff* and *slug* models were run for a two-hour segment where a large wind shift occurred in the second hour. The purpose was to compare concentration footprints from *puff* and *slug* mode results. This study highlights the different manner in which *puffs* and *slugs* are treated in CALPUFF. In the third preliminary study, a detailed examination was made of the concentration output from CALPUFF (*puff* mode) and ISC3 using the Boise meteorological data to help understand the large differences in concentrations between these two models over a multi-hour period involving calm winds and a wind shift.

First Study

The first study was done to see whether CALPUFF would calculate σ_y and σ_z values differently than ISC3. The same standard input file was created for ISC3 and CALPUFF with the idea being that any difference in the way the sigmas were calculated would be evident in the concentration results. In this comparison, CALPUFF was run in both the *puff* and *slug* modes. The models were run for a 2m point source and the basic switch settings for CALPUFF set per Appendix A. The meteorological data were kept constant except for P-G stability category. For each run, the stability category was changed until all six stability categories, A through F, were used for all three models (i.e., ISC3, CALPUFF *puff* model, and CALPUFF *slug* model). A preliminary group of receptors was created with the centerline along the 360° axis and the receptors spaced every 1° for 44°.

The resulting concentrations were compared on a receptor-by-receptor basis. When the same input data were used, all three models produced concentrations that were within a few fractions of a percent of one another (Figure 1). Figure 1 displays six sets of three curves, one set of curves for each stability category. Each curve in each set overlaps the other curves in that set. The only common difference in each set is that both CALPUFF curves are truncated. This can be seen by the extrapolation of the ISC3 thin dashed line after the thick dashed line and thin solid lines of the two CALPUFF curves. This disparity results from CALPUFF concentration values set to zero for receptors that are more than $3\sigma_y$ from the centerline (Appendix E), whereas ISC3 sets concentration values to zero for receptors that are more than $11.75\sigma_y$ from the centerline. However, lateral plume spread in ISC3 is limited to 50° either side of the centerline and may be further decreased by vertical mixing conditions.

Second Study

In the second study, CALPUFF's treatment of emissions, *puffs* versus *slugs*, was evaluated (Appendix E), using synthesized meteorological data. There is a general difference in the extent of the hourly CALPUFF concentration "footprints" using the *puff* and *slug* models (Appendix K). Concentrations produced by the puff model produce a concentration field similar to a concentration field produced by ISC3 but are restricted to the trajectory algorithms in CALPUFF. The extent of each CALPUFF downwind concentration field is limited by the average wind speed occurring over a particular hour. The extent of the downwind concentration field in ISC3 is limited only by the farthest downwind receptor. The extent of the downwind concentration field when the *slug* model is used is the same as that for the *puff* model. However, when the wind direction changes from one hour and to the next, the directional orientation of the *slug* is maintained while the *slug* is advected downwind (Figure 2). During Hour 1, the wind was from

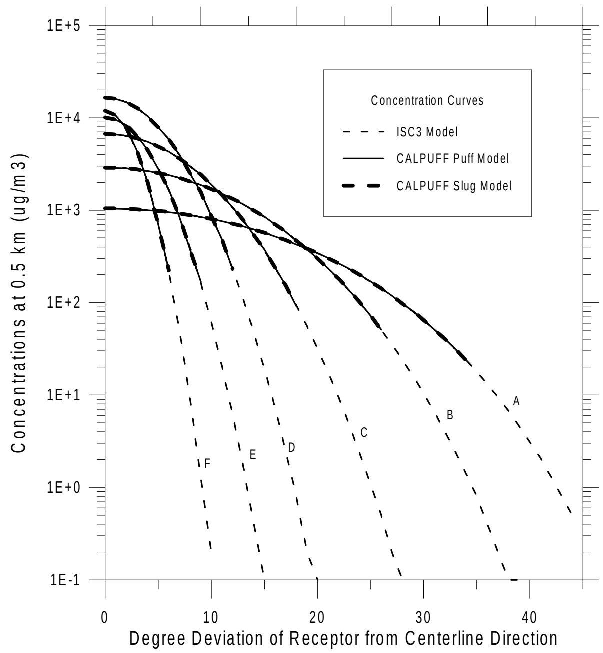


Figure 1. Plot of ISC3 and CALPUFF *slug* and *puff* model concentrations at a distance of 0.5 km from the source for all stability classes. The curves for CALPUFF are truncated because CALPUFF and ISC3 use different y/σ_y criteria for deciding whether to compute a concentration for a given receptor.

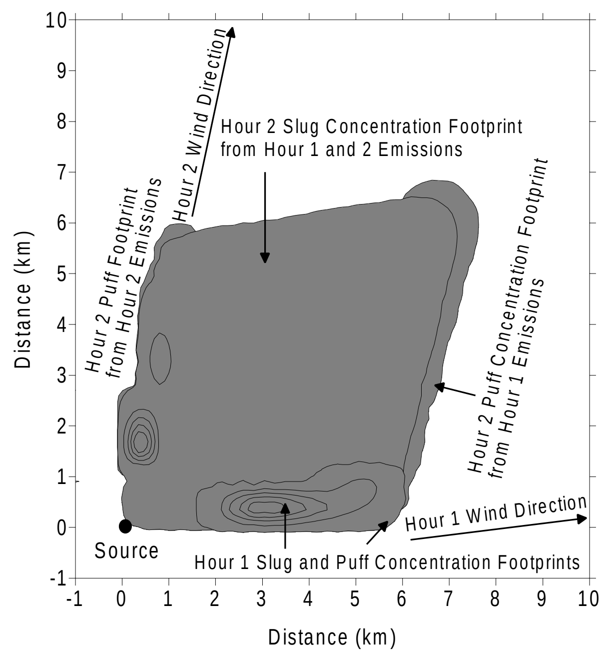


Figure 2. Plot of CALPUFF *slug* and *puff* one-hour concentration footprints during a 2-hour, 70 degree wind shift. Note the broad Hour 2 *slug* area which was advected from the area of the Hour 1 *slug* footprint. This area was coupled with the Hour 2 emissions.

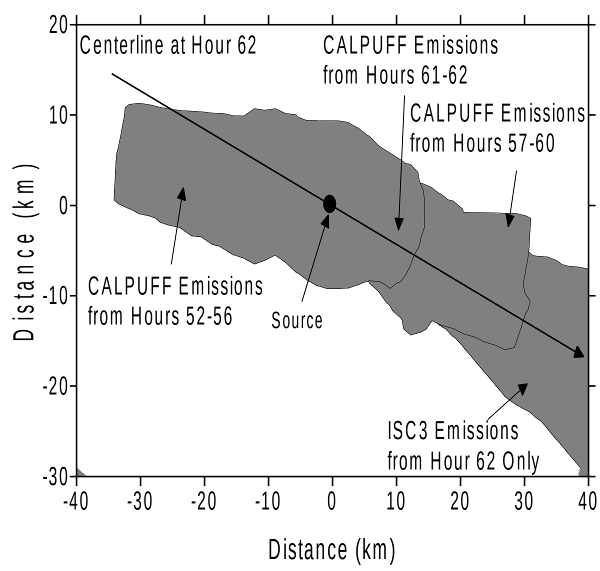


Figure 3. Plot of concentration footprints at Hour 62 from three CALPUFF hourly emission groups and one ISC3 emission group. The Hour 62 ISC3 plume centerline orientation is drawn through the source location. Note the overlap of groups in the 5 to 15km downwind range.

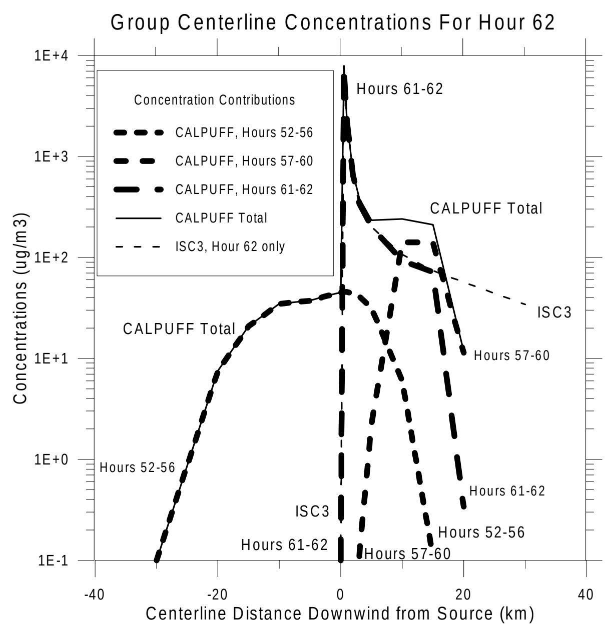


Figure 4. Plot of Figure 3 CALPUFF group and total and ISC3 one-hour concentrations at Hour 62. Note that the CALPUFF total is approximately 50% greater than ISC3 concentrations at 15km.

263°; during Hour 2, the wind switched to 193°. In Hour 1, the *puff* and *slug* model concentration footprints are almost exactly the same. However, in the next hour, the east-west oriented slug is advected north-northeastward. This results in a number of receptors being impacted but at a much lower concentration of about 280 μgm^{-3}. At the end of Hour 2, an area of approximately 25 km^2 has been impacted by the *slug* model. The puff impacts are restricted to relatively narrow corridors.

Note that during Hour 2, the *slug* and *puff* models have been simulating emissions from the source. The emissions have been transported north-northeastward (Figure 2). The concentrations produced by both models are similar but the puff concentrations are higher in the area of the maximum (Appendix K), due to the way in which dispersion is treated in the *slug* model. Since the slug is elongated and the mass of effluent is spread evenly throughout its volume, the newly emitted effluent close to the end of the hour has not had time to be transported past the receptors farther out. At distances of 0.5, 1, 2, 3 and 5km along the 10 degree radial, the Hour 2 slug concentrations are 91, 82, 64, 46, and 11 percent of the respective puff concentrations. While the *slug* model may have a broader spatial impact, its average concentrations are generally lower than those of the *puff* model.

Remember that receptors were placed on rings within the modeled domain and that there were no rings between 5km and 10km. With this arrangement a truncation appeared in the *puff* concentration footprint for Hour 2 beyond 5km from the source, and the actual footprint (appearing as right side Hour 2 in Figure 2) was not detected. (This truncation was not as evident for the Hour 2 *slug* footprint). To address this artifact, a finer Cartesian grid was developed for the second preliminary study that used a spacing of 400 meters and the right side Hour 2 *puff* footprint was then detected and expressed (Fig. 2). Note that the right side Hour 2 *puff* footprint originates from the terminus of the Hour 1 *puff*. The left side Hour 2 *puff* footprint is the result of Hour 2 emissions from the source. Also note the 400 meter grid resolution was not fine enough to properly contour the left side Hour 2 *puff* concentration isopleths. There was no such contouring problem evident within the other *puff* and *slug* concentration footprints. Note that the Hour 2 *slug* footprint is superimposed by the Hour 1 and Hour 2 *puff* footprints and by the exposed area between them.

Third Study

In the third study, a detailed examination was done on the concentration output from CALPUFF (*puff* mode) and ISC3 using the Boise meteorological data to examine the cause of a large difference in concentrations between these two models' results. These concentrations occurred 5 to 15km downwind from the source at Hour 62 and after a 4-hour period of calm winds and then a wind reversal (Figure 3).

During the 10 hours preceding Hour 62, hourly emissions were released into one of three wind regimes. First, there were 5 hours of east-southeasterly winds, followed by 4 hours of calm winds, followed by a 180-degree wind shift for 2 hours. Emissions were advected west-northwesterly, then stagnated but the puffs spread out evenly during this calm wind regime, and finally all emissions were advected east-southeasterly until Hour 62.

The CALPUFF concentration field at Hour 62 consists of three groups of concentrations based upon the prevailing wind direction at the time of emission release. One group had releases during Hours 52 through 56. The next group had releases during the calm wind Hours 57 through 60, and the final group had releases during Hours 61 and 62. The fields were depicted to show their respective group concentration footprints at Hour 62.

In Figure 3, note that all three groups overlap each other in the 5 to 12km range downwind. This is also affirmed in Figure 4, which shows the centerline concentrations oriented on the Hour 62 wind direction for each group, the total of the three groups, and the ISC3 centerline concentrations for the receptors nearest the centerline. The centerline concentrations from the three groups were added together to produce concentrations a factor of two greater than those estimated by ISC3 at 15km.

Leading up to Hour 62, there were four hours of calm wind conditions. During calm winds, CALPUFF assumes that the wind speed is zero. However, unlike ISC3 which treats the calm hour as missing, CALPUFF increases the sigma values of each puff with respect to time. During an hour of calm winds, the puffs have grown to the point that ground-level concentrations in this study were calculated at 0.5 and 1.0 km from the puff centers in all directions for the first hour of calm. After two hours, the effluent reached as far as 2km. The broadness of the Hour 52-56 and Hour 57-60 groups is reflective of the puff spreading during the calm wind period.

Details of this type of dispersion phenomena can be seen in Table 1. During Hour 57, the Hour 57 puff releases penetrated a low mixing height (inversion) and continued to spread horizontally without any concentrations contacting the ground. During the inversion rise in Hour 58, emissions were then mixed to the ground and Hour 57 emissions impacted receptors 0.5, 1 and 2km distance from the source while Hour 58 emissions were dispersed only to receptors at 0.5 and 1 km distance from the source.

3.2.3 Sensitivity Study

One of the major tasks of this study is to understand what types of concentrations will be produced by CALPUFF with respect to ISC3. The results of ISC3 versus CALPUFF using the *puff* and *slug* models were compared for three different climatological regions of the country. The results are displayed as a series of figures plotting the percent difference in concentrations at various downwind distances with only ISC3 results in the denominator. Results consist of maximum and highest of the second highest percent differences for 1-, 3-, 24-hour and annual averages.

