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Executive Summary

The U. S. Air Force uses the Rocket Exhaust Effluent Diffusion Model (REEDM) to estimate the transport and diffusion of exhaust clouds produced by large launch vehicles such as the Titan IV rocket. To help in assessing the model's strengths and weaknesses, the Atmospheric Turbulence and Diffusion Division of NOAA's Air Resources Laboratory conducted a model verification and sensitivity study of REEDM. This report presents the results of these studies. In the model verification, we performed a detailed examination of the physics and mathematical equations used by REEDM to describe buoyant exhaust-cloud rise, the meteorological state of the lower troposphere, and atmospheric dispersion and deposition of effluents. The verification was largely based on the model description given in the REEDM User's Manual. In the sensitivity study, we examined how the REEDM output responded to variations in several key input variables, including mean wind speed, mixing-layer depth, and cloud cover.

From our model verification, we concluded that the basic approach used by REEDM to model the diffusion of rocket-exhaust clouds is physically sound. However, many specific features of the model contain inconsistencies and shortcomings. Some of the shortcomings are not outright errors, but are aspects of the model that we think have become obsolete because of advances in scientific knowledge and computer capability. Among the major problems we found were:

- The approach that REEDM uses to account for vertical variations in atmospheric parameters such as wind speed and direction is overly simplistic.
- The algorithm REEDM uses to estimate mixing-layer depth is reasonable for launches during daylight hours, but it does not work well for night launches when the boundary layer is stable.
- The empirical relations that REEDM uses to estimate the atmospheric turbulence in the crosswind and vertical directions (when no direct turbulence measurements are available) are based on field measurements that may not be representative of the conditions at either the Cape Canaveral Air Station or Vandenberg Air Force Base.
- The model does not properly account for the effects of turbulence on the alongwind diffusion of the ground cloud. In the current version of REEDM, the alongwind diffusion is affected by wind shear but not by turbulence.
- The existing User's Manual is inadequate, mainly because it provides little or no explanation as to how the major equations in the model were derived.

- In launch accidents involving the burning of solid rocket propellant on the ground, the equations REEDM uses to estimate the buoyant rise of the combustion products may overestimate the final stabilization height of the cloud.

Many other problems of varying importance are discussed in the report.

The REEDM sensitivity study indicated that REEDM generally performs as is expected from simple geometric relationships of cloud diffusion. The findings of the sensitivity study included:

- The peak surface concentration C_{peak} was highly sensitive to the ambient temperature profile in the boundary layer and to the mixing-layer depth.
- When the climatological algorithm in REEDM is used to estimate the level of turbulence, the downwind distance D_{peak} to the peak surface concentration can in some circumstances be greatly increased simply by increasing the fractional cloud cover from 5/10 to 6/10. This unrealistic jump in D_{peak} is caused by the procedure used by REEDM to estimate the atmospheric stability category.
- The REEDM estimates of C_{peak} and D_{peak} showed moderate sensitivity to wind-speed shear, but little sensitivity to wind-direction shear. The lack of sensitivity to wind-direction shear is surprising and suggests there may be a problem in the REEDM code.
- When REEDM is run using actual turbulence measurements (instead of the built-in climatological turbulence algorithm), changes in the turbulence parameters had large effects on D_{peak}, but only minor effects on C_{peak}.

These sensitivity results were obtained by varying one input variable at a time while holding the others fixed. This is the most straightforward approach for testing model sensitivity and has the advantage that the results are relatively simple to interpret. The approach is particularly useful for determining whether REEDM behaves as is expected from basic physical relationships that describe atmospheric diffusion. More complicated approaches are available which can provide information about how interactions between input variables affect model sensitivity. However, these approaches have several limitations and generally require a much larger number of model runs.

As a result of our model verification and sensitivity study, we have the following major recommendations regarding REEDM's future use, listed in order of overall importance:

1. The extensive vertical averaging that takes place in the model should be eliminated, so the portions of the exhaust cloud in different vertical layers are affected by different wind and turbulence regimes.

2. The algorithm used by REEDM to estimate mixing depth needs to be modified so that it provides more realistic mixing-depth estimates in stable conditions at night. The current algorithm is designed primarily for unstable boundary layers during the day.

3. The REEDM equations for concentration, dosage, and deposition implicitly assume that the exhaust cloud is transported downwind in a straight line and with a constant speed. This assumption of straight-line cloud transport should be eliminated, since there are often significant spatial variations in the winds at Cape Canaveral Air Station and Vandenberg Air Force Base.

4. Whenever possible, measured turbulence parameters should be used in REEDM instead of the climatological turbulence algorithm. Measurements are strongly preferred both near the surface and at higher altitudes. This may require additional instrumentation at the launch sites.

5. The technique used to estimate the alongwind diffusion of the exhaust cloud should be modified so that it includes the effect of turbulent mixing. Currently, the alongwind diffusion is affected by wind shear but not turbulent mixing.

6. The method REEDM uses to vertically extrapolate the turbulence parameters to higher altitudes (when no measurements are available at these altitudes) should be upgraded to be consistent with current knowledge of boundary-layer structure.

7. The User's Manual should be overhauled and rewritten to clearly show the assumptions and intermediate steps used in the derivation of the REEDM equations and to correct the large number of typographical errors.

The other problems or potential problems that were discovered during the model verification should also be addressed if continued use is to be made of REEDM. The implementation of our recommendations may require extensive modifications to the REEDM code. It may be simpler and less costly to develop a new rocket-effluent model that combines the best features of REEDM with more up-to-date diffusion modeling techniques and recent advances in the study of atmospheric structure and processes. One possibility which may minimize the development effort would be to base a new rocket-effluent model on an existing, up-to-date puff model.

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Rocket Exhaust Effluent Diffusion Model (REEDM) Verification and Sensitivity Study

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ABSTRACT. The Rocket Exhaust Effluent Diffusion Model (REEDM) is used by the U. S. Air Force to estimate the transport and diffusion of exhaust clouds produced by launch vehicles such as the Titan IV rocket. To help in assessing the model's capabilities, the Atmospheric Turbulence and Diffusion Division of NOAA's Air Resources Laboratory has conducted a model verification and sensitivity study of REEDM. The model verification indicated that the basic approach used by REEDM to model rocket-exhaust clouds is physically sound. However, many of the model's specific algorithms contain shortcomings and inconsistencies. Some of these problems can be attributed to aspects of the model that have become obsolete over the years since REEDM was developed. The sensitivity analysis showed that the peak concentration C_{peak} produced by REEDM is highly sensitive to the temperature profile in the boundary layer and to the mixing-layer depth. In some circumstances, the downwind distance D_{peak} to C_{peak} was found to be unrealistically sensitive to cloud cover. Both C_{peak} and D_{peak} showed some sensitivity to wind-speed shear in the boundary layer, but the sensitivity to wind-direction shear was significantly lower than expected. If continued use is to be made of REEDM, it is recommended that several improvements be made to the model. The turbulence algorithms in the model should be upgraded, and the diffusion algorithms should more realistically account for vertical variations of the winds and turbulence. Also, the User's Manual should be updated and improved.

1. Introduction

The Rocket Exhaust Effluent Diffusion Model (REEDM) is designed to estimate the transport and diffusion of pollutant clouds created by the launch of large rocket vehicles such as the Titan IV rocket. It can simulate the effects of vehicle failures as well as normal launches and test firings of rocket motors. The model can estimate air concentrations, dosages, and surface deposition of various chemical species that are created during a particular launch scenario. A general description of REEDM version 7 can be found in the User's Manual prepared by Bjorklund (1990).

The U. S. Air Force uses REEDM to support launches both at the Cape Canaveral Air Station in Florida and at Vandenberg Air Force Base in California. It is important that the diffusion estimates of REEDM be as accurate as possible, both for public safety and for avoiding costly, unnecessary delays in rocket-vehicle launches. To help in assessing the capabilities of the current version of REEDM, the Air Force funded the Atmospheric Turbulence and Diffusion Division (ATDD) of NOAA's Air Resources Laboratory to undertake a model verification and sensitivity study of REEDM. This report presents the results of these studies.

Model verification is the process of assessing the scientific accuracy of a model. The model should be based on sound physics and give good predictions for the "right" reasons. A scientific review of the model formulations is an essential component of verification. A review of the computer code is also required to verify that the mathematical model is properly implemented. Successful verification of a model provides faith in the predictions beyond the limited range of experimental data normally available for testing the model, and confidence in modeling new situations with different meteorological and release conditions. It also provides insights into the limitations of the model.

A sensitivity study examines the way a particular model responds to variations in either input values or internal parameters. The results of such a study are not directly related to model accuracy or physical reality. This is an important point, because the results of sensitivity studies are often misinterpreted. For example, if a model such as REEDM is demonstrated to be relatively insensitive to wind direction fluctuations, this does not imply that wind direction fluctuations are not important in atmospheric dispersion. This result tells us only that the model does not recognize this importance. Another model which explicitly accounts for such fluctuations would exhibit a greater sensitivity. Sensitivity studies are usually performed to check if the model is performing as intended and to detect errors in logic and coding. Generally, the more complex a model, the greater is the likelihood for logic and coding errors. A sensitivity study can also identify the most and least important input variables. This is helpful to the model user because it gives a sense of how accurately the input values must be measured.

The model verification described in Section 3 of this report consists of a detailed examination of the physics and mathematical equations used by REEDM to describe buoyant exhaust-cloud rise, the meteorological state of the lower troposphere, and atmospheric dispersion and deposition of effluents. An effort was made to work through and derive as many of the equations as possible in the time available, and any discrepancies, omissions, and errors are noted. There are three important limitations of this verification. First, no detailed examination of the source-term physics and chemistry was performed, since ATDD does not have expertise in this area. Second, the verification was based mainly on the REEDM description given in the User's Manual (Bjorklund, 1990). Third, the task assigned to us did not include REEDM code verification. Hence, with some exceptions, we do not know whether any of the problems discussed in this report have already been corrected in the code but remain undocumented.

The REEDM sensitivity analysis is described in Section 4. This analysis was conducted by first developing a control run of the REEDM model. Individual input parameters were then systematically varied to determine how much the REEDM output changed from the control run. The results of earlier independent sensitivity studies of REEDM are reviewed and summarized in Section 5.

The conclusions and recommendations that we reached based on the REEDM model verification and sensitivity study are given in Sections 6 and 7. A note by Mr. J. F. Bowers, which has been added to the report as Appendix A, gives a detailed description of how the alongwind diffusion algorithm used in REEDM was derived, and provides some suggestions on how the algorithm could be improved. Appendix B provides comments on nine specific aspects of REEDM that were discussed during a February 1995 meeting in Salt Lake City, Utah.

REEDM is a complicated model that uses a large number of equations to describe various aspects of the rocket-exhaust cloud. It would be impractical to reproduce all these equations in this report, so extensive references are made (particularly in the model verification) to the REEDM User's Manual (Bjorklund, 1990). For brevity, the User's Manual is hereafter abbreviated as UM. To help in distinguishing this report's equations from those in the UM, the equations in this report are identified as R1, R2, *etc.*

2. Overview of REEDM

This report is not intended to replace the UM, so only a brief overview of REEDM is given here. REEDM is designed to estimate the dispersion of exhaust clouds produced by normal rocket launches, test firings of solid rocket boosters, and launch failures. For normal launches, the rocket exhaust initially forms a roughly spherical ground cloud at the launch pad. REEDM estimates the surface concentrations produced by this ground cloud as it disperses downwind. For launch failures, REEDM can model two different scenarios: a conflagration and a deflagration. They mainly differ in whether the failure involves solid or liquid propellant. In a conflagration, an on-pad explosion is assumed to scatter solid propellant over an area around the launch pad. The solid propellant burns on the ground over an extended period of time, so it represents a quasi continuous source. In a deflagration, the liquid propellant tanks rupture and form a large fireball either on the launch pad or above the ground during flight. The fireball represents an instantaneous source of effluent.

For all launch types, REEDM divides the dispersion of the rocket exhaust cloud into two basic phases: a buoyant-rise phase and a passive-diffusion phase. The buoyant-rise phase represents the period of time when the heat released by the propellant combustion causes the exhaust cloud to ascend. The cloud is assumed to have either a spherical (normal launch or deflagration) or cylindrical (booster test or conflagration) distribution during this phase. As the exhaust cloud continues to rise and expand, it eventually looses its buoyancy and stabilizes at some height above the ground. The cloud stabilization height is determined in REEDM by both the heat liberated during the propellant combustion and by the atmospheric temperature structure at the time of the launch.