Table 1
CALPUFF Concentration Estimates under Calm Wind Conditions

Receptor Coordinates		Concentrations ($\mu g m^{-3}$) produced by:		
X	Y	Hour 57 emissions at Hour 57	Hour 57 emissions at Hour 58	Hour 58 emissions at Hour 58
0.00	0.50	0.00	1340.44	2989.86
0.00	1.00	0.00	822.80	315.08
0.00	2.00	0.00	115.98	0.00
0.00	3.00	0.00	0.00	0.00
0.00	5.00	0.00	0.00	0.00
0.09	0.49	0.00	1340.68	2992.90
0.17	0.99	0.00	822.44	314.55
0.35	1.97	0.00	115.86	0.00
0.52	2.95	0.00	0.00	0.00
0.87	4.92	0.00	0.00	0.00

As illustrated in Figures 3 and 4, the explanation of why and how one model produces higher concentrations than another can be complex. The effects of inversions, calm winds, wind shifts, wind reversals, and plume and puff trajectory differences can all lead to enhanced or reduced effluent impact. The results of these interactions are shown in Figures 5 and 6 (the series is continued as Figures L-1 through L-7 in Appendix L).

As shown in Figure 5, the Medford plots contain the largest number of positive percentage differences over the widest range of downwind distances. As was seen in Figures 3 and 4, the results of calm winds and wind reversals can lead to higher than ISC3 average concentrations at respective downwind distances. With the high percentage of calm winds, note also in the annual average panel (Figure 5d) how the differences increase dramatically for the higher stacks as the downwind distance decreases. This is caused by the ISC3 plume not reaching the ground, or not fully dispersing to the ground, whereas CALPUFF can model effluent dispersion with wind reversals for receptors near the stack base.

As shown in Figure 6, the overall difference pattern with respect to stack height and downwind distances among the three sites is remarkably similar. Only the magnitude of the differences and the downwind distance at which the values initially converge is different. The Pittsburgh plots tend to slope downward with respect to the others but overall the patterns remain the same with respect to stack height and downwind distance.

As illustrated in Figures L - 1 through L - 7 (Appendix L), sometimes a pattern or trend can be seen by comparing subsequent or related figures only to find an exception in another figure. All of this may be the result of complex interactions that are likely to occur in any of the climatological regimes. For instance, Medford, Oregon has a high percentage of calm winds. If these calm wind events are coupled with a wind reversal, the same situation illustrated in Figure 3 for Boise, Idaho can occur. The patterns in the percentage differences may reflect a general pattern found at that site but the pattern can be overlaid by a situation often found at another site.

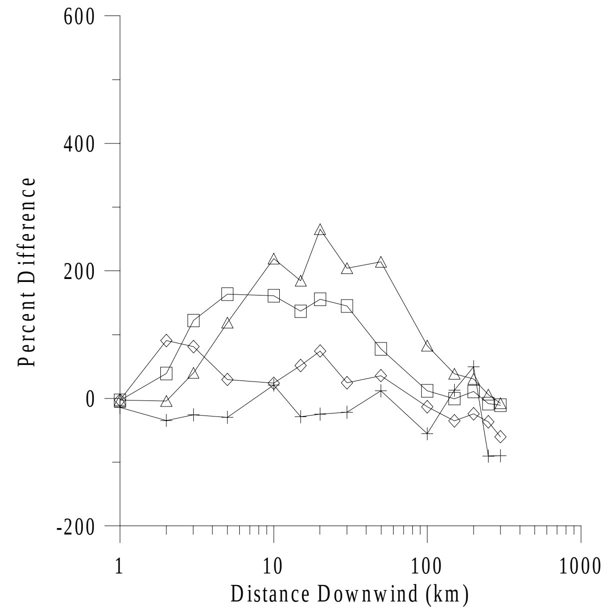


Figure 5a. Results for 1-hour averages using 1990 Medford data.

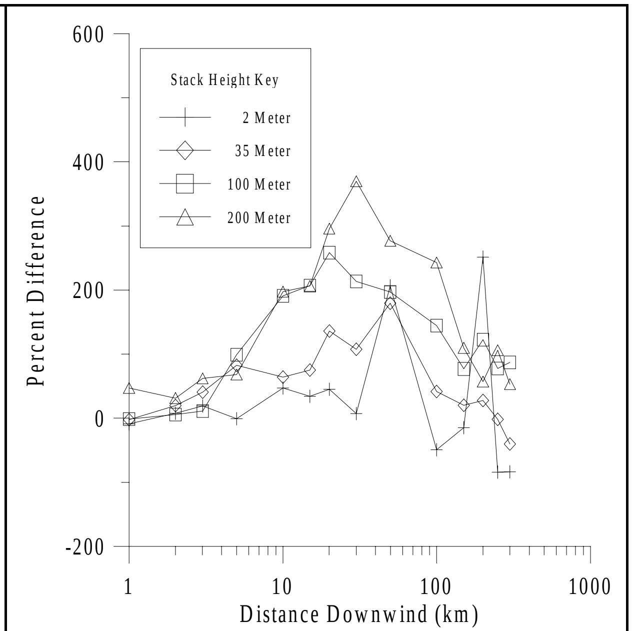


Figure 5b. Results for 3-hour averages using 1990 Medford data.

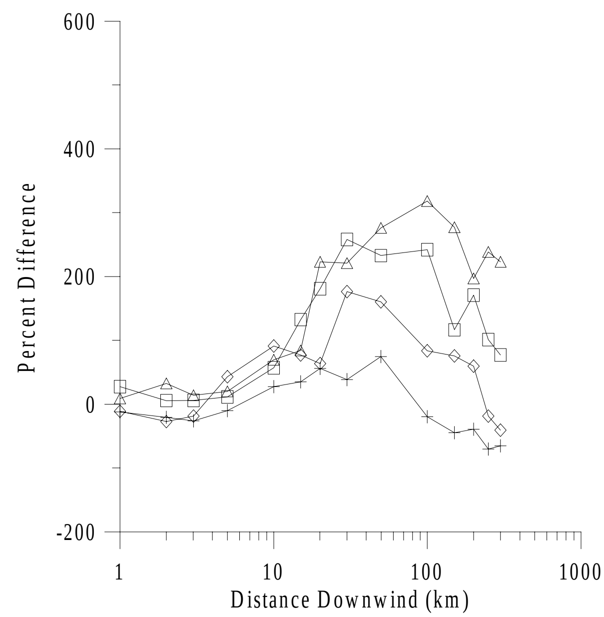


Figure 5c. Results for 24-hour averages using 1990 Medford data.

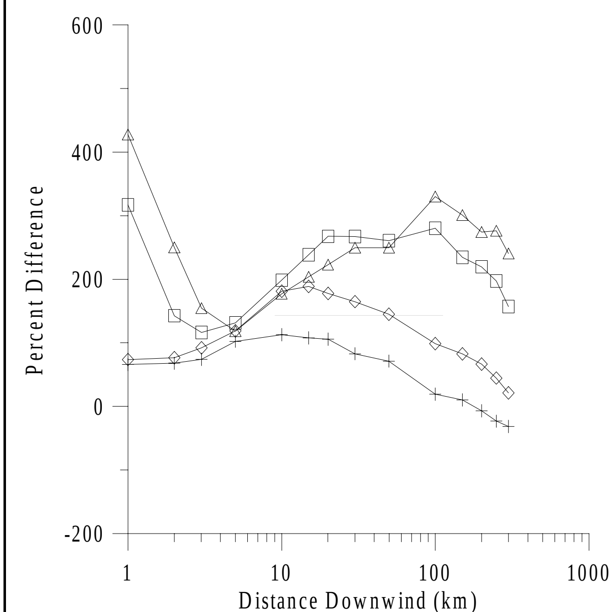


Figure 5d. Results for annual averages using 1990 Medford data.

Figure 5. Percent differences (ISC3 vs. CALPUFF *slug* model) as a function of downwind distance for the highest 2nd high concentrations; 1-, 3-, 24-, and annual averages. Data are for Medford, Oregon. Note: $\%\ Difference = 100\ (\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}})$.

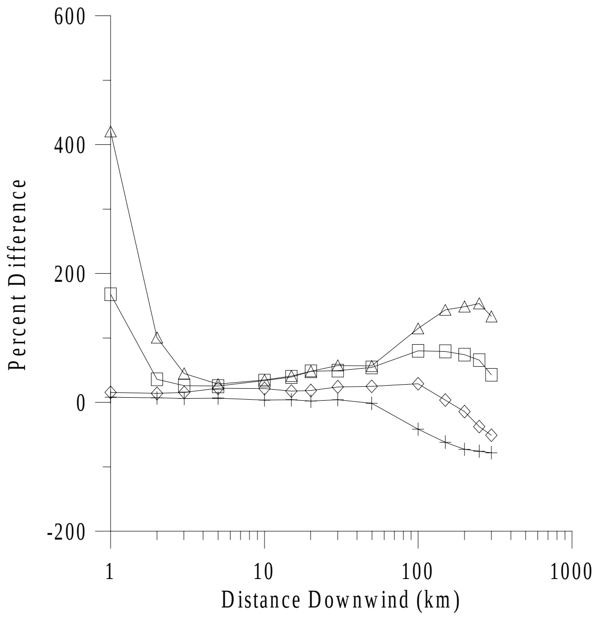


Figure 6a. Results for annual averages using 1991 Boise data.

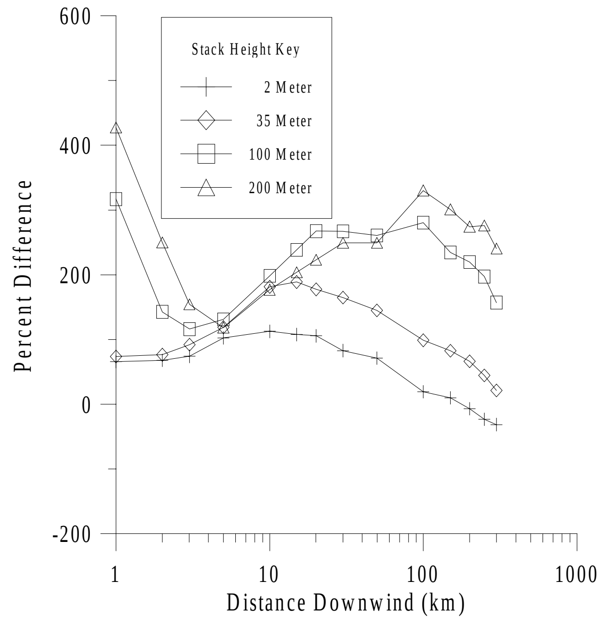


Figure 6b. Results for annual averages using 1990 Medford data (repeat of Fig. 5d).

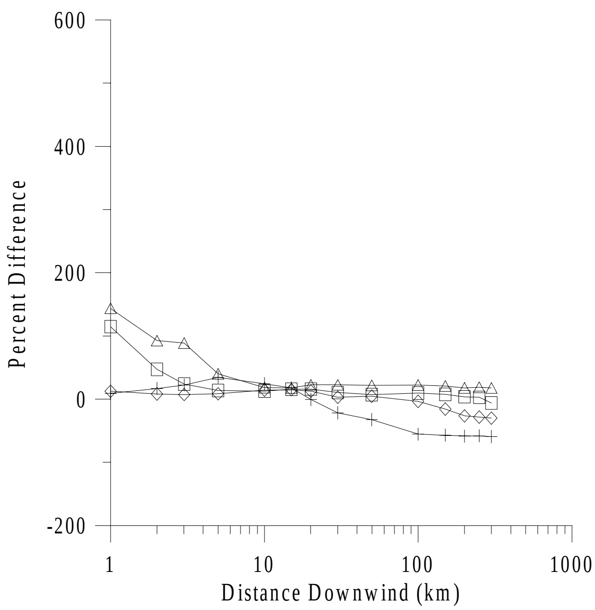


Figure 6c. Results for annual averages using 1964 Pittsburgh data.

Figure 6. Percent differences (ISC3 vs. CALPUFF *slug* model) as a function of downwind distance for annual averages, all three sites. Note: $\%\ Difference = 100\ (\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}})$.

4. Summary and Conclusions

4.1 Steady State Meteorological Conditions

CALPUFF and ISCST3 were run with identical meteorological data sets to compare their estimates. The meteorological data sets were synthesized to represent a variety of wind speeds in each of the six P-G stability categories (54 cases in all). ISC3 was run in the “regulatory default” mode and CALPUFF runs were configured to emulate this mode, which included the simulation of emission releases as *slugs* (versus *integrated puffs*). Receptors were located along a straight line (“due north”) at successively distant intervals. Sources included three elevated point sources (35m, 100m and 200m). Surface releases included a 2m point source and a rectangular area source 500m on a side. A typical volume source was also examined. For point sources, model runs were done for two regimes, one in which the mixing height (Z_i) was set to 3000m, and the other for Z_i = 500m. The latter regime was explored to inspect CALPUFF’s treatment of reflection. For each source type, a comparison matrix was created to assess comparison across all meteorological conditions in terms of a variety of robust statistical indicators.

For all point sources (with Z_i = 3000m), the results indicated good accord between the two dispersion models. For all meteorological conditions, the mean fractional bias across the receptor radial was well below 10%. Maximum residuals at any receptor were on the order of 0.1% of the concentration mean at the incident receptor. While a qualitative inspection of residuals as they appear along the receptor array indicated no distinct pattern of bias, a slight negative bias (CALPUFF relative to ISC3) is apparent for the 2m source, while the reverse is true for the elevated sources. For the low mixing height regime (Z_i = 500m), the comparison results were strikingly similar, suggesting that both CALPUFF and ISC3 treated reflection identically.

The area source was simulated with mixing height set to 3000m. One set of runs was done with initial σ_z set to 0, while the other was set to 2.5m. The best accord was seen for the former case, but for about one fifth of the cases, the mean fractional bias was greater than 10%. The maximum absolute residual was 33% of the concentration mean at the incident receptor. There was an apparent trend toward negative bias (CALPUFF relative to ISC3), but there was substantial variance as well. Mean residuals and mean standard deviations ranged over three orders of magnitude. Accord improved (and variance diminished) with higher wind speeds, which is expected as the slugs are stretched from the point of origin.

With a test version of ISC3 in which the virtual source treatment was “corrected”, the models showed close agreement in their treatment of the volume source. Maximum absolute residual was well below one percent of respective concentration means at incident receptors. For all cases, mean fractional bias was zero. A very slight tendency for negative bias was seen for the stable stability categories, and (as for the area source) variance diminished with higher wind speed. A qualitative inspection of residuals as they appear along the receptor array indicated slightly more bias for receptors in the near field of the source.

4.2 Variable Meteorological Conditions

To examine differences in model estimates when variable meteorological data are used, several studies were done. Actual full-year data sets from three climatologically different sites were used. The sites chosen were Boise, Idaho (1991), Medford, Oregon (1990) and Pittsburgh, Pennsylvania (1964). Using a synthesized meteorological data set, a preliminary set of studies was done to examine (1) differences in the way both models treat lateral σ's (CALPUFF was run using both *puffs* and *slugs*), and (2) *puff* versus *slug* differences within CALPUFF alone. Another study was done using the Boise data to examine the occurrence and location of concentration maxima estimated by ISC3 and the CALPUFF *puff* model. Then for all three sites, extensive sensitivity studies were done in which estimates by ISC3 were compared to CALPUFF (*puff* and *slug* models). In general, 36 - 45 receptors were placed on each of 15 concentric rings at successively more distant intervals.

In general, the differences between CALPUFF and ISC3 concentration results are caused by how emissions are transported and dispersed. CALPUFF limits downwind transport in based on the wind speed while there is no such limitation in ISC3 (it is a plume model). Under calm wind conditions, CALPUFF continues to disperse each puff while the ISC3 model is arbitrarily set to not determine concentrations when the wind speed is less than 1 ms^{-1}. CALPUFF is capable of tracking the puff emitted before, during and after wind shifts and reversals while ISC3 is only concerned with the current hour transport of its plume(s). CALPUFF continues to disperse each puff even when they are above an inversion layer while ISC3 determines its plume is above the inversion layer and cannot be advected to the ground (e.g,. concentrations = 0.0). When the inversion rises above the old puffs, they are dispersed to the ground creating impacts for any nearby receptors.

When all these and other meteorological conditions are recorded on an hourly basis and form a complete year of meteorological data, the effects on concentrations vary between the models and from region to region. The meteorologically induced variations in concentrations do not appear to be so much a regional phenomena, but the variations are related to how the hourly meteorological conditions occur preceding and during a given averaging period. It is possible to have 4 or 5 hours of winds in one general direction followed by 4 hours of calm winds, and then followed by several hours of reversed wind flow. This can occur in any one of the regions. However, the potential frequency of this occurrence may be higher for one region than another. Since calm winds have a causal relationship leading to higher concentrations, then a site such as Medford with a relatively greater incidence of calms (i.e., 22% calm hours versus the other regions having around 6%) will have higher concentrations associated with CALPUFF.

4.3 Conclusion

Even though ISC3 and CALPUFF can be made to produce the same concentrations in a steady state environment, a variable state environment can produce higher-than-ISC3 ground-level concentrations with CALPUFF. Climatological characteristics of a region appear to be a factor, but the accumulation of hour by hour meteorological conditions on the transport of CALPUFF puffs is the key to understanding the differences that are produced by these two models. This should come as no surprise as the meteorological assumptions used in formulating the downwind transport of the ISC3 and CALPUFF effluents and the dispersion from the respective plumes and puffs are different. This is also compounded by the different treatment of dispersion during calm wind conditions.

This complex interaction of transport, vertical mixing, and dispersion have an effect on concentrations with respect to downwind distances in CALPUFF. Occasionally, the accumulation of mass released over several hours will be transported in such a manner that the combined effect is to produce sharp localized maxima in simulated concentration values. The occurrence of such events is not predictable. It seems to occur with greater frequency at Medford. Calm winds play a part in these events. These maxima seem to occur at most locations in the receptor network, at all downwind distances. When they occur, they seem to affect in particular the results for the shorter averaging periods.

Overall trends have been noted in the percentage difference comparisons in simulated concentration values between CALPUFF and ISC3. For taller point sources, there is a trend toward higher concentrations being simulated by CALPUFF in comparison to ISC3. For annual averages, the closer a receptor is to the source and the taller the stack, the greater the chance that the CALPUFF concentration values will be higher than those simulated by ISC3. At the more distant downwind receptor rings, the bias changes direction from CALPUFF yielding higher concentrations, to CALPUFF yielding relatively lower concentrations and sometimes these concentrations are lower than their respective ISC3 counterpart.

5. References

1. Environmental Protection Agency, 1995. User's Guide for the Industrial Source Complex (ISC3) Dispersion Models. Volumes I - III. EPA-454/B-95-003a-c.

2. Environmental Protection Agency, 1995. A User's Guide for the CALPUFF Dispersion Model. EPA-454/B-95-006.

3. Environmental Protection Agency, 1995. SCREEN3 User's Guide. EPA-454/B-95-004.

Appendix A

Switch settings for CALPUFF input file to emulate ISC3's "Regulatory Default" mode

For these comparisons, CALPUFF was run to emulate ISC3's "regulatory mode" (i.e., default). Thus, to ensure equivalence for this emulation, certain of CALPUFF's switches were set as follows:

METFM	= 2	ASCII input file used for input
MSLUG	= 1	Puffs emitted as *slugs*
MDRY	= 0	Dry deposition NOT used, unless specified otherwise
MWET	= 0	Wet deposition NOT used, unless specified otherwise
MSHEAR	= 0	Vertical wind shear NOT modeled
WSCALM	= 0.9999	A value of 1 ms^{-1} for the calm wind speed threshold causes a rounding problem
AVET	= 3	Averaging times for σ's is 60 min; σ_y is adjusted as $(AVET/60)^{0.2}$
MTRANS	= 0	NO transitional plume rise (i.e., final plume rise only)
MDISP	= 3	PG dispersion coefficients for RURAL areas, computed using the ISC multi-segment approximation
MGAUSS	= 1	Vertical dispersion used in the near-field is Gaussian
MCHEM	= 0	NO chemical treatment used
MROUGH	= 0	PG σ_y and σ_z NOT adjusted for roughness
MPARTL	= 0	No partial plume penetration of elevated inversion
MCTADJ	= 1	ISC-type of terrain adjustment
MTIP	= 1	Stack tip downwash used
PLXO(6)		Default wind speed profile power-law exponents for P-G categories A-F
PTGO(2)		Default vertical Θ gradient (Km^{-1}) for stable P-G categories E & F

For all applicable sources, CALPUFF employs buoyancy induced dispersion (BID); a feature enabled in ISC3's regulatory mode. Consistent with ISC3's regulatory default mode, missing data processing was NOT used.

Appendix B

Meteorological conditions for the steady state CALPUFF/ISC3 comparisons[1]

P-G	Wind Speed (ms^{-1})											
A	1.0	1.5	2.0	2.5	3.0							
B	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0			
C	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	8.0	10.0		
D	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0	8.0	10.0	15.0	20.0
E	1.0	1.5	2.0	2.5	3.0	3.5	4.0	4.5	5.0				
F	1.0	1.5	2.0	2.5	3.0	3.5	4.0						

[1]Wind speed is at 10m and values are the same as those used in SCREEN3. For each combination of P-G stability category, comparisons for point sources were made with Z_i = 500m and 3000m. For the area and volume source, Z_i = 3000m.

Appendix C

Characteristics for sources used in the CALPUFF/ISC3 comparisons

Point Sources					
Stack height (m)	X,Y location & base elevation (m)	Emission rate (gs^{-1})	Exit velocity (ms^{-1})	Stack diameter (m)	Temperature (K)
2	0, 0, 0	100	10.0	0.5	300
35	0, 0, 0	100	11.7	2.4	432
100	0, 0, 0	100	18.8	4.6	416
200	0, 0, 0	100	26.5	5.6	425

Ground-level Area Source				
Area (m^2)	Length of side (m)	Emission rate ($gs^{-1}m^{-2}$)	Effective Release Height (m)	Initial σ_z (m)[1]
250,000	500	0.0004	1.0	2.5

Volume Source[2]	
Emission Rate (gs^{-1}):	1.0
Release height (m):	10
Initial σ_y (m):	50
Initial σ_z (m):	20

[1]In one set of comparisons, $\sigma_{z(init)}$ was set to zero.

[2]Parameter values taken from Figure 9 of SCREEN3 User's Guide (Reference 3); buoyancy flux and momentum flux = 0; rural option.

Appendix D

Receptor array used in the steady state CALPUFF/ISC3 comparisons

Receptors are aligned along a 360° radial at these distances (m):

1	100	32	4000
2	200	33	4500
3	300	34	5000
4	400	35	5500
5	500	36	6000
6	600	37	6500
7	700	38	7000
8	800	39	7500
9	900	40	8000
10	1000	41	8500
11	1100	42	9000
12	1200	43	9500
13	1300	44	10000
14	1400	45	15000
15	1500	46	20000
16	1600	47	25000
17	1700	48	30000
18	1800	49	35000
19	1900	50	40000
20	2000	51	45000
21	2100	52	50000
22	2200	53	55000
23	2300	54	60000
24	2400	55	65000
25	2500	56	70000
26	2600	57	75000
27	2700	58	80000
28	2800	59	85000
29	2900	60	90000
30	3000	61	95000
31	3500	62	100000

Appendix E

Puffs versus Slugs: CALPUFF's Two Simulation Modes

CALPUFF may be operated in one of two modes for simulating emissions: *puff* or *slug*. In the *puff* mode, a continuous plume is represented as a number of discrete packets of pollutant material. Most puff models evaluate the contributions of a puff to the concentration at a receptor by a "snapshot" approach, where each puff is "frozen" at particular time intervals, the concentration due to the frozen puff at that time is computed, and the puff is then allowed to move, evolving in size, strength, etc. until the next sampling step. The total concentration at a receptor is the sum of the contributions of all nearby puffs averaged for all sampling steps within the basic time step. A traditional drawback of the puff approach has been the need for the release of many puffs to adequately represent a continuous plume close to the source. Another potential problem arises if the puffs do not overlap sufficiently, causing concentrations at receptors located in the gap between puffs at the time of the "snapshot" to be underestimated, while those at the puff centers are overestimated. One alternative to the problems posed by the "snapshot" approach is the use of the integrated sampling function (originally implemented in MESOPUFF II). This technique is available in CALPUFF as the *integrated puff* approach, and is fully described in Section 2.1.1 of the CALPUFF User's Guide (Reference 2).

Another approach available in CALPUFF uses a non-circular puff (*slug*) elongated in the direction of the wind to eliminate the need for frequent releases of puffs. Thus in the *slug* model, the "puffs" consist of Gaussian packets of pollutant material stretched in the along wind direction. A slug can be visualized as a group of overlapping circular puffs having very small puff separation distances. Actually, the slug represents the continuous emission of puffs, each containing an infinitesimal mass. The concentrations near the endpoints of the slug (both inside and outside of the body of the slug) fall off in such a way that if adjacent slugs are present, the plume predictions will be reproduced when the contributions of those slugs are included (and this is with steady state conditions). As with circular puffs, each slug is free to evolve independently in response to local effects of dispersion, chemical transformation, removal, etc. However, unlike puffs, the endpoints of adjacent slugs are constrained to remain connected (like country sausages). This ensures continuity of a simulated plume without the gaps associated with the puff approach. It should be noted that all receptors lying outside of the slug's $\pm 3\sigma_y$ envelope during the entire averaging time interval are eliminated from consideration. And for those receptors remaining, integration time limits are computed such that sampling is not performed when the receptor is outside of the $\pm 3\sigma_y$ envelope. This technique is available in CALPUFF as the *slug* approach, and is fully described in Section 2.1.2 of the CALPUFF User's Guide (Reference 2).

When initial CALPUFF runs were made for point sources, a disparity was seen between concentration estimates produced by CALPUFF run in the *slug* mode versus those produced by ISC3. This discrepancy was unexpected and the matter was brought to the attention of Earth Tech (CALPUFF's developer). Earth Tech determined that the reason the *slug* model in Version *960612* did not reproduce the plume model (ISC3) was due to the computation algorithm for sigmas. In the *960612* version, the receptor-specific sigma was computed by determining the sigma that the puff would have at the receptor, even if the puff hasn't reached the receptor yet (as does a plume model). This gave nearly exact reproduction of plume results under steady-state conditions.

However, under non-steady conditions and very high sigma growth rates (e.g., under P-G category *A*), this extrapolation can produce puff impacts prematurely (and hence the *causality* effect is compromised somewhat). Therefore, the sigmas were "clipped" at the value at the end of the slug when the receptor is beyond the end of the slug. This arrangement did reasonably well for *causality* effects, but caused some deviation from the plume results under steady state conditions.

As a result of Earth Tech's investigation of this disparity, an experimental version of CALPUFF was made available to EPA for the purposes of this comparison, and all analyses were done with this version. This version compromised between the two solutions described above. The version only allows concentrations to be computed for receptors that are within 4 σ_x (where σ_x is the horizontal puff dispersion parameter) of a puff centroid. This technique was seen to perform much better with respect to both treating *causality* and reproducing plume results, and will be incorporated in the next model to be released (Joe Scire, *pers. comm.*, December 1997).

Appendix F

Summary statistics from performance matrix - point sources (Z_i = 3000m)

Emissions simulated as:	SLUGS[a]
$\overline{\%R}_{min}$ (%)	-0.04 (C1H200)
$\overline{\%R}_{max}$ (%)	0.13 (D1H100)
$R_{i(min)}$ (μgm^{-3})	-8.0 (A3H2 @ 100m)[b]
$R_{i(max)}$ (μgm^{-3})	25.0 (F2p5H2 @ 500m)[c]
$\bar{R}_{min}$ (μgm^{-3})	-0.1 (see footnote e)
$\bar{R}_{max}$ (μgm^{-3})	0.4 (F2p5H2)
$\sigma_{R(min)}$ (μgm^{-3})	0.0 (see footnote e)
$\sigma_{R(max)}$ (μgm^{-3})	3.2 (F2p5H2)
# cases $\overline{FB}$ "out of range":[d]	NONE
$\overline{FB}_{min}$	0.0 (see footnote e)
$\overline{FB}_{max}$	0.02 (D20H100)
$FB_{i(min)}$	-0.18 (A1H2 @ 100km)
$FB_{i(max)}$	0.53 (D20H100 @ 800m)

[a]See text for explanation of (C1H200), etc.