Once the exhaust cloud stabilizes, the passive-diffusion phase of REEDM begins. In this phase, the cloud's motion and diffusion is dominated by the ambient atmospheric winds and turbulence. To characterize the ambient conditions, the model defines two major layers. Layer 1 represents the planetary boundary layer just above the earth's surface, whereas Layer 2 represents the free atmosphere from the top of the boundary layer to about 3050 m AGL. The model uses a bulk-averaging approach to characterize the atmospheric conditions in each major layer. This means that each meteorological variable such as wind speed or wind direction is vertically averaged over the depth of the major layer; the layer-average value is then assumed to be representative for the entire layer.

REEDM further subdivides each major layer into a series of sublayers called meteorological layers in the UM. The boundaries between these sublayers generally correspond to altitudes at which rawinsonde measurements are reported. Thus, the positions of the sublayers are determined more by data availability than by physical changes in atmospheric structure. The sublayers are used for various purposes in REEDM, including the computation of the bulk-average parameters for the major layers and the estimation of ground-level concentration and dosage.

During the passive-diffusion phase, REEDM assumes that the rocket exhaust generally cannot pass from one major layer to the other. (The only exception being the gravitational settling of large acid drops from Layer 2 to Layer 1.) This means that the ground-level concentrations and dosages are mainly determined by the portion of the stabilized exhaust cloud within Layer 1. The exhaust cloud is quite large during this phase, so it is broken up vertically into a series of slabs, with each slab corresponding to one of the sublayers mentioned above. Each slab initially resembles a disk, with a bivariate Gaussian distribution in the horizontal and a uniform distribution in the vertical. The transport and diffusion of each slab is determined by the bulk-average atmospheric parameters for the major layer. Thus, all the slabs in each major layer are transported with the same wind speed and direction and are diffused at the same rate. Reflection terms are used in the model equations to keep the exhaust from diffusing out of the major layers. The concentration, dosage, and deposition of the ground cloud at a given surface location downwind are obtained by summing the contributions from all the slabs making up the cloud.

3. REEDM Verification

During the verification process, we reviewed the REEDM mathematical formulations as they are described in the UM. Overall, we believe that the basic features of

REEDM—the distinction between buoyant-rise and passive-diffusion phases, and the division of the exhaust cloud into a series of vertical slabs—are physically sound. Any improved version of REEDM would likely retain these basic features. However, many specific features of REEDM contain inconsistencies and shortcomings that are addressed in the following subsections. Some of the shortcomings we discuss are not outright errors, but aspects of the model that we feel have become obsolete.

3.1. General Comments

The description of the REEDM model, as documented in the UM, must be characterized overall as inadequate. A typical model user or reader of this document would not have much comprehension of how the model was derived and put together. Many equations, including the dosage and deposition algorithms that involve long, complicated expressions, are presented as *fait accompli* with no rationale or justification; all or most of the steps leading to these equations are omitted. Additional problems for the reader are caused by the lack of consistency in the literature citations. Some citations in the UM are given by number and others by author name. Since the References at the back of the UM are listed numerically, it is difficult to look up citations in the text that are only given by author name.

The review was made more difficult by the relatively obscure nature of the references for key assumptions and equations. Many of the references listed at the end of the UM are old private-company or government-agency reports that are not easily accessible to any but the most determined reader with ample time. An accompanying "science" document, which explains the basis for the model and other details missing in the UM, would have been very helpful, but there is no indication that such a document exists.

One feature of REEDM that stands out is the large amount of vertical averaging that takes place. Instead of allowing atmospheric parameters such as the wind speed and direction to vary with height, the model uses bulk parameters that are obtained by averaging over the entire depth of the major layers. This averaging seems to be a legacy from the model's early history, when computer resources were much more limited than today. With present computer resources, it is no longer necessary to accept the loss of physical realism that is associated with this vertical averaging. One of the major ways REEDM can be improved is to eliminate the vertical averaging and allow parts of the exhaust cloud at different heights to be affected by different winds and turbulence. Any vertical averaging that is retained in the model should be used only to eliminate "noise" in the rawinsonde data. (Rawinsondes inherently provide quasi instantaneous measurements of atmospheric variables rather than time-average measurements, so the resulting profiles can have a jagged appearance.)

REEDM distinguishes between two different launch failure modes: a conflagration and a deflagration. During an actual launch failure, it is possible (even likely) that both modes will occur together. Two independent runs of REEDM would seem to be necessary in this case: one for the conflagration and another for the deflagration. Other than a single reference to Knight and Prince (1988), no justification is given in the UM for why the conflagration and deflagration modes are treated independently.

A confusing feature of REEDM is that a distinction is made between instantaneous and continuous sources in the buoyant-rise computations but not in the dispersion and deposition computations. In some launch modes, the cloud rise is computed using a formula for instantaneous sources, whereas in others a formula for bent-over continuous plumes is used. In all scenarios, however, the downwind dispersion and deposition are computed using a vertical series of slabs, with each slab being treated as an instantaneous puff. It is not clear how a cloud that starts out being treated as a bent-over continuous plume can suddenly be transformed into a series of instantaneous puffs.

When performing averages of the horizontal wind vector, REEDM averages the wind speed and direction instead of the u and v Cartesian components. Examples of this in the UM include Eqs. (18) and (19), Eq. (27), and Eq. (108). Averaging the wind speed and direction can produce errors when the wind-vector angles are large. The average of a westerly wind and an easterly wind, according to this approach, is incorrectly computed to be a southerly wind. Even for small angles, problems occur for winds near north: the average of a 5° and a 355° wind is incorrectly computed to be a 180° wind. It is not clear from the UM whether the averaging algorithms used in the REEDM code account for these kind of problems. Of course, such problems could be eliminated by averaging in rectangular Cartesian coordinates instead of polar coordinates.

There are many inconsistencies in variable definitions, units, and equation numbers in the UM. Most of the equation numbers in the List of Symbols are wrong and need correction. There are also many errors and omissions in the text, such as incorrect or missing literature references and incorrect table or equation numbers. We have generally avoided mentioning specific typographical and notational errors in this report unless these errors caused problems in our understanding of the model physics.

3.2. Specific Comments

3.2.1. *Launch Types*

Two key assumptions of REEDM given on p. 10 of the UM are that the primary exhaust products of concern for all but the deflagration mode are produced by the solid propellant, and that the heat liberated by the deflagration of liquid propellant does not contribute to the plume rise of the solid propellant combustion products. These assumptions are not justified in the UM, except for a reference to a private-company report by Knight and Prince (1988).

3.2.2. *Mixing-depth Estimation*

On p. 13 of the UM, it is recommended that users ignore inversions with tops less than 200 m above the ground when estimating the depth H_m of the turbulent mixing layer (*i.e.*, the depth of Layer 1 in the model). Such inversions are also ignored in the mixing-depth algorithm given in Section 3.5 of the UM. The reason given for this recommendation is that the high initial velocities and temperatures of the rocket exhaust will easily overcome these inversions. While it is true that such low-level inversions may have little effect on the rise of the buoyant ground cloud, they can have a significant influence on the vertical profile of turbulence near the ground. Hence, they can still be highly important during the period after the ground cloud has stabilized, when ambient winds and turbulence are dispersing the cloud.

A more fundamental problem with the mixing-depth algorithm used in REEDM is that it assumes the top of the boundary layer is always capped by a stable layer. This is a good assumption for unstable and even for near-neutral conditions, but it generally does not work in stable conditions. At night, the lowest stable layer is usually right at the surface, and a second stable layer is often found at the top of the previous afternoon's convective boundary layer (*e.g.*, Stull, 1988). The bases of these stable layers have no direct relation to the depth of the turbulent mixing. Estimating the mixing depth is therefore more difficult at night than during the day.

The most direct way to estimate the mixing depth at night is to use available tower and sodar measurements to determine how rapidly the turbulence decreases with height. Another possibility is to use the equation $H_m \approx b[u_* L/f]^{1/2}$, where u_* is the friction velocity, L is the Monin-Obukhov length, f is the Coriolis parameter, and b is a constant roughly equal to 0.4. This equation was first derived by Zilitinkevich (1972) and is valid once the nighttime boundary layer has reached a quasi-steady state. Estimates of u_* and L can be obtained using wind and temperature profiles (*e.g.*, Berkowicz and Prahm, 1982) or surface energy budgets (van Ulden and Holtslag, 1985).

The formula given above for H_m is based on some fairly simple assumptions about boundary-layer structure, and it thus does not account for the complex flow features that can be present in a coastal environment. It is therefore recommended that this formula be tested with observations at Cape Canaveral Air Station and Vandenberg Air Force Base before it is used on a routine basis.

3.2.3. *Plume Rise*

For normal launches and deflagrations, REEDM treats the ground cloud as an instantaneous source during the buoyant-rise phase. The buoyant rise of this cloud is given by [Eq. (1) in the UM]

$$\frac{d^2\left(\overline{w}r^3\right)}{dt^2} = -S\,\overline{w}r^3 \,, \tag{R1}$$

where $\overline{w}$ is the cloud's mean vertical velocity, r is the cloud radius, t is time, and S is a stability parameter. No derivation of this equation is given in the UM. References are given to Briggs (1969, 1970), but neither of these references deals with instantaneous sources. It is possible to derive Eq. (R1) by starting with the equations for instantaneous sources given by Morton *et al.* (1956) and assuming that the cloud's potential temperature changes only by entrainment of ambient air.

Equation (2) in the UM, which is supposed to be the solution of Eq. (R1) above, is incorrect. The first term on the right side of this equation does not have the proper units. The correct form of this equation is

$$\overline{w}r^3 = \begin{cases} \dfrac{F_b}{\sqrt{S}} \sin(\sqrt{S}\,t) + F_m \cos(\sqrt{S}\,t) & \text{for } S > 0; \\ \dfrac{F_b}{\sqrt{-S}} \sinh(\sqrt{-S}\,t) + F_m \cosh(\sqrt{-S}\,t) & \text{for } S < 0. \end{cases} \tag{R2}$$

Here, F_b is the buoyancy flux and F_m is the initial value of $\overline{w}r^3$. This is the equation that is actually being used in the subroutine CRISE within the REEDM source code.

To obtain Eq. (R2) from Eq. (R1), it must be assumed that the stability parameter S remains constant during the cloud's ascent. This is true only within each meteorological sublayer defined in REEDM. Equation (R1) should therefore be applied individually to each of these sublayers, and the variables in Eq. (R2) should be initialized based on the cloud's condition at the bottom of the current meteorological sublayer, not the condition at the time of the cloud's formation. In particular, t represents the time elapsed since the cloud first entered the sublayer, and the factors F_b and F_m should be based on the cloud's buoyancy and vertical velocity when it first entered the sublayer.

Because of the large size and high temperature T_c of the rocket exhaust cloud, the buoyant acceleration is better defined as $g(\rho - \rho_c)/\rho_c$ or $g(T_c - T)/T$ instead of the expression $g(\rho - \rho_c)/\rho$ given in the UM. The effective density of the fluid being driven by the buoyant force is approximately constant and equal to the density of the cloud instead of the density of air. The expression used in REEDM is a reasonable approximation only at larger downwind distances (Briggs, 1972). This may make some difference in the cloud stabilization height.

On p. 18 of the UM, it is stated that the instantaneous cloud-rise equations are applied to each meteorological sublayer k defined by the rawinsonde record. This agrees with what has been said in the foregoing paragraphs. However, at the top of UM p. 19, the stability parameter S is said to be averaged over a vertical layer. Although the vertical layer is not explicitly defined, one could infer that it is one of the two major layers in REEDM. These statements on pp. 18 and 19 are contradictory, since averaging S over a major layer would eliminate the need to apply the cloud-rise equations to each sublayer k. It is thus unclear exactly how the cloud-rise equations are employed in REEDM.

In the definition of the initial buoyancy flux F_{bo} on UM p. 18, the cloud density ρ_c should be used instead of the ambient density ρ. The definition of F_{bo} will then be consistent with what has been said above regarding the buoyant acceleration. [This comment also applies to the buoyancy flux F_b for continuous sources, as defined by Eq. (12) on p. 20 of the UM.] For a deflagration, REEDM assumes according to UM p. 18 that 5% of the total solid propellant effective heat contributes to the buoyancy flux F_{bo}. No explanation is given as to why this 5% is added.

In Section 3.1.2 of the UM, the equations that REEDM uses for the buoyant rise of a continuous effluent release (*i.e.*, a conflagration scenario) are presented. These equations are valid for the case of a bent-over plume (*e.g.*, Briggs, 1975), and they thus should not be used in light winds. As is the case with the instantaneous-cloud equations, the continuous-plume equations assume that the stability parameter S is constant with height, so they should be applied to each REEDM sublayer individually.