[b]This value for R_i is 0.03% of $\bar{\chi}$ $\left(= \frac{\chi_{CALPUFF} + \chi_{ISC3}}{2}\right)$ at this receptor. $\chi_{CALPUFF}$ = 24836 μgm^{-3}; χ_{ISC3} = 24844 μgm^{-3}

[c]This value for R_i is 0.13% of $\bar{\chi}$ at this receptor. $\chi_{CALPUFF}$ = 19040 μgm^{-3}; χ_{ISC3} = 19015 μgm^{-3}

[d]There were 216 distinct cases. The "goal" for this range is: $-0.10 \le \overline{FB} \le 0.10$

[e]There is no unique run associated with this value.

Appendix G

Summary statistics from performance matrix - area source (emissions simulated as *slugs*)

Initial σ_z (m):	**0**		**2.5**	
$\overline{\%R}_{min}$ (%)	-1.5	(F1AREA)	-3.2	(F1AREA)
$\overline{\%R}_{max}$ (%)	-0.07	(see footnote a)	-0.66	(see footnote a)
$R_{i(min)}$ (μgm^{-3})	-1537	(F1AREA @ 3500m)[b]	-4212	(F1AREA @ 300m)
$R_{i(max)}$ (μgm^{-3})	561	(E1AREA @ 100m)[c]	0.08	(A1AREA @ 85km)
$\bar{R}_{min}$ (μgm^{-3})	-548	(F1AREA)	-969	(F1AREA)
$\bar{R}_{max}$ (μgm^{-3})	-1.1	(D20AREA)	-10.5	(D20AREA)
$\sigma_{R(min)}$ (μgm^{-3})	2.4	(D20AREA)	28.3	(D20AREA)
$\sigma_{R(max)}$ (μgm^{-3})	510	(F1AREA)	895	(F1AREA)
# cases $\overline{FB}$ "out of range":[d]		10		19
$\overline{FB}_{min}$	-0.16	(see footnote a)	-0.19	(F1AREA)
$\overline{FB}_{max}$	-0.02	(see footnote a)	-0.04	(see footnote a)
$FB_{i(min)}$	-0.39	(E1AREA @ 4000m)	-0.40	(E1AREA @ 4000m)
$FB_{i(max)}$	0.05	(A1AREA @ 85km)	0.05	(A1AREA @ 85km)

[a]There is no unique run associated with this value.

[b]This value for R_i is 33% of $\bar{\chi}$ $\left(= \frac{\chi_{CALPUFF} + \chi_{ISC3}}{2}\right)$ at this receptor. $\chi_{CALPUFF} = 3869\ \mu gm^{-3}$; $\chi_{ISC3} = 5406\ \mu gm^{-3}$

[c]This value for R_i is 2.2% of $\bar{\chi}$ at this receptor. $\chi_{CALPUFF} = 25719\ \mu gm^{-3}$; $\chi_{ISC3} = 25158\ \mu gm^{-3}$

[d]There are 54 distinct cases. The "goal" for this range is: $-0.10 \le \overline{FB} \le 0.10$

Appendix H

ISCST3's Treatment of Virtual Sources

For volume sources and point sources subject to building wake dispersion, ISC3 makes use of a *virtual source* to simulate an initial plume size. That is, if a source has a finite size at the point of release, its initial σ_y and σ_z are "matched" to a point on the corresponding dispersion curve. Because these curves prescribe the dispersion parameters as a function of distance (starting with a value of zero at a downwind distance equal to zero), matching the curve to a source with a non-zero initial sigma entails shifting the apparent position of the source upwind. This shift is known as the *virtual position* of the source. If x_v denotes the distance of the virtual location of the source upwind of its actual location, then the value of the dispersion parameter at some distance (x) downwind of the source should be evaluated at the modified distance $(x + x_v)$.

ISC3 adopts this general method, but modifies its implementation in the following way. Because the P-G curves for σ_z are expressed as the function ax^b, where the parameters a and b themselves depend on the distance, "the ISC model programs check to ensure that the x_v used to calculate σ_z at $(x + x_v)$ is calculated using coefficients a and b that correspond to the distance category specified by the quantity $(x + x_v)$." (Vol. II of the ISC3 User's Guide (Section 1.1.5.2, p. 1-20) with the notation for the virtual distance changed from x_z to x_v. The term x_v is calculated using Equation 1-36.)

The result of this implementation is that the virtual distance becomes a function of receptor distance downwind of the source, and in fact x_v is reevaluated at each receptor the plume encounters as it moves downwind. Thus, the computed curve of σ_z as a function of distance is no longer the continuous P-G curve. This error is illustrated in the following figures. ISC3 was applied to a volume source with an initial σ_z of 5m and 20m, respectively, and concentrations were obtained at receptors within 1000m, for both P-G stability classes A and F (Figs. H-1 to H-4). Using strategically placed write statements in CALC1.FOR (one of ISCST3's files), the computed virtual distances and the corresponding σ_z values were written to a diagnostic file. These values were then plotted in the figures below as open squares (virtual distances) and as solid circles (σ_z) in the figures below. Figures H-1 and H-2 are for the P-G A stability category, while Figures H-3 and H-4 are for P-G F.

In Figure H-1, the virtual distance begins at 33.76m, and grows in steps corresponding to the "distance ranges" (Table 1-3 of Vol. II) for this P-G curve to almost 120m. The corresponding σ_z values "jump" each time a new virtual distance is used. The same phenomenon can be seen in the other figures, and the departure (ISC3 σ_z versus P-G σ_z) increases with downwind distance. Had more receptors been placed near each of the transition points, a clear "break" in the σ_z curve would have been resolved.

For the purpose of the CALPUFF/ISC3 comparison, ISCST3 was re-configured so that a single value of the virtual distance is computed as a joint function of P-G category and initial σ_z, with due regard for the distance ranges imposed on selecting a & b. This single value is then added to all receptor distances, and the corresponding value for σ_z computed. Figure H-1 indicates the resulting contour (depicted with open triangles) and suggests the *continuous* P-G curve for stability class A, for a virtual location 33.76m upwind of x = 0m.

A version of ISC3 with a corrected virtual source algorithm (dated *97363*), as was used in this comparison, was released in January 1998 and uploaded to EPA’s SCRAM web site for public use.

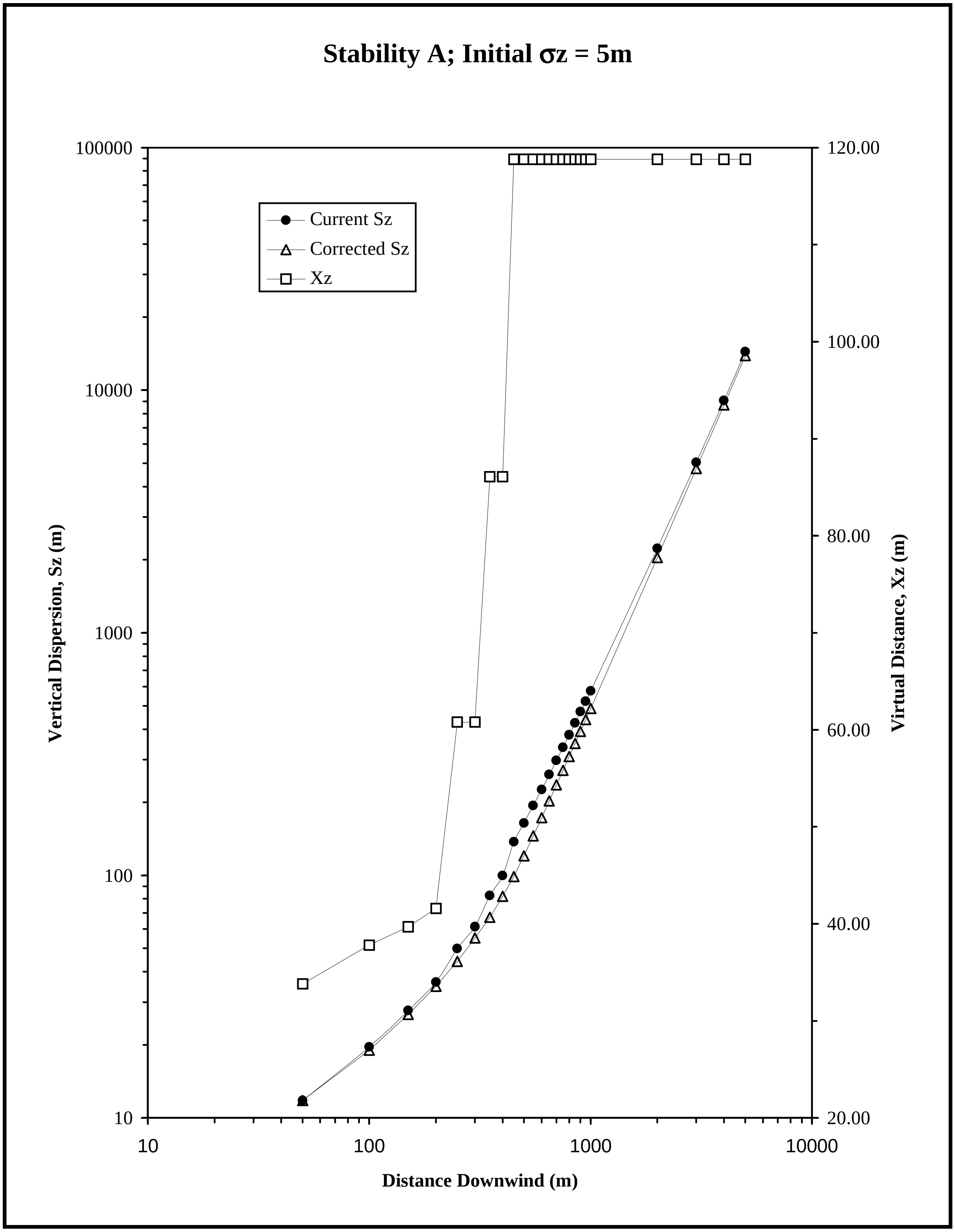


Figure H-1. Profile of σ_z with distance (m); P-G A and $\sigma_{z(init)}$ = 5m.

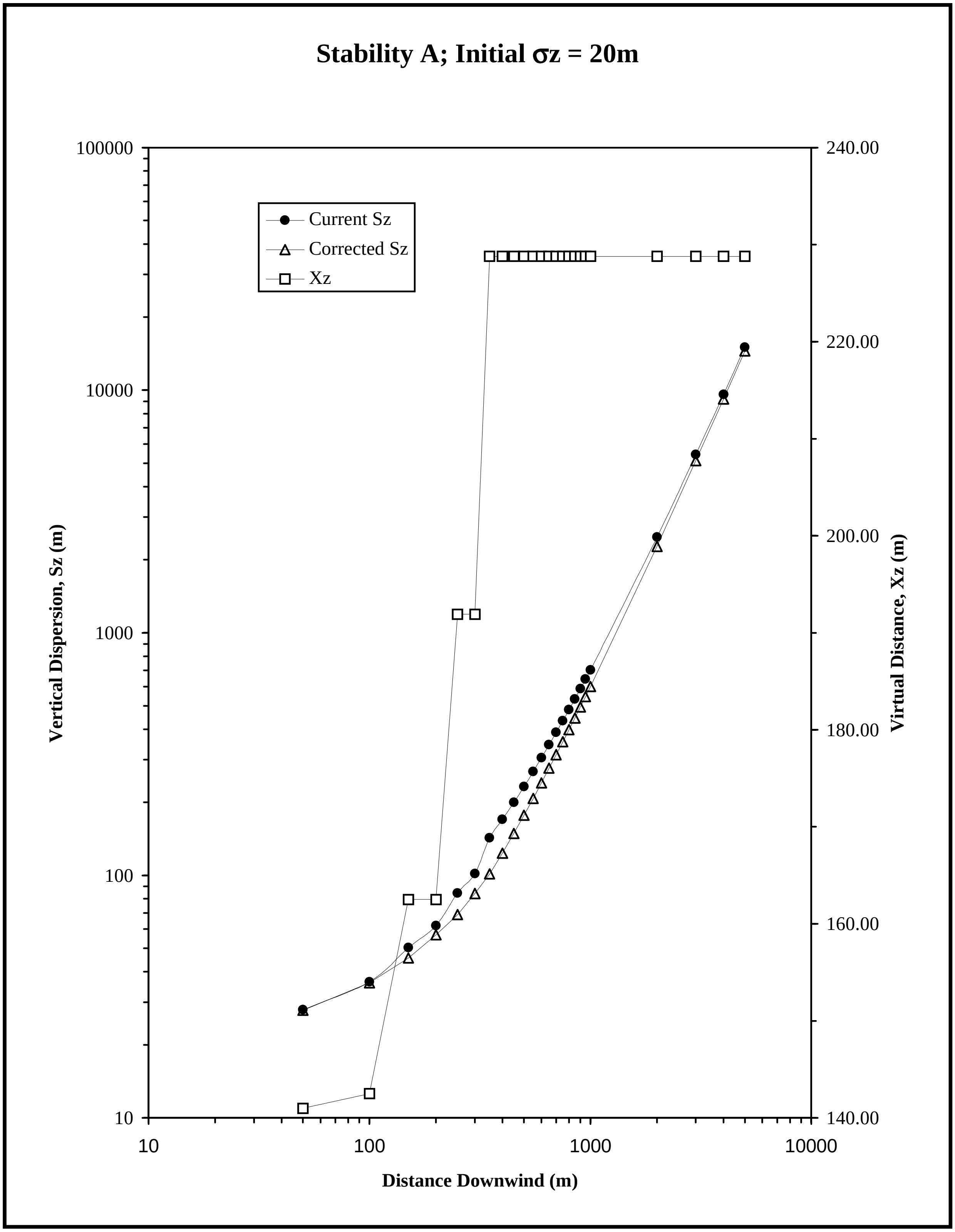


Figure H-2. Profile of σ_z with distance (m); P-G A and $\sigma_{z(init)}$ = 20m.

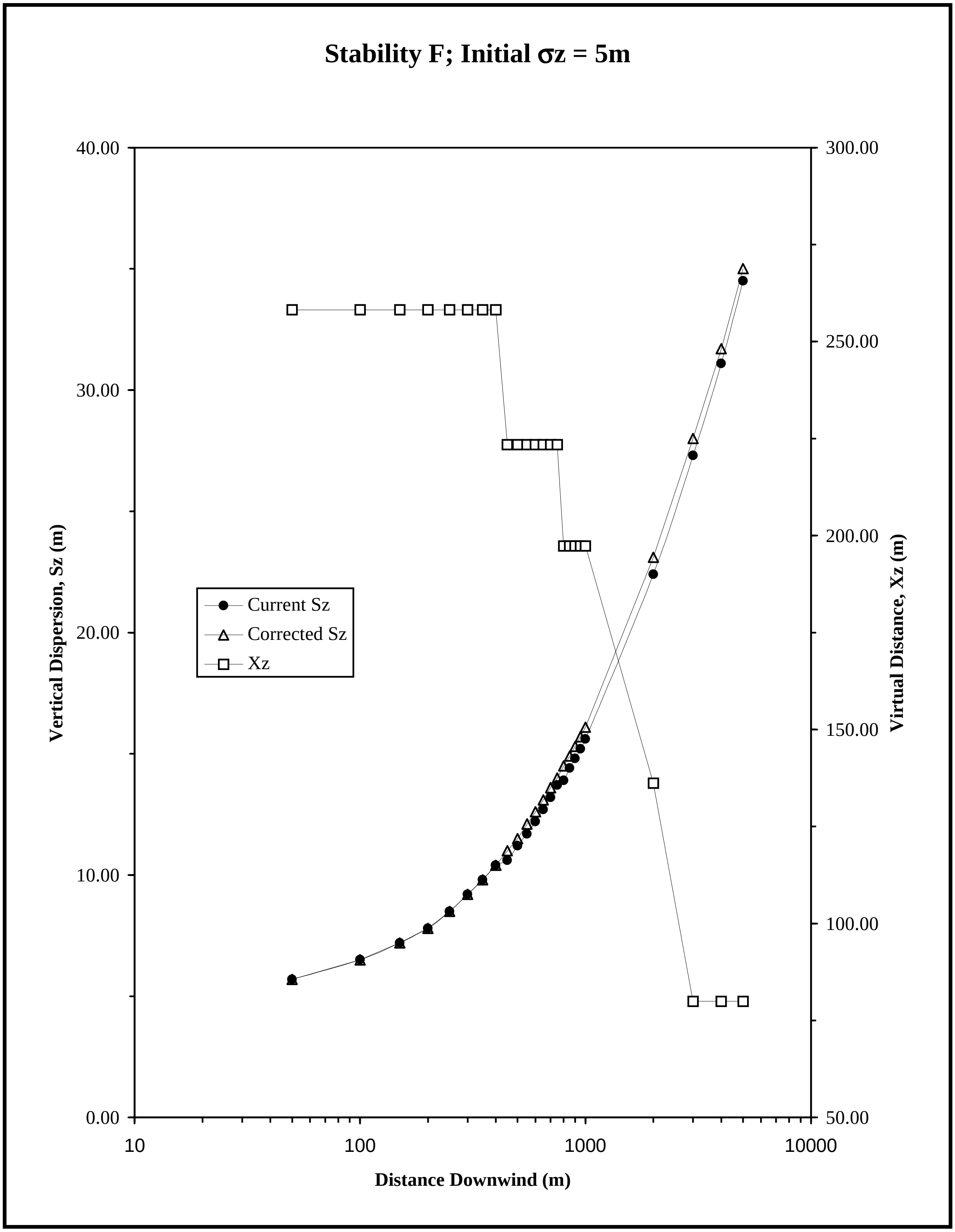


Figure H-3. Profile of σ_z with distance (m); P-G F and $\sigma_{z(init)}$ = 5m.

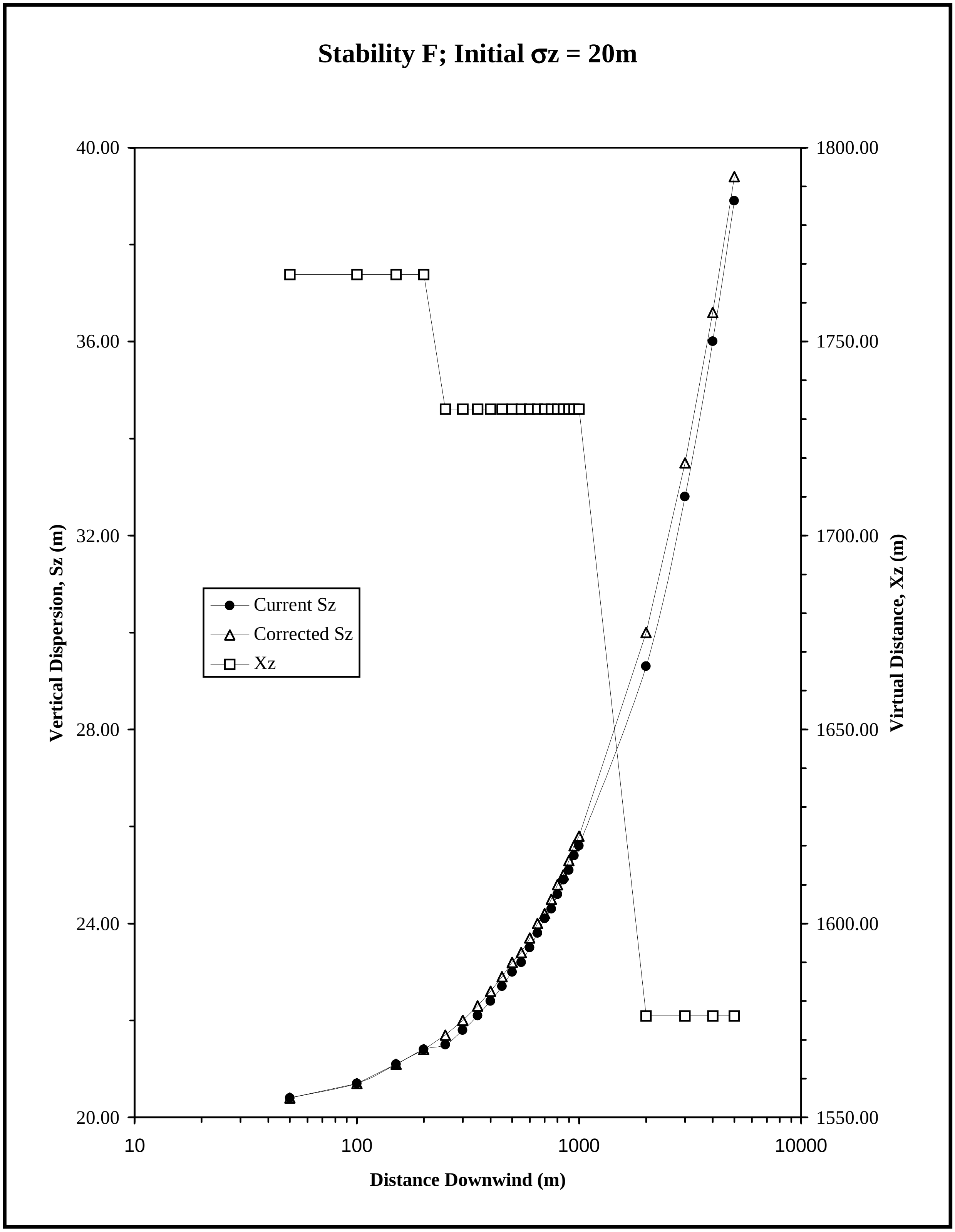


Figure H-4. Profile of σ_z with distance (m); P-G F and $\sigma_{z(init)}$ = 20m.

Appendix I

Summary statistics from performance matrix - volume source

Emissions simulated as:	SLUGS
$\overline{\%R}_{min}$ (%)	-0.07 (see footnote a)
$\overline{\%R}_{max}$ (%)	0.01 (see footnote a)
$R_{i(min)}$ (μgm^{-3})	-0.92 (F1VOL @ 200m)[b]
$R_{i(max)}$ (μgm^{-3})	0.15 (C1VOL @ 200m)[c]
$\bar{R}_{min}$ (μgm^{-3})	-0.2 (F1VOL)
$\bar{R}_{max}$ (μgm^{-3})	0.0 (see footnote a)
$\sigma_{R(min)}$ (μgm^{-3})	0.0 (see footnote a)
$\sigma_{R(max)}$ (μgm^{-3})	0.22 (F1VOL)
# cases $\overline{FB}$ "out of range":[d]	NONE
$\overline{FB}_{min}$	0.0 (see footnote a)
$\overline{FB}_{max}$	0.0 (see footnote a)
$FB_{i(min)}$	-0.18 (A1VOL @ 100km)
$FB_{i(max)}$	0.06 (A1VOL @ 85km)

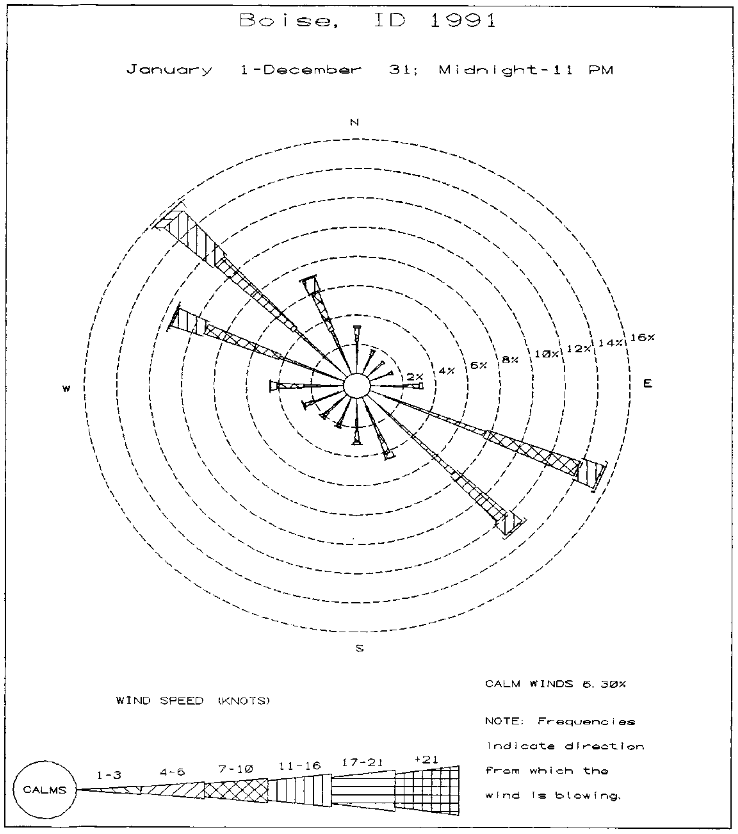
[a]There is no unique run associated with this value.

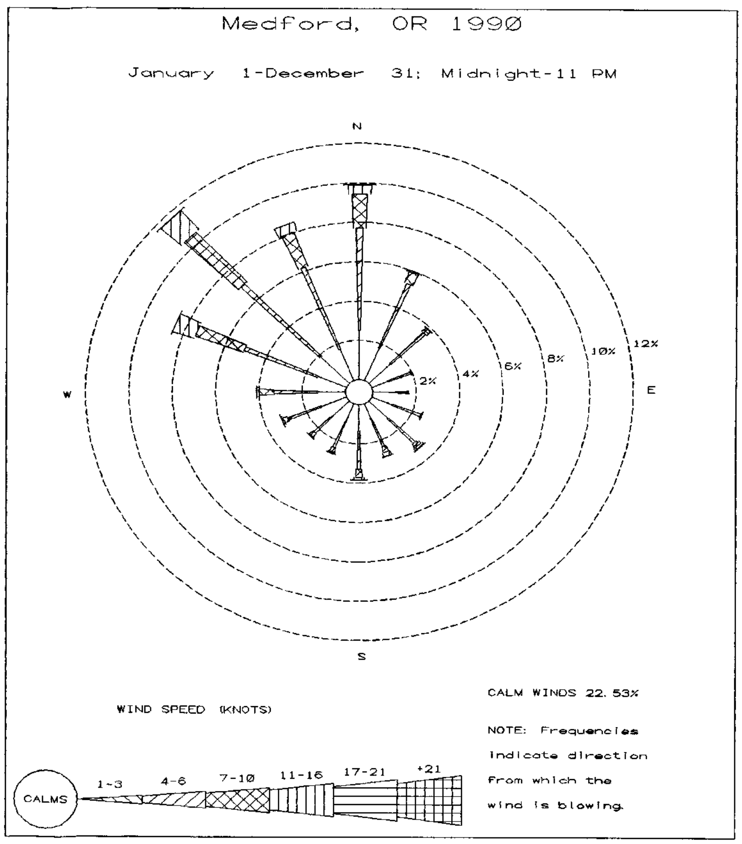
[b]This value for R_i is 0.4% of $\bar{\chi}$ $\left(= \frac{\chi_{CALPUFF} + \chi_{ISC3}}{2}\right)$ at this receptor. $\chi_{CALPUFF} = 238.6\ \mu gm^{-3}$; $\chi_{ISC3} = 239.5\ \mu gm^{-3}$

[c]This value for R_i is 0.1% of $\bar{\chi}$ at this receptor. $\chi_{CALPUFF} = 135.1\ \mu gm^{-3}$; $\chi_{ISC3} = 135.0\ \mu gm^{-3}$

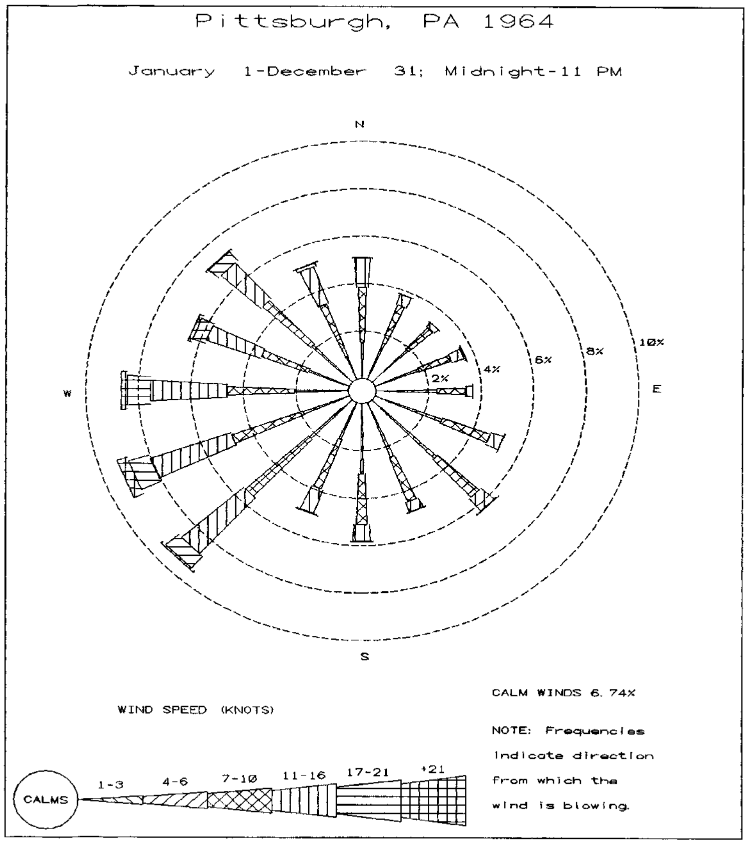
[d]There were 54 distinct cases. The "goal" for this range is: $-0.10 \leq \overline{FB} \leq 0.10$

Appendix J
Wind Rose Patterns





Appendix J, continued.