Equation (11) in the UM is used to compute the time t_k it takes for the plume from a continuous release to reach a height z_k corresponding to the bottom of the kth sublayer in REEDM. This equation requires some additional assumptions that are not stated in the UM. Namely, it is assumed that the initial plume radius r_o and the initial momentum parameter F_m are zero. If these assumptions are not made, Eq. (11) becomes

$$t_k = \frac{-2}{\sqrt{S}} \arctan\left\{ \left[6\frac{\gamma_e F_b}{\overline{u}_s S} - (r_o + \gamma_e z_k)^3 + r_o^3 \right]^{-1} \left[\frac{3\gamma_e F_m}{\overline{u}_s \sqrt{S}} - \sqrt{9\frac{\gamma_e^2 F_m^2}{\overline{u}_s^2 S} + 6\left[(r_o + \gamma_e z_k)^3 - r_o^3\right] \frac{\gamma_e F_b}{\overline{u}_s S} - \left[(r_o + \gamma_e z_k)^3 + r_o^3\right]^2} \right] \right\}, \quad \text{(R3)}$$

and UM Eq. (13), which describes the stabilization height z_s for a continuous plume, becomes

$$z_s = \left[\frac{6F_b}{\overline{u}_s \gamma_e^2 S} + \frac{r_o^3}{\gamma_e^3} \right]^{1/3} - \frac{r_o}{\gamma_e}. \quad \text{(R4)}$$

In these equations, γ_e is a dimensionless entrainment parameter, and $\overline{u}_s$ is a mean wind speed representative of the layer extending from the ground to the height z_s. Some sample calculations indicate that the value of t_k obtained from Eq. (R3) is larger than that obtained from the REEDM equation, whereas the value of z_s obtained from Eq. (R4) is smaller than that obtained from REEDM.

Suppose, for example, that $S = 1.1 \times 10^{-4}\,\mathrm{s}^{-2}$, $\overline{u}_s = 5\,\mathrm{m\,s}^{-1}$, $\gamma_e = 0.5$, $r_o = 10\,\mathrm{m}$, and $F_b = 33.4\,\mathrm{m}^4\,\mathrm{s}^{-3}$. Equation (R4) then predicts that $z_s = 94\,\mathrm{m}$, whereas the REEDM equation predicts a value of 113 m. If $F_m = 0$ and $z_k = 50\,\mathrm{m}$, then Eq. (R3) gives $t_k = 95\,\mathrm{s}$, whereas REEDM gives 57 s. If F_m is increased to a value of $250\,\mathrm{m}^4\,\mathrm{s}^{-2}$, then t_k falls to 88 s. These calculations suggest that it may be important to retain the dependence on r_o and F_m when using the bent-over-plume equations. By setting these variables to zero, REEDM may be overestimating the cloud stabilization height and underestimating the ground-level concentration for a conflagration event.

3.2.4. *Initial Position and Dimensions of Stabilized Ground Cloud*

As the ground cloud rises from the launch pad to its stabilization height, it travels downwind some distance as a result of the ambient winds. The initial position of the stabilized ground cloud is therefore not directly above the launch pad in most cases. To account for this, REEDM uses the variables R_{ck} and θ_{ck}, which respectively represent the horizontal distance and direction of the stabilized ground cloud relative to the launch pad. A subscript k is used with these variables to indicate that separate values are computed for each of the k sublayers in the model. (This is one of the few cases in which REEDM uses the rawinsonde data directly without first averaging over the depth of a major layer.)

For dosage and concentration computations, R_{ck} and θ_{ck} are computed using Eqs. (21) and (22) in the UM. However, there is confusion in the UM whether θ_{ck} is defined using a mathematical convention with angles increasing counterclockwise starting from east, or using a navigational convention with angles increasing clockwise starting from north. Equation (22) in the UM implies that a navigational convention is used, but Eq. (15), which defines a different value of θ_{ck} used for acid-drop deposition, seems to use a mathematical convention.

Another problem with Eqs. (21) and (22) is the appearance of the term $\overline{u}_k(t_s - t_k)$, where $\overline{u}_k$ is the mean wind in sublayer k, t_k is the time it takes the ground cloud to rise from the launch pad to the bottom of sublayer k, and t_s is the time it takes the ground cloud to reach its stabilization height. This term is supposed to account for the horizontal drift of the cloud between the times t_k and t_s. However, this term rests on the assumption that the cloud material that reaches sublayer k at time t_k stops rising and only moves horizontally from t_k to t_s. No justification is given for this assumption. In fact, this assumption to some extent contradicts REEDM's overall treatment of the rising ground cloud as an intact sphere. A more plausible assumption, which is consistent with a rising sphere, is that the cloud material that reaches sublayer k at time t_k continues to rise to higher levels, whereas new material reaches sublayer k from below. With this assumption, Eqs. (14) and (15) in the UM would better describe the stabilized cloud's horizontal position instead of Eqs. (21) and (22).

For the sublayer that contains the stabilization height z_s of the ground cloud, REEDM uses a different equation [UM Eq. (26)] in the computation of R_{ck} and θ_{ck} than it does for other sublayers. However, UM Eq. (26) has a number of problems that make it difficult to understand. It is not clear, for example, why the time t_R required for the launch vehicle to reach z_s should be relevant in the sublayer that contains z_s. Another problem is that this equation requires instantaneous sources to somehow move faster than the ambient wind. For continuous sources, the equation does not have the correct units; presumably, the factor Δz_M that appears on the right side of the equation should actually be Δt_M. Finally, it is not explained why separate equations for instantaneous and continuous sources are required for the sublayer containing z_s but not for other sublayers.

In Section 3.2.3 of the UM, a distinction is made between "elliptical" and "spherical" distributions for the stabilized ground cloud. The only difference between the two distributions is that the spherical distribution has some extra cloud material near the ground. It is not clear why the terms "elliptical" and "spherical" are used to describe these distributions. Moreover, no explanation is given why the extra material near the ground in the "spherical" distribution should have a fixed horizontal radius of 50 m. Both distributions also assume that a portion of the rocket-exhaust trail extends vertically above the top of the stabilized ground cloud. This part of the exhaust trail is assumed to have a horizontal radius of about 200 m [the standard deviation σ_m in Eqs. (33) and (34) of the UM is given a value of 93 m, which roughly corresponds to a radius of 200 m], but no mention is made of where this number came from.

3.2.5. *Source Strengths and Characteristics*

In the discussion of cloud acid drops in Section 3.2.4. of the UM, the acid-drop settling velocity V_j is introduced. There is no mention in the UM as to how V_j is computed for the drop-size categories j, except for the statement on p. 46 that the drop diameter at the top of each meteorological layer is used in the computation of V_j.

On p. 26 of the UM, the variable $h_j(r)$ is defined as the height above ground at which acid drops within a certain size category j start to fall out of the ground cloud. This height varies with the horizontal distance r from the cloud's center, since the vertical velocity within the cloud is greatest near the center and falls off towards the cloud's edges. According to the UM, REEDM replaces the continuous variable $h_j(r)$ with the discrete variable $h_{k,j}$, which varies with the drop-size category j and with the vertical sublayer k. It is unclear how the dependence of $h_j(r)$ on the horizontal radius r is replaced by a dependence of $h_{k,j}$ on the vertical sublayer k.

Equation (38) on p. 28 of the UM is difficult to interpret, in part because the variables r and r_k are not consistently defined. r is first defined as the cloud radius on p. 16 of the UM, then as a normalized radius on p. 26. r_k is defined as the cloud radius in layer k on UM p. 24, and then as the normalized radius at which the net velocity V_j' equals zero on pp. 27–28. Additional confusion is caused by using the notation $F_j(k)$ for the drop fraction, which looks very similar to the mass $F\{k\}$.

Once the ground cloud has stabilized, REEDM divides the total mass of the exhaust material among the various meteorological sublayers. Equation (39) of the UM is supposed to determine how the mass is distributed for normal launches and deflagrations, but this equation cannot be correct. Two of the four cases on the right side of this equation have the wrong units for a mass. The equation also indicates that the stabilized ground cloud will not initially reach to the ground if the radius r_s of the stabilized cloud is less than the stabilization height z_s. If this is true, there is no justification for distinguishing between the "elliptical" and "spherical" cloud forms used in REEDM, since they both give the same result. In the second case on the right side of Eq. (39), the volume V_k should not appear in the denominator. It would make more sense if this case contained the ratio of V_k to the total cloud volume $4\pi r_s^3/3$. The third case should also contain a volume ratio, and the variables t_R and Δt_k should be added together. The variable K that appears in the denominator of the third case is presumably a typographical error.

3.2.6. *Reaction Products*

In Table 3-1 on p. 32 of the UM, it is not entirely clear what the molecular weights in the first row represent. They could be either the molecular weights of a stoichiometric mixture of A-50 and N_2O_4 or the molecular weights of the reaction products.

Equation (52) on p. 36 of the UM is used to determine temperature of a fireball created during a deflagration. No explanation is given as to how this equation was derived. The validity of this equation is questionable, since the units on the right side of this equation do not agree with those on the left side.

In Section 3.2.5.3 of the UM, there is some confusion regarding the decay of N_2O_4 after a deflagration. Any unreacted oxidizer that is present after a deflagration should produce a mixture of N_2O_4 and NO_2, since these species coexist in a chemical equilibrium in the gas phase. Section 3.2.5.3 discusses the decay of NO_2 into HNO_3, but says nothing about the decay of N_2O_4. It is not clear whether N_2O_4 also decays into HNO_3 or has its own decay products.

3.2.7. *HCl Distribution*

The description of HCl in Section 3.3 of the UM seems to be specifically tailored to the Space Shuttle. It is unclear whether REEDM is also used to compute HCl deposition for other launch vehicles. If so, it may not be reasonable to assume that the drop-size distribution for these other launch vehicles is the same as that for the Space Shuttle.

In computing the size distribution of HCl drops, REEDM assumes that the drops are of unit density (p. 40 in the UM). It is not clear whether this a good assumption. For highly concentrated HCl drops, the drop density could be significantly above unity.

The average mean diameter *AMD* of the acid-drop distribution is computed in REEDM using the equation [Eq. (62) in the UM]

$$AMD = \exp\left[\ln(MMD) - 1.5\ln^2(\sigma_g)\right] \ , \qquad \text{(R5)}$$

where *MMD* is the mass median diameter and σ_g is the geometric standard deviation of the acid-drop mass distribution. The constant for the second term should be 3.0 (see Cadle, 1975, p. 26) instead of 1.5; the mass and number lognormal distributions are related by Kapteyn's law (Herdan, 1960; Rao and Satterfield, 1983) which gives the value of 3.0 for this constant.

In UM Eq. (79) for the Reynolds number, the purpose of the multiplication factor 10^{-2} should be clearly stated. It apparently is a unit conversion factor, so the units of the various parameters in this equation need to be specified.

3.2.8. *Turbulence Parameterizations*

To estimate the diffusion of the ground cloud, REEDM must estimate the turbulence parameters σ'_A and σ'_E, which are defined respectively as the standard deviations of the wind direction in the horizontal and vertical directions. These parameters can be estimated either with direct field measurements or with a climatological procedure described in Section 3.4.1 of the UM.

The climatological procedure used by REEDM for estimating σ'_A and σ'_E below heights of 100 m is based on some empirical analyses going back to the 1960s. Although this procedure is not erroneous, it does not take advantage of developments in surface-layer and mixed-layer scaling. Furthermore, it is largely based on measurements taken at only two sites: White Sands Missile Range in New Mexico and Round Hill Field Station in Massachusetts. The turbulence profiles at these sites may be quite different from those at Cape Canaveral Air Station and Vandenberg Air Force Base. It may be worthwhile to replace the existing procedure with a more modern approach based on the standard deviations σ_v and σ_w of the lateral and vertical velocity components. In most of the current models for boundary-layer structure (*e.g.*, Panofsky and Dutton, 1984; Hicks, 1985; Stull, 1988), σ_v and σ_w are estimated using the friction velocity u_*, the Monin-Obukhov length L, and the mixing layer depth H_m. The angular standard deviations σ'_A and σ'_E within sublayer k can then be estimated respectively as $\sigma_v/\overline{u}_k$ and $\sigma_w/\overline{u}_k$, where $\overline{u}_k$ is the mean wind speed in the sublayer. Such an approach would at least have some basis in theory, would be more general, and would more naturally account for variations in height and surface roughness.