Appendix K

CALPUFF Concentrations Estimated by *Integrated Puff* and *Slug* Model

Coordinates		Hour 1	Hour 2	
X	Y	Puff	Puff	Slug
0	0.5	0	0	0
0	1	0	0	0
0	2	0	0	0
0	3	0	0	0
0	5	0	0	0
0.09	0.49	0	4400.88	4011.7
0.17	0.99	0	4606.96	3785.43
0.35	1.97	0	2366.87	1525.9
0.52	2.95	0	1408.23	658.51
0.87	4.92	0	670.78	74.94
0.17	0.47	0	0	75.18
0.34	0.94	0	0	211.99
0.68	1.88	0	0	284.43
3.19	2.82	0	0	271.96
1.71	4.7	0	0	233.71
0.25	0.43	0	0	93.83
0.5	0.87	0	0	234.87
1	1.73	0	0	284.04
1.5	2.6	0	0	266.32
2.5	4.33	0	0	229.02
0.32	0.38	0	0	108.62
0.64	0.77	0	0	248.26
1.29	1.53	0	0	282.78
1.93	2.3	0	0	262.57
3.21	3.83	0	0	226.52
0.38	0.32	0	0	118.39
0.77	0.64	0	0	254.07
1.53	1.29	0	0	261.61
2.3	1.93	0	0	261.61
3.83	3.21	0	0	226.13
0.43	0.25	0	0	122.47
0.87	0.5	0	0	255.92
1.73	1	0	0	281.55
2.6	1.5	0	0	261.75
4.33	2.5	0	0	227.49
0.47	0.17	0	0	120.31
0.94	0.34	0	0	254.23
1.88	0.68	0	0	282.08
2.82	1.03	0	0	263.61
4.7	1.71	0	0	230.65
0.49	0.09	4445.83	0	103.69
0.99	0.17	4593.7	0	234.05
1.97	0.35	2440.53	0	269.69
2.95	0.52	1413.91	0	254.14
4.92	0.87	678.28	0	226.08
0.5	0	0	0	0

Puff vs. ISC3	*Slug* vs. ISC3

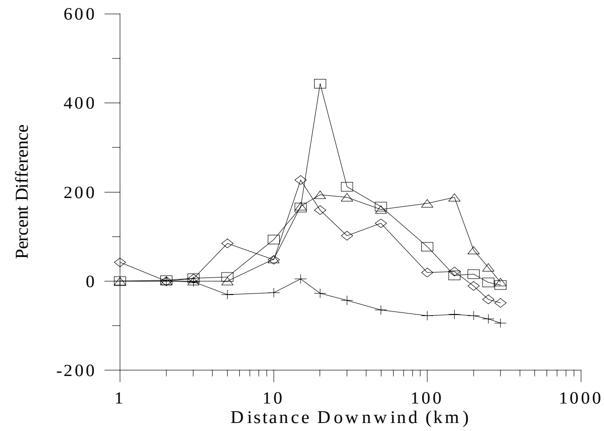


Figure L-1(a). Boise meteorological data.

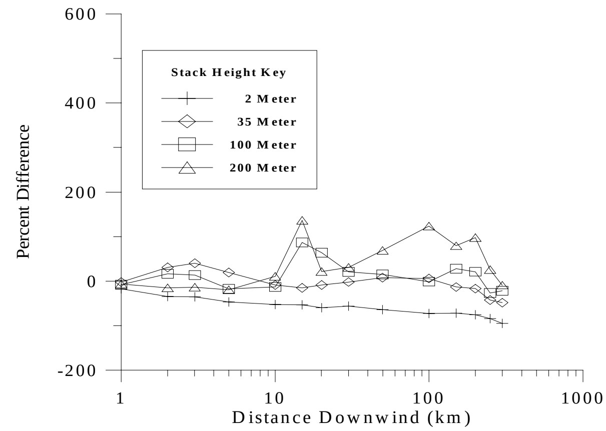


Figure L-1(b). Boise meteorological data.

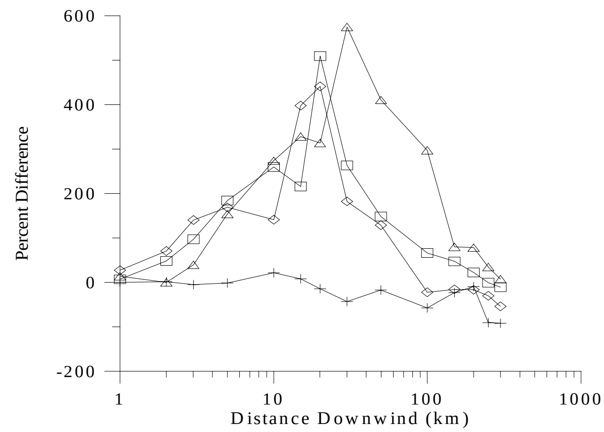


Figure L-1(c). Medford meteorological data.

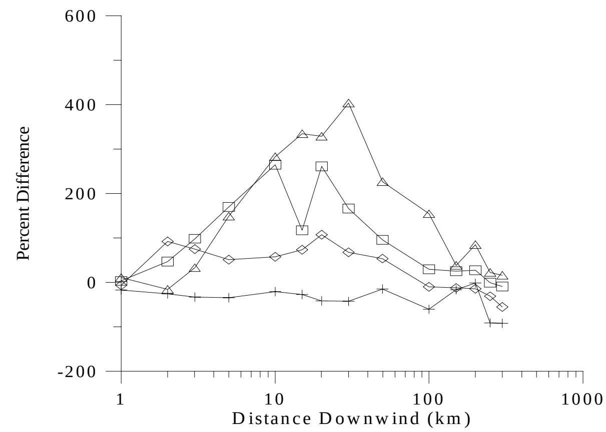


Figure L-1(d). Medford meteorological Data.

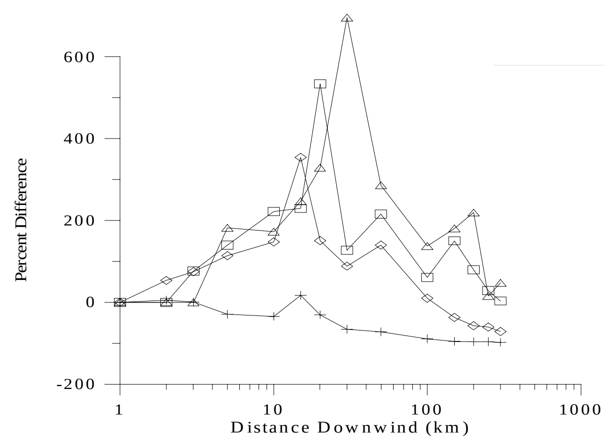


Figure L-1(e). Pittsburgh meteorological data.

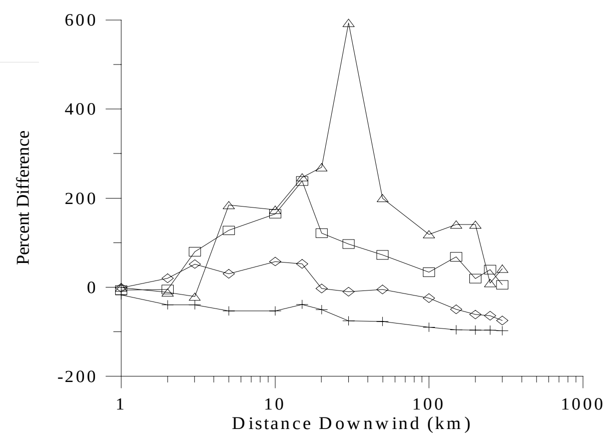


Figure L-1(f). Pittsburgh meteorological data.

Figure L-1. Maximum 1-hour average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*.
Note: $\% \; Difference = 100 \; (\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}})$.

Puff vs. ISC3 | *Slug* vs. ISC3

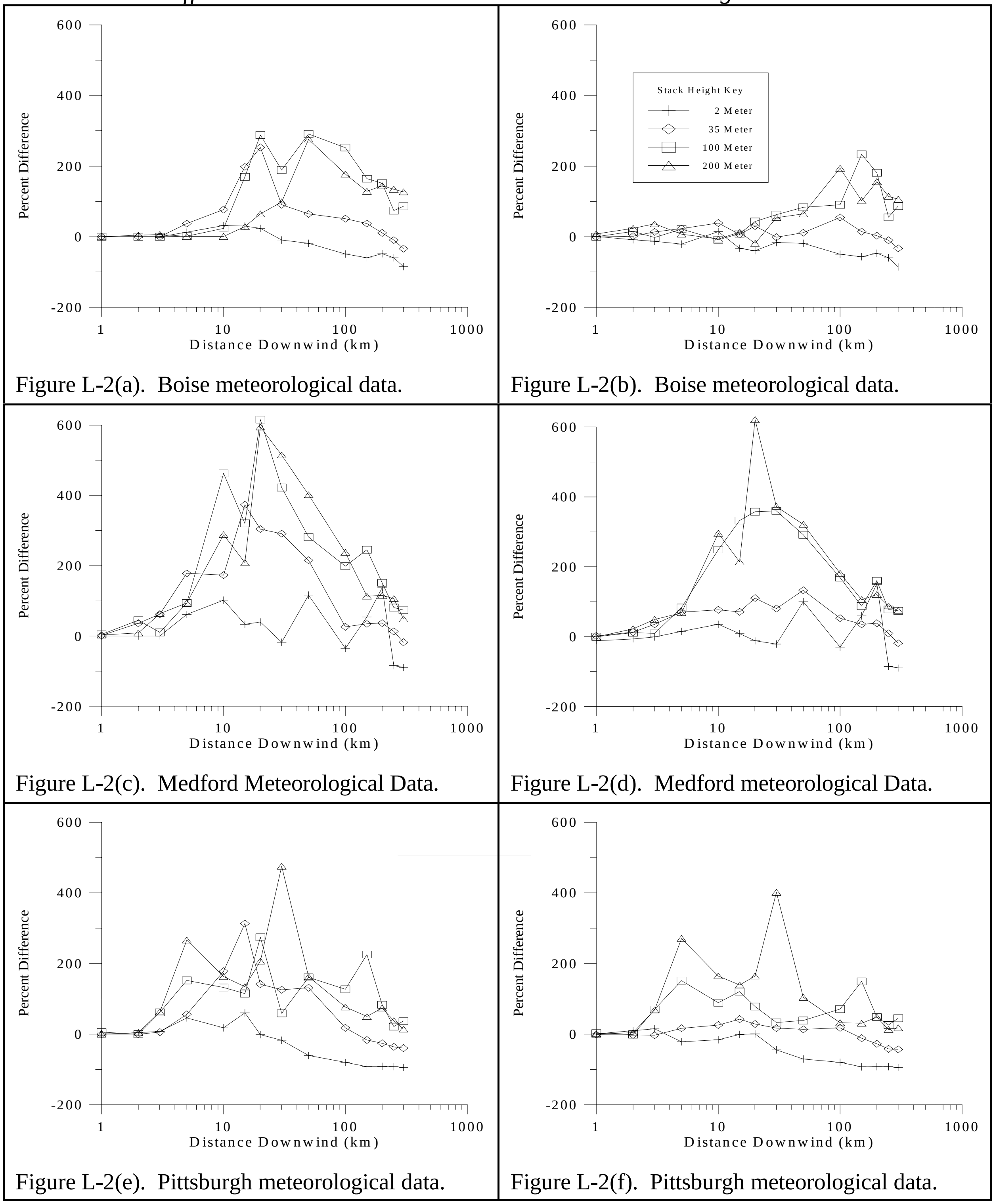


Figure L-2(a). Boise meteorological data.

Figure L-2(b). Boise meteorological data.

Figure L-2(c). Medford Meteorological Data.

Figure L-2(d). Medford meteorological Data.

Figure L-2(e). Pittsburgh meteorological data.

Figure L-2(f). Pittsburgh meteorological data.

Figure L-2. Maximum 3-hour average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*.
Note: $\%\ Difference = 100\ (\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}})$.

Puff vs. ISC3 | *Slug* vs. ISC3

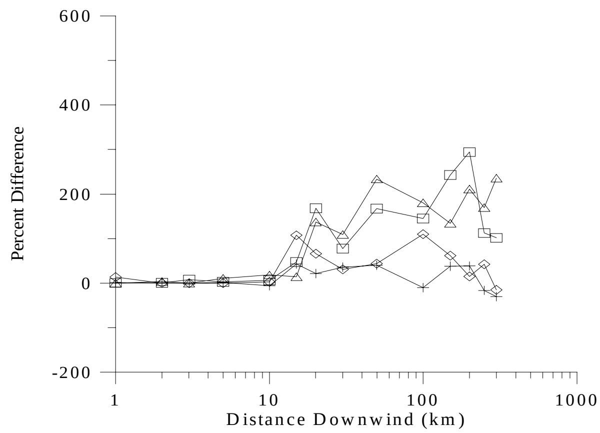


Figure L-3(a). Boise meteorological data.

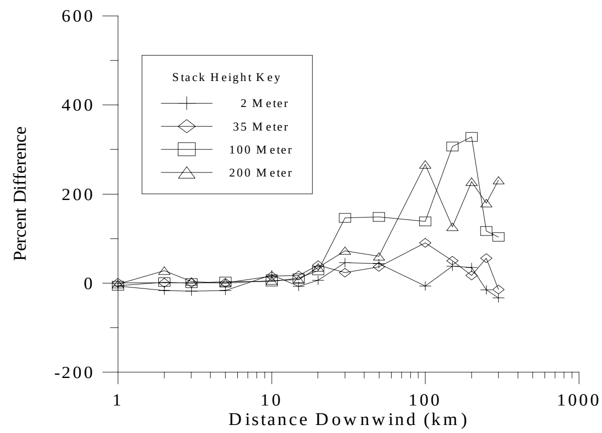


Figure L-3(b). Boise meteorological data.

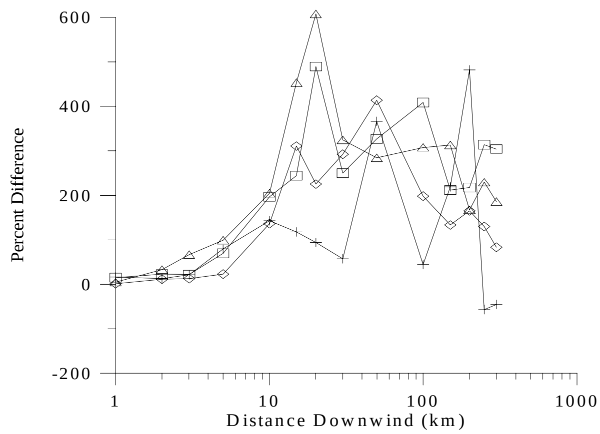


Figure L-3(c). Medford meteorological data.

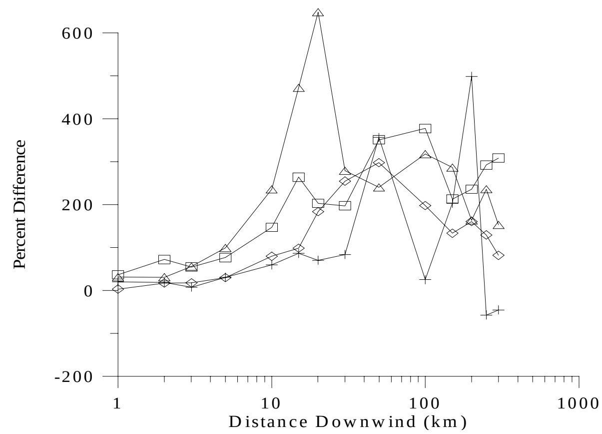


Figure L-3(d). Medford meteorological data.

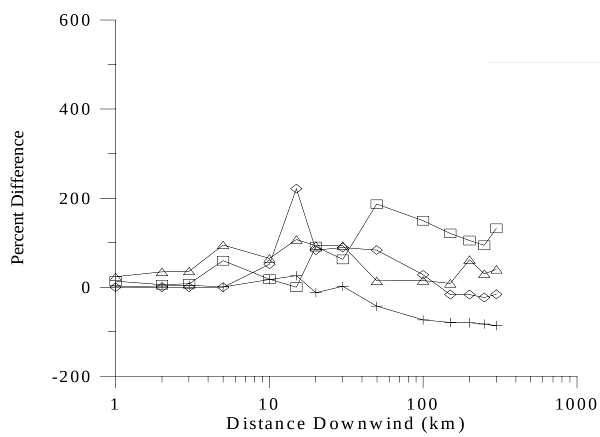


Figure L-3(e). Pittsburgh meteorological data.

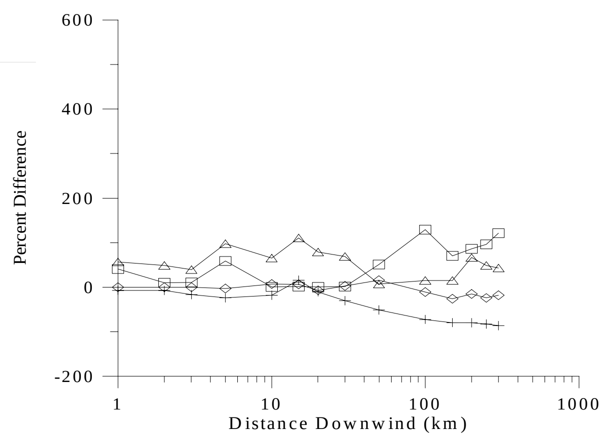


Figure L-3(f). Pittsburgh meteorological data.

Figure L-3. Maximum 24-hour average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*.
Note: $\%\ Difference = 100\ (\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}})$.

Puff vs. ISC3 | *Slug* vs. ISC3

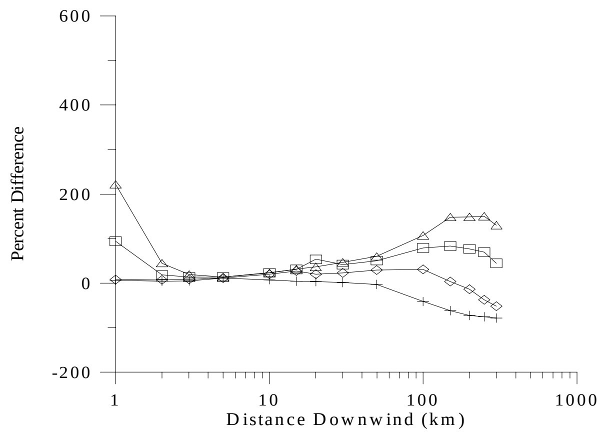


Figure L-4(a). Boise meteorological data.

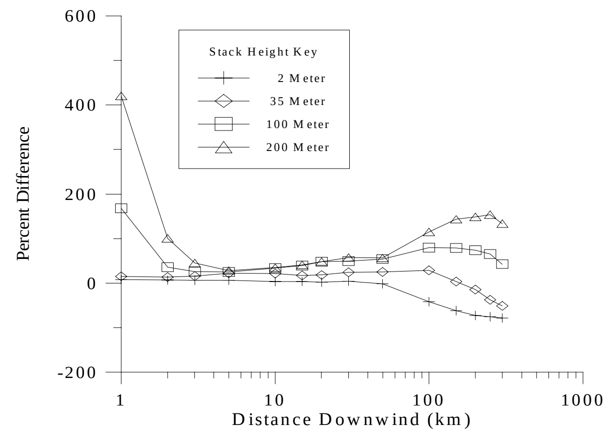


Figure L-4(b). Boise meteorological data.

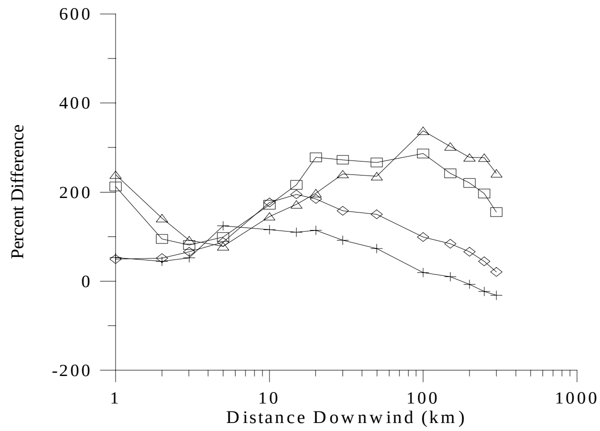


Figure L-4(c). Medford meteorological data.

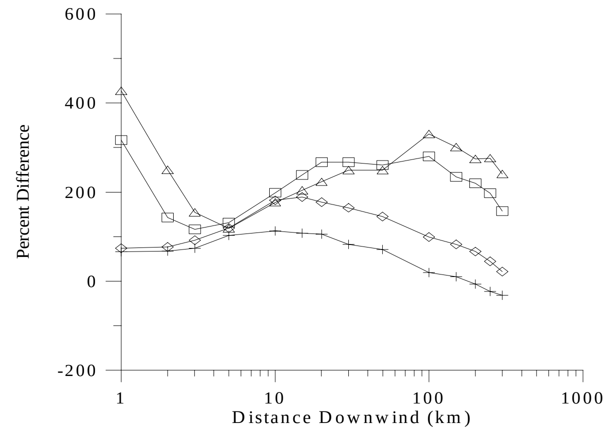


Figure L-4(d). Medford meteorological data.

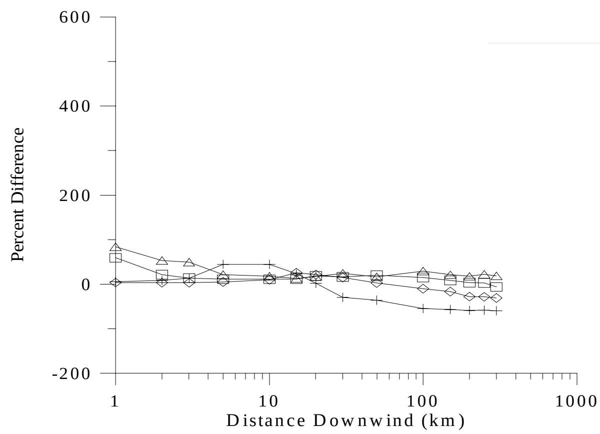


Figure L-4(e). Pittsburgh meteorological data.

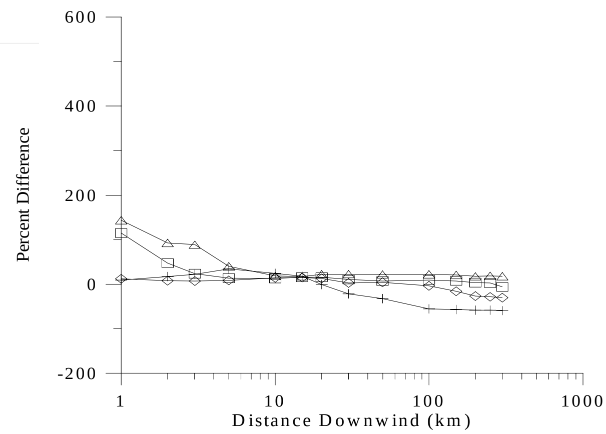


Figure L-4(f). Pittsburgh meteorological data.

Figure L-4. Maximum annual average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*.
Note: $\% \; Difference = 100 \left(\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}}\right)$.

Puff vs. ISC3 | *Slug* vs. ISC3

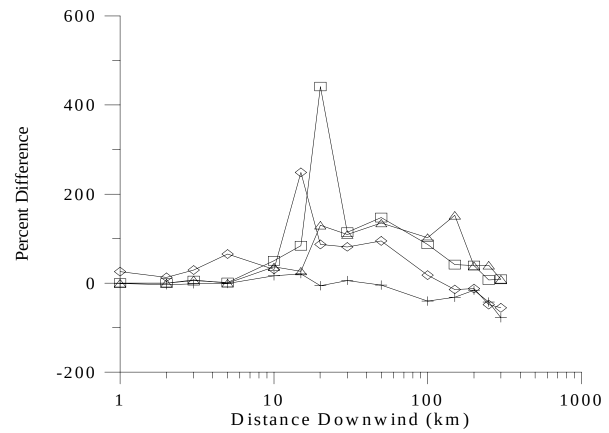


Figure L-5(a). Boise meteorological data.

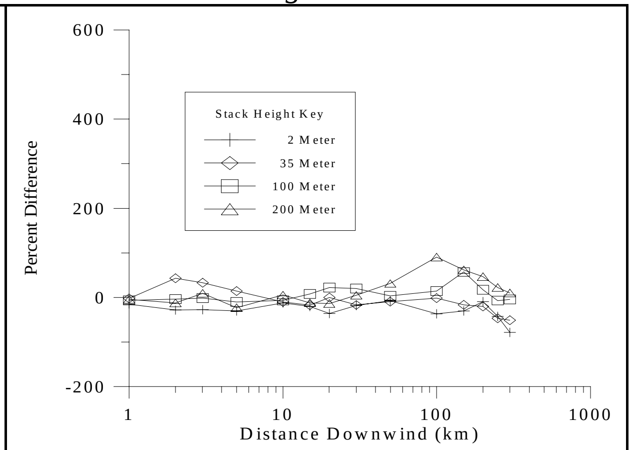


Figure L-5(b). Boise meteorological data.

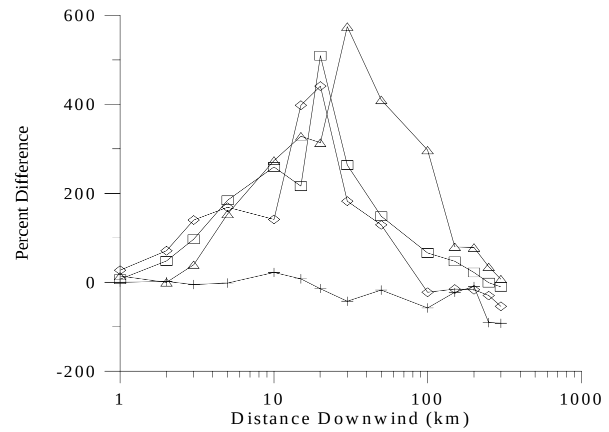


Figure L-5(c). Medford meteorological data.