To use a similarity based model for σ_v and σ_w in REEDM, the friction velocity u_* and Monin-Obukhov length L must be estimated. This can be done using wind and temperature profiles from towers (*e.g.*, Berkowicz and Prahm, 1982) or using surface energy budgets (van Ulden and Holtslag, 1985). Of course, direct measurements of σ_v and σ_w (or σ'_A and σ'_E) are always preferred over the climatological estimates discussed here. Such measurements are now quite feasible using three-dimensional sonic anemometers.

Another problem with the climatological procedure used by REEDM is that the same power-law formulas [Eqs. (84) and (85) in the UM] are used for all heights up to 100 m AGL. This implies that the atmospheric surface layer is always about 100 m deep. A surface-layer depth of 100 m is fairly reasonable for daytime conditions, but nighttime surface layers are usually much shallower. Moreover, it makes more sense to use the mixing layer depth H_m, which is already computed in REEDM, to estimate the surface-layer depth. The top of the surface layer is usually taken to be at $0.1H_m$.

The climatological procedure initially produces estimates of σ'_A and σ'_E that are valid for a roughness length z_o of 10 cm. To adjust for different values of z_o, REEDM assumes, according to Eqs. (82) and (83) of the UM, that $\sigma'_A \propto z_o^{0.2}$ and $\sigma'_E \propto z_o^{0.15}$. From surface-layer similarity in neutral conditions, it is easy to show that

$$\begin{aligned} \sigma'_A &= \frac{C_2 k_a}{\ln(z/z_o)} , \\ \sigma'_E &= \frac{C_3 k_a}{\ln(z/z_o)} , \end{aligned} \qquad \text{(R6)}$$

where k_a is the von Kármán constant, z is height, and C_2 and C_3 are other empirical constants. The proper multiplication factor to account for the surface roughness is thus $\ln(z/10\,\text{cm})/\ln(z/z_o)$ for both σ'_A and σ'_E. This would suggest that the power laws in Eqs. (82) and (83) should be the same. (Of course, the factor $\ln(z/10\,\text{cm})/\ln(z/z_o)$ could be used in place of the power laws, since it is consistent with surface-layer similarity.)

In Eq. (92) of the UM, the horizontal standard deviation σ'_A is adjusted to account for the time t_s required for the ground cloud to reach its stabilization height. This adjustment does not make sense. REEDM uses two phases to describe the diffusion of the ground cloud: a buoyant-rise phase and a passive-diffusion phase. The turbulence parameter σ'_A is used to quantify the ambient turbulence during the second phase. There is no reason why it should depend on t_s. After all, the level of ambient turbulence will be the same whether t_s is 90 s or 180 s. The t_s adjustment is apparently designed to increase the effective sampling time τ of σ'_A from its initial value of 600 s.

Determining the effects of the sampling time on turbulent diffusion is a complicated issue (Eckman, 1994), but a simple estimate for the proper value of τ for REEDM can be obtained by considering the size of the stabilized ground cloud. Initially, the cloud has a horizontal radius of about 1 km, and turbulent diffusion over a downwind distance of 30 km could increase the horizontal size to something on the order of 5–10 km. The sampling time used for σ'_A should therefore at least be long enough to include the effects of turbulent eddies with length scales of 5-10 km. For a wind speed of $5\,\text{m}\,\text{s}^{-1}$, this requires a sampling time of about 30 min.

At the top of p. 58 in the UM, it is stated that the mixing-layer depth H_m can be optionally adjusted upward if H_m is less than the stabilized height z_s of the ground cloud. The adjustment ensures that H_m is greater than z_s. This adjustment of H_m may be useful for investigating "worst-case" dispersion scenarios, but it has no physical justification. Since z_s is a characteristic of the ground cloud and H_m is a characteristic of the ambient atmosphere, there is no reason to believe that H_m depends on z_s (although z_s can depend on H_m). The adjustment to H_m therefore should not be made on a routine basis.

3.2.9. *Dosage and Concentration Computations*

REEDM uses UM Eq. (103) to estimate the dosage due to the portion of the cloud in sublayer k. Unfortunately, no derivation or references are given for this equation. To obtain this equation, it is necessary to assume an instantaneous release of cloud material in sublayer k with a bivariate Gaussian distribution in the horizontal and a uniform distribution in the vertical. A partial-reflection approach with partial reflection coefficient γ_j (the subscript j representing one of the acid-drop size categories) is used to account for surface deposition. In computing the dosage from this instantaneous release, it is assumed that the cloud advects past the downwind point x at a constant, layer-average speed $\overline{u}_L$ and that the cloud's standard deviation σ_{xL} in the alongwind direction does not vary much during the cloud's passage at x.

Equation (103) in the UM contains a number of inconsistencies. A factor of $\overline{u}_L$ should appear in the denominator, although this is apparently just a typographical error (Bowers, 1995, personal communication). Since the equation contains the coefficient γ_j, it can apparently be used for either the gaseous or acid-drop portions of the cloud. But the variable $F\{k\}$ only represents the gaseous mass. (It is not a fraction, as erroneously stated on UM p. 67.) For application to HCl drops in size category j, $F\{k\}$ should be replaced by the product $M\{\mathrm{H_2O, HCl}\}F_j(k)$. To make the situation more complicated, the evaporation of the HCl drops must be considered. This means that both the drop mass $M\{\mathrm{H_2O, HCl}\}F_j(k)$ and the settling velocity V_j are not constant. Another inconsistency is that a tilted cloud centerline is not included in UM Eq. (103), whereas it does appear in Eq. (115).

Although we were aware of the basic assumptions involved in the derivation of UM Eq. (103), we were still not able to obtain all of the reflection terms. There were sign differences between our reflection terms and those in Eq. (103), with our results having better agreement with Healy (1968). Our results also did not contain the $\pm 2z_{BL}$ that appears in several of the terms in Eq. (103). These differences need to be investigated further if the dosage estimates are to be relied on.

The partial reflection coefficient γ_j is computed using Eq. (104) in the UM. No explanations or references are given as to where this equation came from. The upper and lower limits for V_j in the second case on the right side of this equation should be interchanged.

In the definition of x_{rz} on UM p. 67, a "vertical point source" is mentioned. We assume this should be "virtual point source", as is the case in the definition of x_{ry}.

UM Eq. (106) for the lateral standard deviation σ_{yL} uses the outdated concept of a virtual point source to account for the effects of the initial cloud size. With this concept, the diffusion of a cloud with a finite initial size σ_{yo} is assumed to be equivalent to that of a point source located some distance x_v upwind of the real source. The distance x_v is adjusted so that the virtual cloud has the lateral width σ_{yo} at the location where the real cloud is released. Although the virtual-source concept may have had some utility in the past, it is physically incorrect because it assumes that turbulent diffusion is a Markov process (*i.e.*, it has no "memory"). Since turbulent diffusion is not generally Markovian, the diffusion of the virtual source is not the same as that of the real source. In the near field, for example, the virtual-source concept gives the expression

$$\sigma_{yL} = \sigma'_{AL} x + \sigma_{yo} \, . \tag{R7}$$

It can be shown from basic diffusion theory (*e.g.*, Pasquill and Smith, 1983) that the correct equation for near-field diffusion is

$$\sigma_{yL} = \sqrt{{\sigma'_{AL}}^2 x^2 + \sigma_{yo}^2} \, . \tag{R8}$$

The cloud diffuses less rapidly with Eq. (R8), because the fluid particle velocities are correlated over time.

The first term on the right side of UM Eq. (107) is missing a factor of α.

To calculate the peak concentration, REEDM must estimate the cloud standard deviation σ_{xL} in the alongwind direction. Equations (111) and (112) in the UM indicate that σ_{xL} is assumed to be affected by the vertical wind-speed shear $\Delta\overline{u}_L$ but not by the ambient turbulence. The failure to include the effect of turbulence means that σ_{xL} will be underestimated by REEDM in most situations, resulting in an overestimate of concentration. A simple remedy for this problem, which is used in most puff models, is to assume that the growth of σ_{xL} due to turbulence is the same as the growth of σ_{yL}; the values of σ_{xL} and σ_{yL} may still differ as a result of wind-speed and direction shear. The discussion in Appendix A provides another approach for estimating σ_{xL} that can account for both turbulence and wind-speed shear.

The parameterization of wind-speed shear given by UM Eq. (112) is based on the work of Saffman (1962) and Tyldesley and Wallington (1965). To obtain this result, it is necessary to assume that the vertical eddy diffusivity is constant with height and that the wind speed varies linearly with height. Moreover, the effect of turbulent diffusion in the downwind direction is neglected. These assumptions are not very representative of flow near the earth's surface (especially in a coastal environment or over complex terrain), so it is not clear whether Eq. (112) is a good parameterization of the effects of speed shear.

The constant 0.28 in UM Eq. (112) results from the assumption that the cloud diffusion occurs near the surface. For a release into a free-shear layer with no boundaries (*i.e.*, well above the surface), the work by Smith (1965) indicates that a constant of 0.58 should be used instead of 0.28. Since the ground cloud from a rocket launch can rise to quite high altitudes, the free-shear constant may be more realistic. Interestingly, some field experiments conducted in the 1970s indicated that a constant of 0.6 fit the diffusion measurements better than 0.28 (see Appendix A). Since these experiments used surface releases, the larger constant was interpreted as resulting from the effect of turbulence. Still, it is interesting that the purely theoretical constant of 0.58 obtained by Smith (1965) for free-shear layers is close to the empirically derived value of 0.6.

The variable Φ in UM Eq. (112) is used to distinguish between two of the cases. This variable is not defined and is not included in the List of Symbols. From the context, we can infer that Φ is the potential temperature, although θ^* is used to denote virtual potential temperature on p. 16 of the UM.

The approach that REEDM uses to account for wind shear in UM Eqs. (106) and (111) is unrealistic when the directional shear is large. These equations have a basic inconsistency in that σ_{xL} and σ_{yL} are defined in rectangular Cartesian coordinates, whereas the wind shear is specified in polar coordinates. A more consistent approach is to specify the wind shear in rectangular Cartesian coordinates, so that σ_{xL} is affected by the vertical shear of the alongwind component u, and σ_{yL} is affected by the shear of the crosswind component v. Consider a scenario in which a wind-direction reversal occurs in Major Layer 1. This reversal leads to a large shear in u but little or no shear in v. Hence, the direction reversal should enhance the alongwind diffusion σ_{xL} while having little effect on σ_{yL}. The response of REEDM to this scenario is unrealistic, since the directional shear of 180° is used in UM Eq. (106) to enhance the crosswind diffusion.

3.2.10. *Deposition Computations*

It would have been helpful to have some explanation and intermediate steps leading to UM Eq. (115) for the deposition. We could not derive many of the terms in this equation. It was difficult for us to determine whether the differences between our results and Eq. (115) were due to errors or to unspecified assumptions. Another confusing aspect of Eq. (115) is that the mass $F\{k\}$ of gaseous material is used instead of the mass $M\{H_2O, HCl\}F_j(k)$ of HCl drops. Since REEDM allows deposition only by gravitational settling and washout, the gaseous mass $F\{k\}$ should not influence the deposition.

The present deposition approach in REEDM ignores deposition by mechanisms such as turbulent and Brownian diffusion, chemical adsorption, inertial impaction, and thermal and electrical processes. Turbulent transfer, which is the dominant deposition mechanism for gases and small droplets, can be usually accounted by deriving the deposition algorithms in terms of a deposition velocity which incorporates both gravitational and nongravitational contributions. See Rao (1981) for details. The treatment of deposition is an area in which REEDM can be improved.

Although REEDM supposedly can only account for deposition by gravitational settling and washout, we discovered that an absorption coefficient for gases can be provided to REEDM as an input parameter (UM, p. 99). This coefficient, which varies from 0 to 1, clearly represents a simple parameterization of dry deposition for gases. We could find no description in the UM of how this coefficient is used in the concentration and deposition equations.

3.2.11. *Wind-Field Model*

In section 5.1 of the UM, a wind-field model based on the so-called shallow-water equations is described. The top of the mixing layer is assumed to be the interface between higher density air below and lower density air above. Apparently, warmer air from the upper layer cannot be entrained into the lower layer, so the interaction of the upper layer with the lower layer is limited to reducing gravity waves in the lower layer. Since the UM does not cite any comparisons of this model with wind observations in complex terrain, it is not clear how well this approach works. If this approach is to be retained in REEDM, it needs to be tested more thoroughly with field measurements.