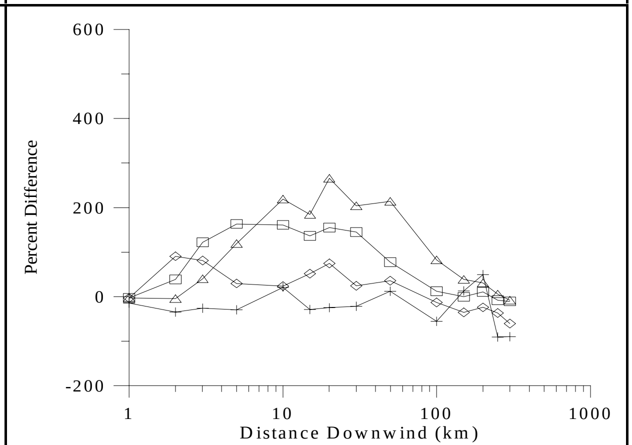


Figure L-5(d). Medford meteorological data.

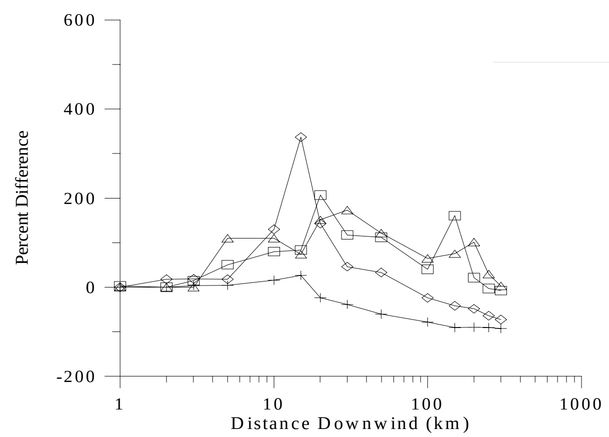


Figure L-5(e). Pittsburgh meteorological data.

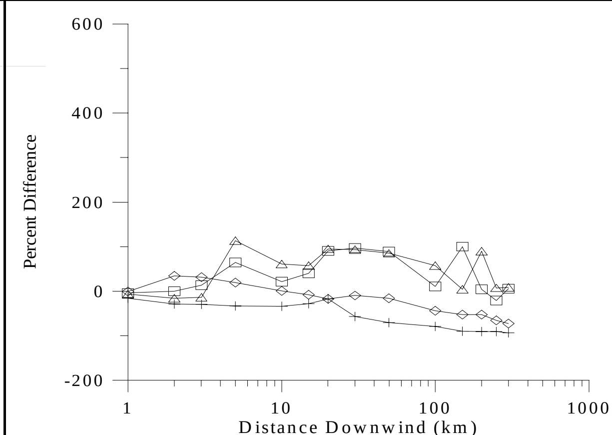


Figure L-5(f). Pittsburgh meteorological data.

Figure L-5. Highest of the second highest 1-hour average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*.
Note: $\%\ Difference = 100\ (\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}})$.

Puff vs. ISC3 | *Slug* vs ISC3

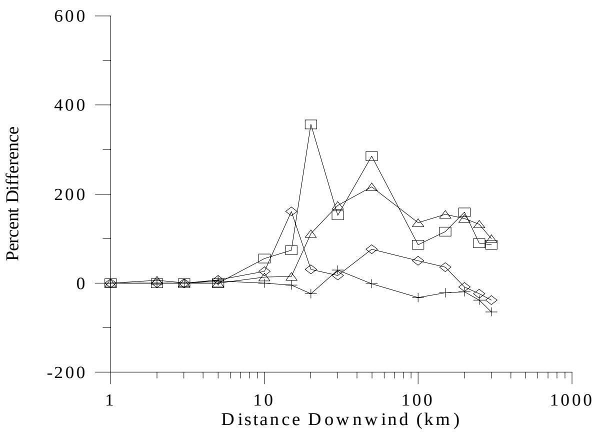


Figure L-6(a). Boise meteorological data.

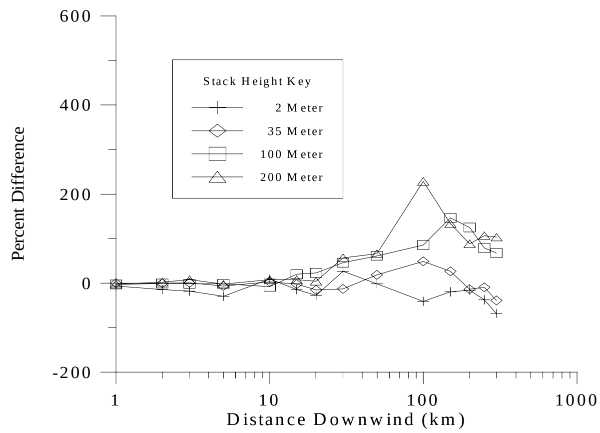


Figure L-6(b). Boise meteorological data.

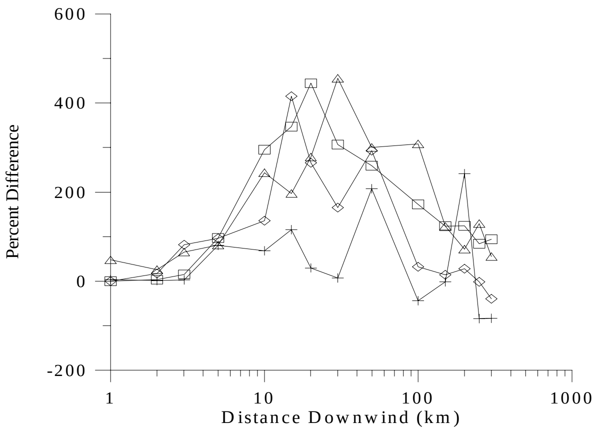


Figure L-6(c). Medford meteorological data.

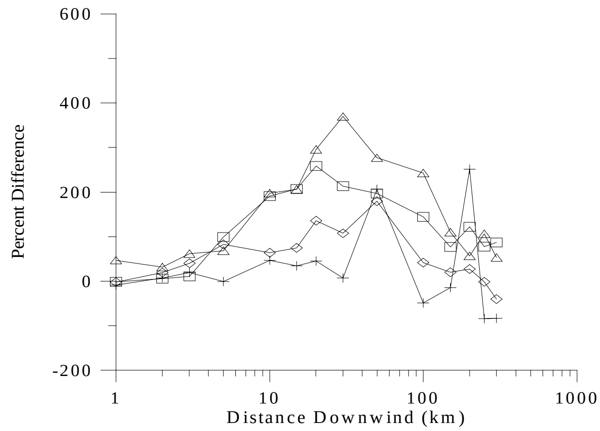


Figure L-6(d). Medford meteorological data.

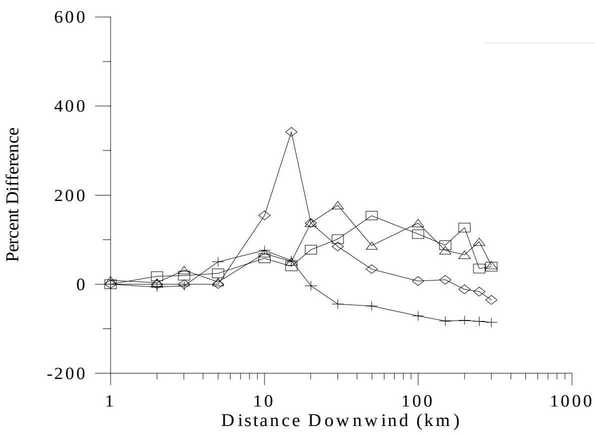


Figure L-6(e). Pittsburgh meteorological data.

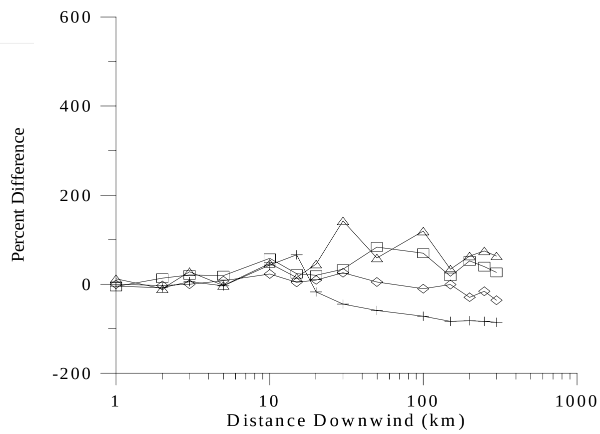


Figure L-6(f). Pittsburgh meteorological data.

Figure L-6. Highest of the second highest 3-hour average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*.
Note: $\%\ Difference = 100\ \left(\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}}\right)$.

Puff vs. ISC3 | *Slug* vs. ISC3

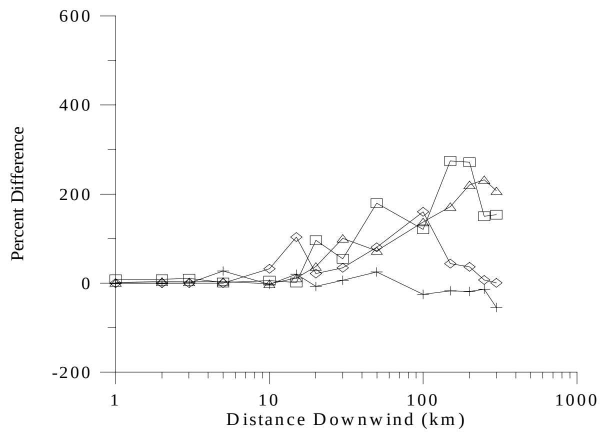


Figure L-7(a). Boise meteorological data.

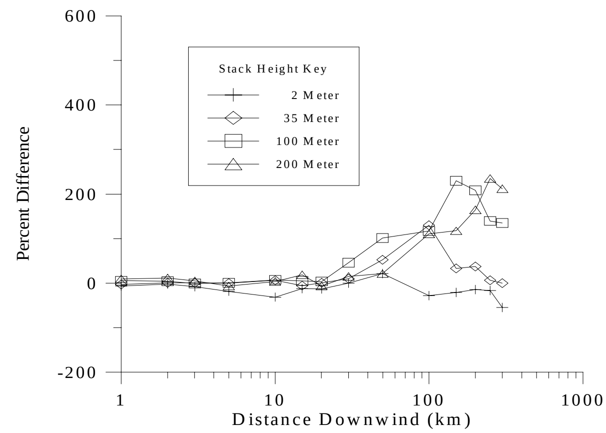


Figure L-7(b). Boise meteorological data.

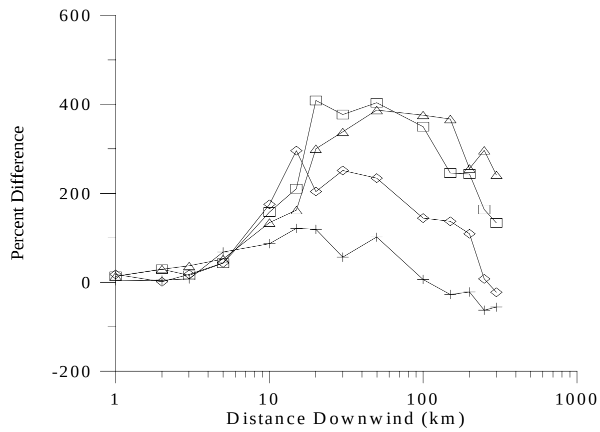


Figure L-7(c). Medford meteorological data.

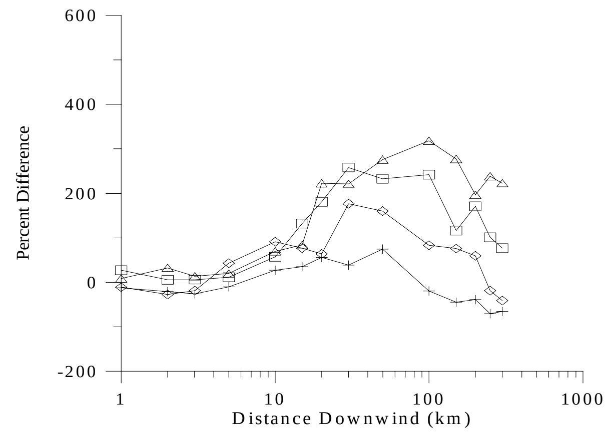


Figure L-7(d). Medford meteorological data.

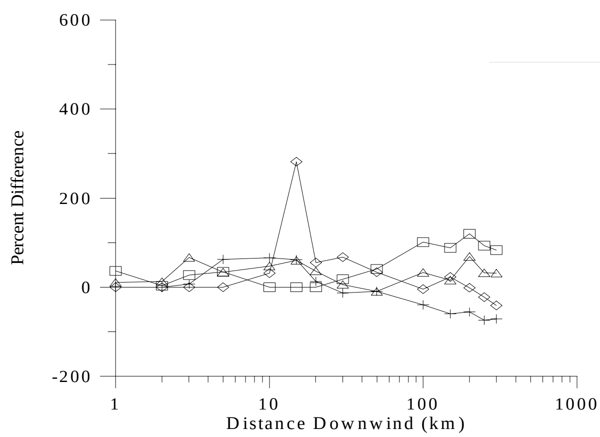


Figure L-7(e). Pittsburgh meteorological data.

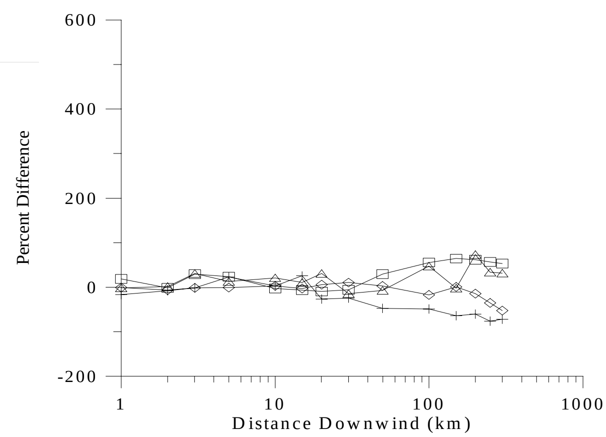


Figure L-7(f). Pittsburgh meteorological data.

Figure L-7. Highest of the second highest 24-hour average concentrations by distance. Figures a, c, & e show CALPUFF *puffs*, whereas figures b, d, & f show *slugs*. Note: $\%\ Difference = 100\ \left(\frac{\chi_{CALPUFF} - \chi_{ISC3}}{\chi_{ISC3}}\right)$.