The shallow-water equations used in REEDM require the hydrostatic assumption, so the resulting winds are valid only when the variations in terrain elevation have horizontal length scales much larger than the mixing-layer depth H_m. For a mixing-layer depth in stable conditions of, say, 100 m, the model will only apply to terrain variations having length scales of roughly a kilometer or more. At Vandenberg Air Force Base, the wind-field model may not properly account for smaller scale terrain features having length scales of a kilometer or less. The model is also likely to become progressively less useful for terrain length scales greater than 20–30 km because it lacks the Coriolis force (*e.g.*, Peng *et al.*, 1995). Thus, the model is likely to be applicable for terrain length scales between roughly one kilometer and a few tens of kilometers when H_m is about 100 m.

On UM p. 75, an adjustment procedure is described for cases when the calculated mixing layer depth is less than 30 m. The model arbitrarily resets the u and v components to zero and the layer depth to 30 m. It was concluded that "wind fields in the immediate vicinity of higher elevations under these conditions appear to be reasonable." This is a qualitative statement that needs to be supported with a quantitative evaluation of the wind-field model.

It is not clear how the wind-field model described in Section 5 of the UM is integrated with the diffusion algorithms in REEDM. Both UM Eq. (103) for the dosage and UM Eq. (115) for the deposition implicitly assume that the puffs are moving in straight lines with the speed $\overline{u}_L$. If the wind-field model causes the puffs to deviate from constant straight-line motion, then it seems that Eqs. (103) and (115) would no longer be valid. This potential inconsistency with the wind-field model is not addressed in the User's Manual, and no alternatives to Eqs. (103) and (115) are provided for cases when the transport is not along straight lines.

4. REEDM Sensitivity to Meteorological Input Data

A sensitivity study seeks to determine the changes in model output due to variations in model input values. We chose to vary only one input parameter at a time while holding the others fixed. REEDM is designed to use tower and sodar turbulence measurements if they are available. These measurements are used in the model to calculate the dispersion rate of the stabilized ground cloud. Vandenberg Air Force Base currently uses REEDM in this measured-turbulence mode. If tower and sodar turbulence measurements are not available, REEDM makes climatological estimates of the wind-direction standard deviations σ'_A and σ'_E based on wind speed and solar radiation. This climatological-turbulence mode of REEDM is currently used at the Cape Canaveral Air Station. In our study, we examined the sensitivity of REEDM to both modes of turbulence estimation. Differences were observed in the sensitivity of the two modes.

4.1. Meteorological Input Variables

To estimate atmospheric conditions during a rocket-vehicle launch, REEDM uses rawinsonde profiles of wind speed and direction, temperature, and pressure. Mixing-layer depths are either calculated using the rawinsonde temperature profile or provided manually by the user. We have found that manually specifying the mixing depth is more reliable. The UM also strongly recommends that the mixing depth be manually specified. If the climatological-turbulence mode of REEDM is used, cloud cover and ceiling height must also be specified in the input data. Otherwise, tower and sodar measurements of the velocity standard deviations σ_v and σ_w must be provided in the REEDM input.

By adjusting various quantities in the REEDM input data, we tested the sensitivity of REEDM to the following variables:

1. Wind speed
2. Wind-speed shear

3. Wind-direction shear
4. Boundary-layer lapse rate
5. Surface-layer stability
6. Mixing-layer depth
7. Cloud cover and ceiling (climatological-turbulence mode)
8. Boundary-layer turbulence (measured-turbulence mode)

For the first six of these variables, the model sensitivity was tested by developing a series of idealized rawinsonde profiles. A control profile was established, and single elements of this profile (such as wind speed, wind direction, or temperature) were changed to create new profiles, which were then used in the sensitivity runs. The control rawinsonde profile had the following features:

1. Constant wind speed of $5\,\mathrm{m\,s^{-1}}$
2. Constant wind direction of 270°
3. Unstable surface layer extending to 91 m AGL with the vertical temperature gradient dT/dz determined from surface-layer similarity using a Monin-Obukhov length of −40 m
4. Neutrally stratified well-mixed layer from 91 to 1554 m AGL with $dT/dz = -9.77°\mathrm{C\,km^{-1}}$ (adiabatic lapse rate)
5. Capping inversion from 1554 to 1737 m AGL with $dT/dz = 0.0°\mathrm{C\,km^{-1}}$
6. Free troposphere lapse rate from 1737 to 3627 m AGL with $dT/dz = -6.5°\mathrm{C\,km^{-1}}$
7. Turbulence parameterization
   a) Climatological-turbulence mode: clear skies
   b) Measured-turbulence mode: $\sigma'_A = 0.2\,\mathrm{rad}$, $\sigma'_E = 0.12\,\mathrm{rad}$
8. Launch time: 24 May 1995, 1400 LST
9. Normal launch of a Titan IV rocket; HCl plume considered

Table 1 lists the test runs used in the sensitivity calculations. Runs A through E explored variations in stability of the surface and mixing layers. For brevity we call Run B a stable mixing layer even though the stable stratification would tend to suppress vertical mixing. Run E was designed to investigate how sensitive the model is to a combination of Runs A and D, but it has no physical significance regarding real-world temperature profiles. Runs F and G adjusted the layer-average wind speed $\overline{u}_L$ in Major Layer 1. For testing wind-speed shear, Runs H through J used a linearly increasing wind

Table 1. REEDM runs that were used to evaluate model sensitivity. All the model input variables were the same as in the control run except for the modified values listed in the third column.

Run	Description	Modified values
A	Stable surface layer	$dT/dz = -4.77°\mathrm{C\,km^{-1}}$ from 0–91 m
B	Stable mixing layer	$dT/dz = -8°\mathrm{C\,km^{-1}}$ from 91–1554 m
C	Stable boundary layer	Combination of A and B
D	Unstable mixing layer	$dT/dz = -11°\mathrm{C\,km^{-1}}$ from 91–1554 m
E	Stable surface layer with unstable mixing layer	Combination of A and D
F	Low wind speed	$\overline{u}_L = 1\,\mathrm{m\,s^{-1}}$
G	High wind speed	$\overline{u}_L = 10\,\mathrm{m\,s^{-1}}$
H	Wind speed shear	$\Delta\overline{u}_L = 4\,\mathrm{m\,s^{-1}}$ from 0–1554 m
I	Wind speed shear	$\Delta\overline{u}_L = 8\,\mathrm{m\,s^{-1}}$ from 0–1554 m
J	Wind speed shear	$\Delta\overline{u}_L = 16\,\mathrm{m\,s^{-1}}$ from 0–1554 m
K	Wind direction shear	$\Delta\theta_L = 20°$ from 0–1554 m
L	Wind direction shear	$\Delta\theta_L = 40°$ from 0–1554 m
M	Wind direction shear	$\Delta\theta_L = 80°$ from 0–1554 m
N	Low mixing depth	$H_m = 1000\,\mathrm{m}$
O	High mixing depth	$H_m = 2000\,\mathrm{m}$
P	Low cloud ceiling	Ceiling = 1600 m, Cloud cover = 6/10
Q	Low cloud ceiling	Ceiling = 1600 m, Cloud cover = 10/10
R	High cloud ceiling	Ceiling = 3200 m, Cloud cover = 6/10
S	High cloud ceiling	Ceiling = 3200 m, Cloud cover = 10/10
T	Low turbulence	$\sigma'_A = 0.1\,\mathrm{rad}$, $\sigma'_E = 0.06\,\mathrm{rad}$
U	High turbulence	$\sigma'_A = 0.4\,\mathrm{rad}$, $\sigma'_E = 0.24\,\mathrm{rad}$

speed given by

$$\overline{u}(z) = 5\,\mathrm{m\,s^{-1}} + \Delta\overline{u}_L \left[\frac{z - H_m/2}{H_m}\right] , \qquad \text{(R7)}$$

where H_m is the height of the mixing layer, and $\Delta\overline{u}_L$ is the total change in wind speed from the ground to the top of the mixing layer. Equation (R7) keeps the average wind speed in the mixing layer at $5\,\mathrm{m\,s^{-1}}$, which is the same as in the control run. When $\Delta\overline{u}_L$ exceeds $10\,\mathrm{m\,s^{-1}}$, Eq. (R7) produces negative wind speeds near the surface. This only occurs for Run J, and is interpreted as a wind-direction reversal, so that the mean wind speed in the mixing layer remains at $5\,\mathrm{m\,s^{-1}}$. Above H_m, the wind speed was held constant at the value $\overline{u}(H_m)$.

For testing wind-direction shear (Runs K, L, and M), the wind direction was changed linearly with height between $270° - \Delta\theta_L/2$ at the ground to $270° + \Delta\theta_L/2$ at the top of the mixing layer, with $\Delta\theta_L$ representing the total change in wind direction within the mixing layer. The mean transport wind direction was 270°.

4.2. Output Variables

There are many variables in REEDM that could potentially be considered in a sensitivity analysis. To keep the analysis manageable, we selected the following key variables for examination:

1. Exhaust cloud stabilization height z_s
2. Peak surface concentration C_{peak} of HCl
3. Downwind distance D_{peak} to C_{peak}
4. Maximum 30-minute-average surface concentration C_{avg}
5. Downwind distance D_{avg} to C_{avg}
6. Layer-average turbulence parameters σ'_{AL} and σ'_{EL}

In assessing the sensitivity of the concentrations C_{peak} and C_{avg} in REEDM, it is important to also consider the downwind distances D_{peak} and D_{avg} at which these concentrations occur. Consider as an example a situation in which a change in a single input variable can double the value of D_{peak} while leaving C_{peak} unaffected. Clearly, this has important consequences for public safety, even though the value of C_{peak} is not sensitive to this particular input variable.

4.3. Results

The results of the sensitivity tests are presented in Tables 2 and 3 as normalized values relative to the control-run output (e.g., C_{peak} for run A divided by C_{peak} for the control run). Values close to unity indicate little change from the control run, and we interpret this as low sensitivity. "CLIM" indicates runs that used the climatological-turbulence mode of REEDM, and "MEAS" indicates those that used the measured-turbulence mode.

4.3.1. *Stabilization Height*

The stabilization height z_s computed for the control run was 1452 m. From Runs B, C, D, and E in Table 2, it is clear that z_s is sensitive to the thermal stratification in the mixing layer. This is to be expected, since in REEDM the cloud rise for a normal

Table 2. Results of the REEDM model sensitivity analysis for surface concentrations, downwind distances, and cloud stabilization height. For each variable, the ratio of the value obtained for a particular run to the value obtained for the control run is given.

	Ratio								
	C_{peak}		D_{peak}		C_{avg}		D_{avg}		z_s
Run	CLIM	MEAS	CLIM	MEAS	CLIM	MEAS	CLIM	MEAS	
A	0.98	0.98	1.00	1.00	0.98	0.98	1.00	1.00	1.00
B	2.29	2.29	0.82	0.83	1.80	1.80	0.91	0.92	0.75
C	2.31	2.30	0.82	0.83	1.80	1.78	0.91	0.92	0.75
D	0.56	0.56	1.00	1.00	0.62	0.62	1.09	1.08	1.20
E	0.55	0.55	1.00	1.00	0.61	0.61	1.09	1.08	1.21
F	0.81	1.00	0.73	0.75	3.91	4.81	0.73	0.83	1.00
G	1.00	1.00	1.27	1.17	0.50	0.49	1.36	1.25	1.00
H	0.88	0.96	1.18	1.00	0.92	0.99	1.27	1.00	1.00
I	0.55	0.87	1.82	1.00	0.79	0.98	2.18	1.08	1.00
J	0.63	0.71	0.91	1.00	0.81	1.00	1.00	1.08	0.99
K	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
L	0.98	0.99	1.00	1.00	1.00	1.01	1.00	1.00	1.00
M	0.93	0.94	1.00	0.92	1.02	1.03	1.00	1.00	1.00
N	1.61	1.64	0.64	0.67	1.22	1.25	0.73	0.67	0.78
O	0.71	0.71	1.18	1.25	0.84	0.83	1.27	1.25	1.17
P	0.91	–	1.82	–	0.91	–	1.82	–	1.00
Q	1.01	–	2.18	–	1.01	–	2.27	–	1.00
R	1.01	–	1.09	–	1.01	–	1.09	–	1.00
S	1.01	–	1.09	–	1.01	–	1.09	–	1.00
T	–	1.01	–	1.67	–	1.01	–	1.75	1.00
U	–	1.00	–	0.58	–	0.99	–	0.58	1.00

Table 3. Results of the REEDM model sensitivity analysis for σ'_{AL} and σ'_{EL}. For each variable, the ratio of the value obtained for a particular run to the value obtained for the control run is given.

	Ratio			
	σ'_{AL}		σ'_{EL}	
Run	CLIM	MEAS	CLIM	MEAS
A	1.01	1.01	1.00	1.00
B	0.95	0.96	1.00	1.00
C	0.97	0.96	1.00	1.00
D	1.02	1.02	1.00	1.00
E	1.03	1.03	1.00	1.00
F	1.45	1.00	1.11	1.00
G	0.88	1.00	0.89	1.00
H	0.85	0.98	0.76	0.98
I	0.52	0.97	0.39	0.97
J	1.50	0.97	1.15	0.97
K	1.00	1.00	1.00	1.00
L	1.00	1.00	1.00	1.00
M	1.00	1.00	1.00	1.00
N	1.01	1.03	1.04	1.08
O	1.06	1.05	1.03	1.00
P	0.52	–	0.46	–
Q	0.37	–	0.38	–
R	0.87	–	0.89	–
S	0.87	–	0.89	–
T	–	0.51	–	0.52
U	–	1.99	–	1.98

launch is mainly a function of the ambient temperature profile and propellant heat content. The mixing-layer stratifications specified in cases B through E are fairly weak, representing a change in potential temperature of $+1.77°\mathrm{C\,km^{-1}}$ in cases B and C, and $-1.23°\mathrm{C\,km^{-1}}$ in cases D and E. However, these stratifications changed z_s by 20–25%.

The stabilization height is also sensitive to changes in the mixing depth (Runs N and O). For these runs, the height of the capping inversion in the control profile was adjusted to correspond to the value of H_m given in Table 1. This inversion is fairly effective in halting the buoyant rise of the cloud, so z_s tends to move in tandem with H_m.

4.3.2. *Peak Surface Concentration and Downwind Distance*

The results in Table 2 for C_{peak} and D_{peak} are presented graphically in Figs. 1 and 2 as percentage changes from the control run. To understand some of the sensitivities in these figures, it is useful to consider a simple model in which the part of the stabilized ground cloud within the boundary layer is represented as a three dimensional Gaussian puff with σ_x, σ_y, and σ_z representing the respective standard deviations in the alongwind, crosswind, and vertical directions. The puff's center is at an elevation h ($\approx z_s$) above the ground. If the ratios σ_x/σ_z and σ_y/σ_z are assumed to be constant with downwind distance [an assumption which has frequently been invoked (e.g., Panofsky and Dutton, 1984, p. 237) to estimate maximum concentrations], it can be shown from the Gaussian puff equation that C_{peak} will occur at the downwind distance for which $\sigma_z = h/\sqrt{3}$. Hence, C_{peak} for this Gaussian puff will follow the proportionality

$$C_{peak} \propto \frac{1}{\sigma_x \sigma_y h} . \qquad \text{(R9)}$$

This equation is valid at the downwind distance D_{peak}, so we can assume that $\sigma_y \approx \sigma'_{AL} D_{peak}$. In REEDM, the alongwind diffusion σ_x is assumed to remain constant at its initial value σ_{xo} unless the wind-speed shear $\Delta\overline{u}_L$ is nonzero. For no wind-speed shear, we can therefore write Eq. (R9) as

$$C_{peak} \propto \frac{1}{\sigma_{xo} \sigma'_{AL} D_{peak}\, h} , \qquad \text{(R10)}$$

whereas for cases with wind-speed shear we can write

$$C_{peak} \propto \frac{\overline{u}_L}{\Delta\overline{u}_L\, \sigma'_{AL} D^2_{peak}\, h} . \qquad \text{(R11)}$$

This latter equation uses the relation $\sigma_x \propto \Delta\overline{u}_L D_{peak}/\overline{u}_L$, which is based on Eqs. (111) and (112) in the UM.

If we make the simple assumption that $\sigma_z \approx \sigma'_{EL} D_{peak}$ at the point where the peak concentration occurs, the condition $\sigma_z = h/\sqrt{3}$ leads to the expression

$$D_{peak} \approx \frac{h}{\sqrt{3}\, \sigma'_{EL}} . \qquad \text{(R12)}$$

REEDM's treatment of the stabilized ground cloud is much more complicated than the simple assumptions used to obtain Eqs. (R9)–(R12), but these equations are still useful for interpreting some of the results of the sensitivity analysis. In applying these equations, it should be noted that they apply only to the portion of the ground cloud that can be mixed down to the surface. Hence, h may not be the same as the stabilization height z_s if much of the ground cloud is above the top of the mixing layer.

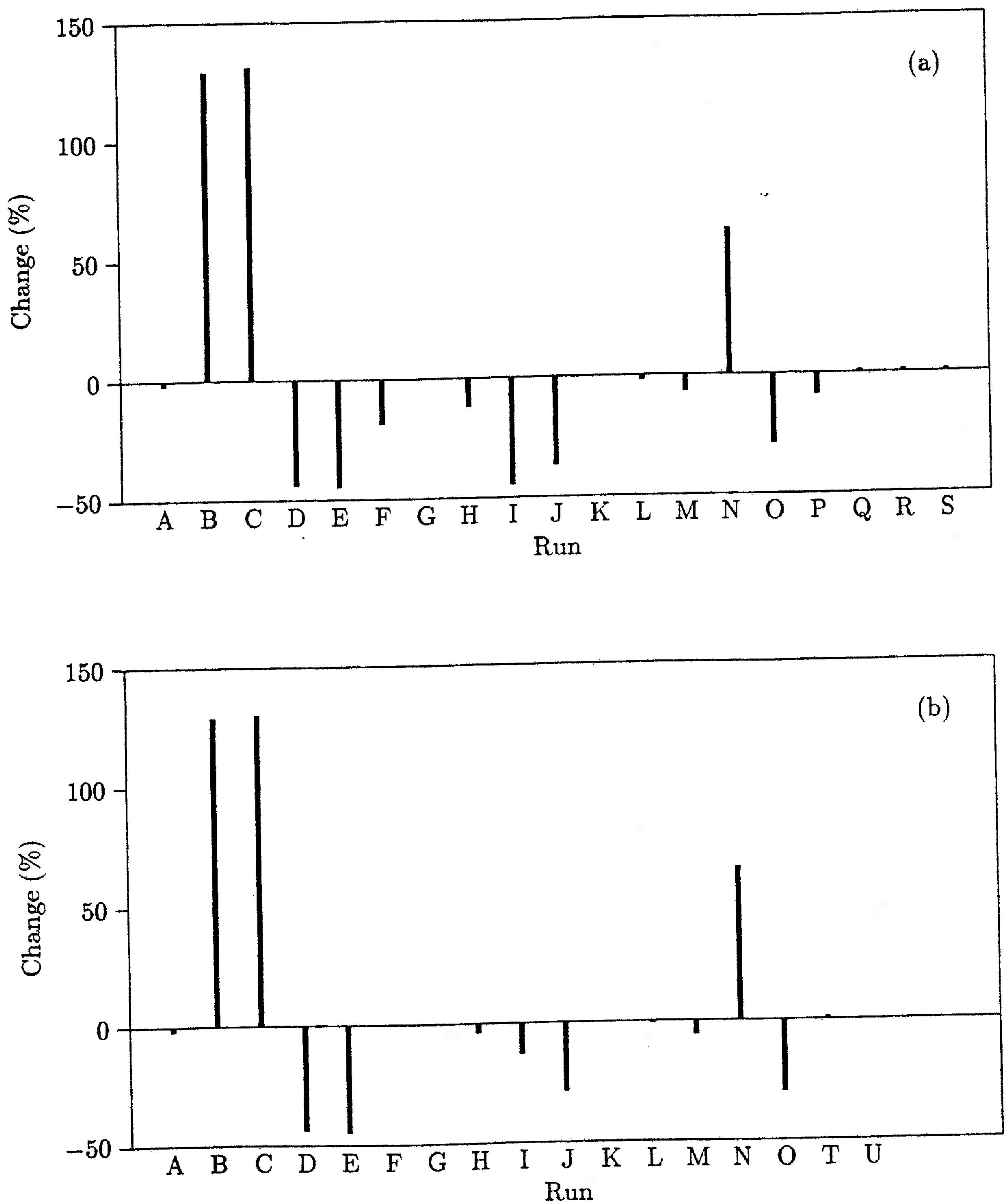

Figure 1. Variation of the peak concentration C_{peak} for each of the REEDM sensitivity runs. The values are plotted as percentage changes from the control run. (a) is for the CLIM runs, and (b) is for the MEAS runs.

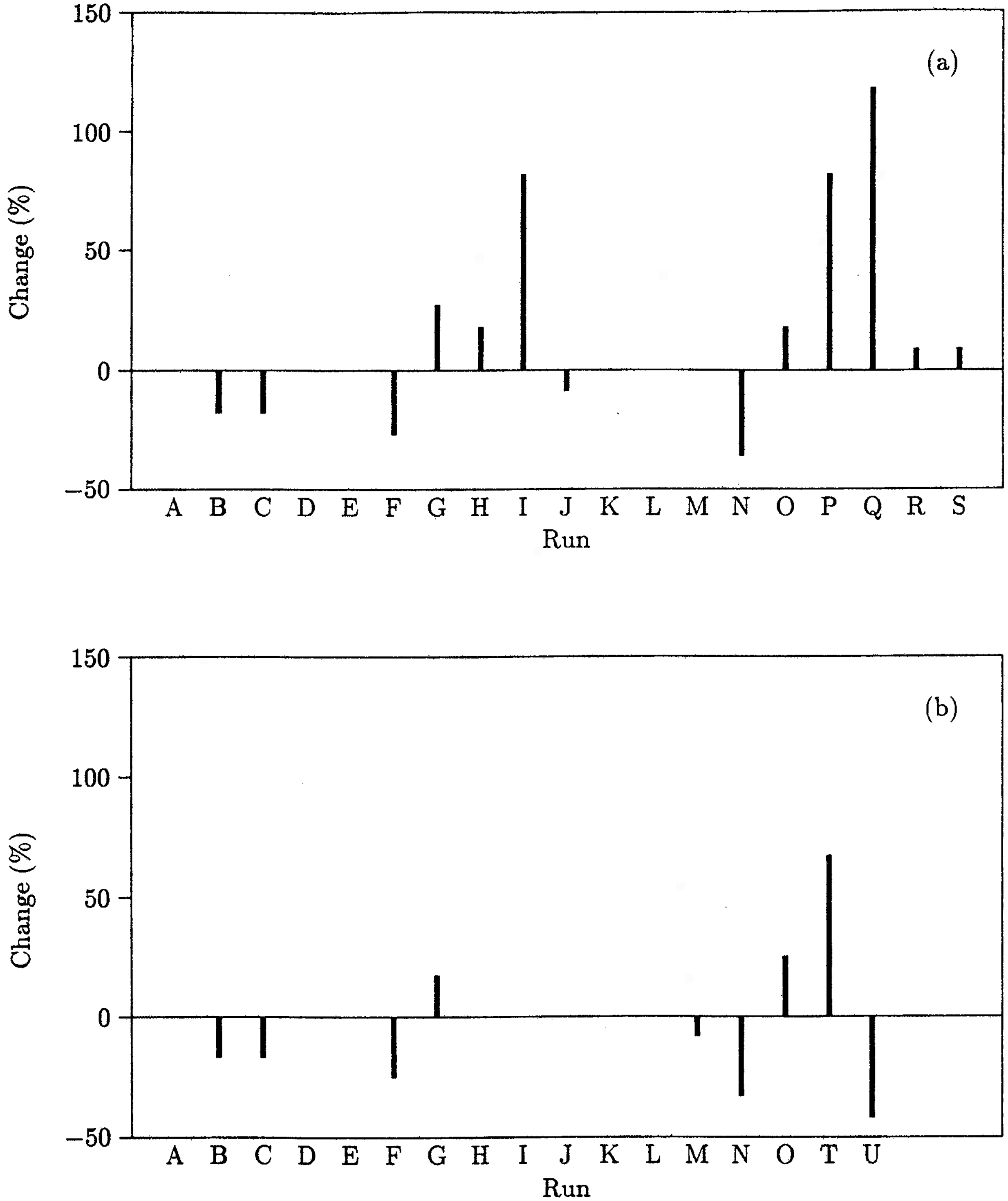

Figure 2. Variation of the downwind distance D_{peak} to the peak concentration C_{peak} for each of the REEDM sensitivity runs. The values are plotted as percentage changes from the control run. (a) is for the CLIM runs, and (b) is for the MEAS runs.

It is clear from Fig. 1 that the peak concentration computed by REEDM is sensitive to changes in the mixing-layer temperature profile, Runs B, C, D and E. This sensitivity is due to the effect of the temperature profile on the stabilization height z_s. For Runs B and C, z_s is smaller than in the control run, and from Eq. (R10) we would expect h to be smaller and the peak concentration to be higher. For Runs D and E, z_s and h are larger and the peak concentrations are smaller. Equation (R12) indicates that D_{peak} should also show significant sensitivity to the mixing-layer stability, but this is not the case in Fig. 2. This is because the mixing-layer stability in Runs B through E also affected the initial size of the ground cloud. In Runs B and C, the initial vertical dimension of the ground cloud is about 24% smaller than in the control run, and it is about 19% larger in Runs D and E. These differences in the initial size of the stabilized cloud are due to Eq. (30) in the UM, which requires the cloud radius after stabilization to be directly proportional to z_s.

In the derivation of Eq. (R12), we did not account for the initial value σ_{zo} of σ_z. If we assume that σ_z at the downwind distance D_{peak} is approximated by $\sigma_z^2 \approx \sigma_{zo}^2 + {\sigma'_{EL}}^2 D_{peak}^2$, then Eq. (R12) can be replaced with

$$D_{peak} \approx \frac{1}{\sigma'_{EL}} \sqrt{\frac{h^2}{3} - \sigma_{zo}^2}\,. \qquad \text{(R13)}$$

For Runs B through E, this equation indicates that the effect of h on D_{peak} is offset to some extent by the effect of σ_{zo}, making D_{peak} less sensitive to changes in the temperature profile than C_{peak}.

The H and I CLIM runs in Fig. 1 show a stronger sensitivity to wind-speed shear than the corresponding MEAS runs. In both the CLIM and MEAS runs, the wind-speed shear $\Delta\overline{u}_L$ increases the ground cloud's alongwind diffusion. As indicated by Eq. (R11), the speed shear should reduce C_{peak}. But for the CLIM runs, the speed shear also has a strong affect on the turbulence parameters σ'_{AL} and σ'_{EL}, as can be seen in Table 3. From Eq. (R12), we see that the smaller values of σ'_{EL} in the CLIM runs should significantly increase D_{peak}, and this is just what is observed for the H and I CLIM runs in Fig. 2. The increases in D_{peak} will magnify the effects of the speed shear in Eq. (R11), which explains why the H and I CLIM runs show more sensitivity than the corresponding MEAS runs.

The J CLIM run, which is the run with the most wind-speed shear, does not have quite the same behavior as Runs H and I in Figs. 1 and 2. This run has a smaller value of D_{peak} than the control run, and the decrease in C_{peak} is somewhat less than in CLIM Run I. Run J behaves differently because the wind-speed shear is large enough to cause a wind-direction reversal within the mixing layer. At the height where this flow reversal occurs, the wind speed is small, and the climatological turbulence algorithm in REEDM computes large values of σ'_A and σ'_E at this height. The high level of turbulence near the flow-reversal height is enough to increase the layer-average parameters σ'_{AL} and σ'_{EL}, as seen in Table 3. D_{peak} is therefore reduced in CLIM Run J as a result of the larger value of σ'_{EL}. According to Eq. (R11), a reduction in D_{peak} tends to offset any increases in $\Delta\overline{u}_L$ and σ'_{AL}, so that C_{peak} is not reduced as much in CLIM Run J as it is in Run I. The aberrant behavior of CLIM Run J indicates that the climatological turbulence algorithm in REEDM may have problems when a flow reversal is present.

A reduction in the mixing-layer depth (Run N) results in larger peak concentrations and smaller values of D_{peak}. The opposite behavior is observed for Run O. These results are in agreement with Eqs. (R10) and (R12), considering that the effective cloud height h is smaller in Run N and larger in Run O. The value of C_{peak} shows somewhat greater sensitivity to the mixing-layer depth than D_{peak}, because it is inversely proportional to both h and D_{peak} in Eq. (R10).

The value of C_{peak} shows moderate sensitivity to low wind speeds in CLIM Run F. The reason for this is not entirely clear. Because of the lower wind speed, the CLIM estimates of σ'_{AL} and σ'_{EL} are larger than those for the control run (Table 3). Hence, a smaller value of D_{peak} is expected from Eq. (R12) and is observed in Fig. 2a. In Eq. (R10), however, the effect of an enhanced value of σ'_{AL} should be largely offset by the smaller value of D_{peak}. It is possible that the gravitational settling of HCl droplets is affecting the results in Run F. This settling is not accounted for in the simple derivation of Eqs. (R9)–(R12). Settling may also account for the sensitivity of D_{peak} to wind speed in MEAS Runs F and G. Since σ'_{EL} is unaltered in these MEAS runs, Eq. (R12) indicates D_{peak} should not change. But in Fig. 2, the sensitivity of D_{peak} in MEAS Runs F and G is about the same as that in the corresponding CLIM runs.

The CLIM values of D_{peak} are highly sensitive to cloud cover when the cloud ceiling is at 1600 m AGL (Runs P and Q in Fig. 2a). When the cloud ceiling is lower than 2134 m AGL and the cloud cover is greater than 5/10, REEDM reduces the net radiation index used in the computation of σ'_{AL} and σ'_{EL}. A reduction of σ'_{EL} leads to an increase in D_{peak}, which is what is observed in Fig. 2a. The values of C_{peak} are not altered much in Runs P and Q, because the decreased values of σ'_{AL} in Eq. (R10) are offset by the increased values of D_{peak}.

Runs T and U in Fig. 2b indicate that D_{peak} is sensitive to the measured level of turbulence. This is in agreement with Eq. (R12), where D_{peak} is inversely proportional to σ'_{EL}. The values of C_{peak} for Runs T and U are very close to the control value, since the variations of σ'_{AL} in Eq. (R10) are offset by the variations in D_{peak}.

Both C_{peak} and D_{peak} are relatively insensitive to the wind-direction shear in Runs K, L, and M. This is surprising, since the 80° directional shear in Run M should, according to Eq. (106) in the UM, diffuse the cloud horizontally about as effectively as a turbulence level of $\sigma'_{AL} = 0.32\,\mathrm{rad}$. When looking more closely at the output of REEDM for Run M, we discovered that it seems to be using a value of 16.9° for $\Delta\theta'_L$ instead of the 80° that would be expected from Eq. (108) in the UM. This indicates that the REEDM code may be using a different technique for computing $\Delta\theta'_L$ than is described in the UM.

4.3.3. *Average Surface Concentration and Downwind Distance*

The sensitivity results for C_{avg} and D_{avg} are shown graphically in Figs. 3 and 4. Simple expressions for these variables can be obtained using an approach similar to that used to obtain Eqs. (R9)–(R12). To simplify matters, we assume that the concentration averaging time t_A is longer than the residence time of the cloud at a fixed downwind location. With this assumption, the inverse dependence of C_{avg} on σ_x is replaced by an inverse dependence on the product $\overline{u}_L t_A$. If this replacement is made in the Gaussian puff equation, it is easy to show that the peak time-average concentration occurs at the downwind distance D_{avg} for which $\sigma_z = h/\sqrt{2}$. Hence, the expression for C_{avg} corresponding to Eq. (R10) is

$$C_{avg} \propto \frac{1}{\overline{u}_L \, t_A \, \sigma'_{AL} D_{avg} \, h} \,, \tag{R14}$$

and the expression for D_{avg} corresponding to Eq. (R12) is

$$D_{avg} \approx \frac{h}{\sqrt{2}\, \sigma'_{EL}} \,. \tag{R15}$$

Equation (R15) indicates that D_{avg} should be slightly larger than D_{peak}, but both distances should show about the same sensitivity to variations in h and σ'_{EL}. Although it cannot be seen from the ratios in Table 2, the values of D_{avg} computed by REEDM were indeed generally either slightly larger than or equal to the values of D_{peak}. A comparison of Figs. 2 and 4 also indicates that D_{avg} and D_{peak} have about the same sensitivity, which is in agreement with Eqs. (R12) and (R15).

After accounting for the different vertical-axis scales in Figs. 1 and 3, it can be seen that with the exception of Runs F and G, C_{peak} and C_{avg} follow about the same pattern. Runs F and G are the only two which used a layer-averaged wind speed $\overline{u}_L$ that differs from the control run. From Eqs. (R10) and (R14), we expect that C_{avg} is inversely proportional to wind speed whereas C_{peak} is not. Hence, C_{avg} shows much greater sensitivity to wind speed.

C_{avg} is not as sensitive to wind-speed shear (Runs H through J) as C_{peak}. Speed shear tends to dilute the cloud by increasing the alongwind diffusion parameter σ_{xL}. However, a larger value of σ_{xL} also increases the residence time of the cloud at a fixed location. For C_{avg} in Runs H through J, the increased dilution of the cloud caused by wind-speed shear is largely offset by the increased residence time of the cloud.

4.3.4. *Turbulence Parameters*

Table 3 lists the control-normalized turbulence parameters σ'_{AL} and σ'_{EL} for the various sensitivity runs. Some of the results in this table have already been discussed

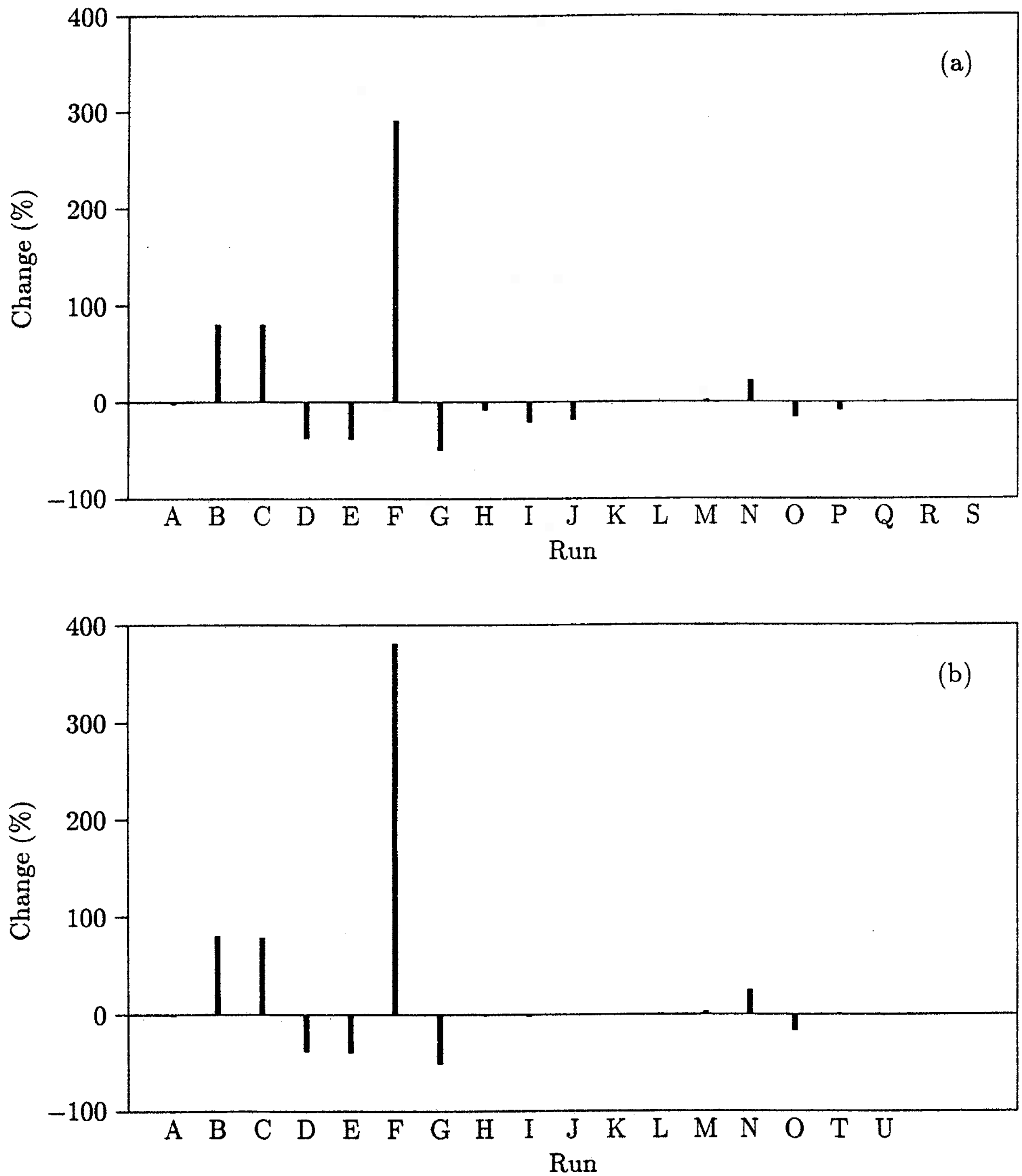

Figure 3. Variation of the average concentration C_{avg} for each of the REEDM sensitivity runs. The values are plotted as percentage changes from the control run. (a) is for the CLIM runs, and (b) is for the MEAS runs.

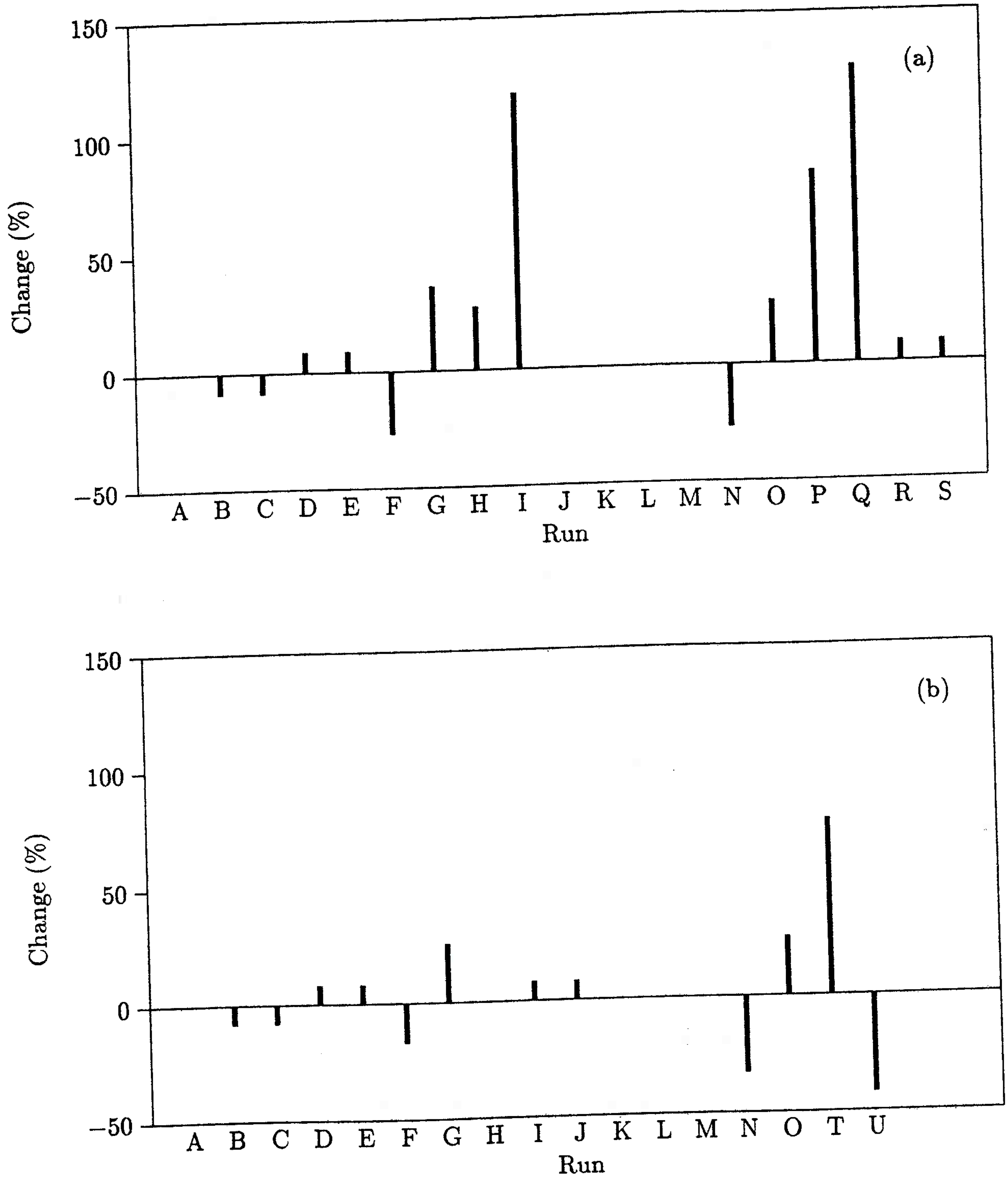

Figure 4. Variation of the downwind distance D_{avg} to the average concentration C_{avg} for each of the REEDM sensitivity runs. The values are plotted as percentage changes from the control run. (a) is for the CLIM runs, and (b) is for the MEAS runs.

in previous sections. For the MEAS runs, only Runs T and U should show significant variations from the control run. The values in Table 3 do exhibit this behavior, with variations of less than 10% for runs A through O. These minor variations are likely due to the way REEDM reduces the turbulence levels in the top 20% of the mixing layer.

The variations seen for the CLIM values of σ'_{AL} and σ'_{EL} are largely due to variations in wind speed and net radiation index. These are the two variables that determine the CLIM turbulence values near the surface (UM, p. 52). In Runs F and G, the variations in σ'_{AL} and σ'_{EL} result from the changes in wind speed. In Runs P and Q, the cloud cover produced a decrease in the net radiation index.

The situation is somewhat more complicated in CLIM Runs H through J. The turbulence levels are altered in these runs because of the way REEDM uses the rawinsonde wind profile to compute σ'_A and σ'_E at higher altitudes. At heights z above 100 m in a convective boundary layer, REEDM uses the equations (see UM p. 53) $\sigma'_A(z) = \sigma_v/\overline{u}(z)$ and $\sigma'_E(z) = \sigma_w/\overline{u}(z)$, where the velocity variances σ_v and σ_w are assumed to be constant with height. Since the wind speed $\overline{u}(z)$ increases with height in Runs H and I, $\sigma'_A(z)$ and $\sigma'_E(z)$ must decrease with height above 100 m. The layer-average values σ'_{AL} and σ'_{EL} are therefore lower in Runs H and I than in the control run. CLIM Run J differs from Runs H and I in that a flow reversal occurs at about 300 m above the ground. Wind speeds are very low at altitudes near this reversal, and the computed values of $\sigma'_A(z)$ and $\sigma'_E(z)$ are therefore large at these altitudes. The high turbulence levels near the flow reversal are responsible for the larger values of σ'_{AL} and σ'_{EL} observed in CLIM Run J.

It is notable that atmospheric thermal stratification (Runs A to E) has little or no effect on the CLIM turbulence in Table 3. This is not surprising given that CLIM turbulence estimates in REEDM only take into account the wind speed and net radiation index. However, REEDM indirectly accounts for thermal stratification in that Runs A through E would, in a real-world situation, occur at different times of the day (or probably not at all for Run E), when the net radiation index would be different.

5. Previous Sensitivity Studies

In addition to the present study, sensitivity studies of REEDM have been performed by The Aerospace Corp. (Womack, 1995) and R. Nyman of ACTA, Inc. (Hudson *et al.*, 1991). In this section we summarize these results.

5.1. The Aerospace Study

The Aerospace study (Womack, 1995) examined the sensitivity of the peak concentration, the 60 s time-averaged concentration, the exhaust cloud stabilization height, and the downwind distance to the point of peak concentration. A normal launch of a Titan IV was considered. The model input variables investigated were:

1. Meteorological profile
2. Percentage of HCl in rocket exhaust cloud
3. Air entrainment coefficient
4. Ground absorption coefficient for gases
5. Vehicle propellant temperature
6. Cloud cover
7. Initial exhaust-cloud radius

All other factors were held constant. A factorial design was used to identify which of the seven factors listed above had the most effect on the REEDM outputs. Each of the factors was assigned two values: a "high" value and a "low" value. The model sensitivity was then evaluated by making multiple runs of REEDM using different combinations of the "high" and "low" values. A full factorial design using all possible combinations of the seven factors would require 128 REEDM runs. Since performing such a large number of runs would be time consuming, Womack decided to use a fractional factorial design requiring only 16 REEDM runs. Of course, this reduction in the number of model runs is not free. Some information regarding interaction effects is lost, and it becomes more difficult to isolate the effects of a single factor.

The "high" and "low" values used in the fractional factorial design were 20% and 15% for the percentage of HCl, 0.64 and 0.50 for the entrainment coefficient, 100% and 0% for the ground absorption coefficient, and 10°C and 20°C for the propellant temperature. Two different rawinsonde profiles from Vandenberg Air Force Base were used as the "high" and "low" settings for the meteorological profile. The "low" profile had a mean wind speed of $9.4\,\mathrm{m\,s^{-1}}$ and an inversion layer at 898 m AGL, whereas the "high" profile had a mean wind speed of $1.9\,\mathrm{m\,s^{-1}}$ and an inversion layer at 312 m AGL. The cloud cover was set at either 0/10 or 10/10, and the initial cloud radius was either 86 m or 58 m.

Womack's results indicated that the most important factors in REEDM are the entrainment coefficient, ground absorption (reflection) coefficient, and meteorological profile. These conclusions are of course dependent on the assumed "high" and "low" settings for the seven factors. Significant interaction effects were also observed between some of the factors. Because of these interaction effects, Womack concluded that simple sensitivity studies which vary one factor at a time are not adequate.

However, there are some shortcomings to Womack's fractional factorial analysis. Because only 16 model runs were performed (out of a possible 128), some of the interaction effects of the factors were not considered. Also, fractional factorial designs have a problem with aliasing (Walpole and Myers, 1978), in which the main effects of the factors cannot be distinguished from certain interaction effects. In Womack's design, for example, the main effect of the entrainment coefficient cannot be distinguished from the interaction effects of the meteorological profile, propellant temperature, and initial cloud radius. This aliasing problem can make it difficult to interpret the sensitivity results from a fractional factorial design.

Another problem stems from the "high" and "low" settings used for the meteorological profile. These two rawinsonde soundings had different mean wind speeds and mixing-layer depths. It is also likely that the temperature profiles and vertical wind shear were different. An additional difference between the "high" and "low" meteorological profiles was that the measured-turbulence mode of REEDM was used at the "low" setting, whereas the climatological-turbulence mode was used at the "high" setting. With so many differences between the two settings, it becomes nearly impossible to assign any physical significance to REEDM's sensitivity to the meteorological profile.

A final caveat regarding factorial design is that it assumes the effects of the factors are additive. Thus, there is an implicit assumption in Womack's analysis that the overall sensitivity of REEDM to the seven factors can be obtained by summing over the effects of each factor and then accounting for interaction effects. It is not clear whether this assumption is valid (*e.g.*, the effects of the factors might be multiplicative instead of additive).

5.2. The ACTA Study

The ACTA study (Hudson *et al.*, 1991) used about 200 REEDM cases with different meteorological inputs to assess the response of the centerline concentrations and total dosage outputs. The meteorological inputs that were tested included wind speed, wind direction, temperature lapse rate, and wind shear. The test cases were based on a Titan IV vehicle and used three of the launch modes provided by REEDM: a normal launch, a conflagration, and a deflagration. Table 4 summarizes the sensitivity results obtained in the ACTA study.

The REEDM sensitivity to wind speed was investigated by using a vertically constant wind speed between about 1 and $9\,\mathrm{m\,s^{-1}}$. For the normal launch, the peak concentration C_{peak} was found to be nearly constant with wind speed, which is also what was found in Fig. 1 of this report for MEAS runs F and G. For a deflagration, C_{peak} was approximately constant until wind speeds dropped below about $3.6\,\mathrm{m\,s^{-1}}$, at which point C_{peak} decreased with decreasing wind speed. It is not clear why the dependence of C_{peak} on wind speed is different for a deflagration than it is for a normal launch. Possibly, the source-term computations for a deflagration have some kind of wind-speed dependence that is not obvious from the equations given in Section 3.2.5 of the UM. The peak concentration in a conflagration event was found to increase

Table 4. Summary of the results obtained in the ACTA sensitivity study of REEDM.

Varied input variable	Response in REEDM peak concentration		Response in REEDM peak dosage	
Wind speed	Normal:	Peak is constant in magnitude, but moves upwind with increasing wind speed.	Normal:	Peak reduces in inverse proportion to wind speed.
	Conflagration:	Peak increases linearly with wind speed.	Conflagration:	Peak decreases approximately linearly with increasing wind speed.
	Deflagration:	Gradual increase in peak with increasing wind speed. Increase is more pronounced with low cloud stabilization height.	Deflagration:	Peak decreases with increasing wind speed. Most pronounced with low cloud stabilization height.
Dry bulb lapse rate	Normal:	Peak increases linearly with increasing stability and moves upwind.	Normal:	Peak increases approximately linearly with increasing stability and moves upwind.
	Conflagration:	Same as normal launch.	Conflagration:	Same as normal launch.
	Deflagration:	Same as normal launch	Deflagration:	Same as normal launch.
Wind shear	Normal:	Peak decreases nonlinearly with increasing shear. Greatest change with light winds and when directional shear exceeds 90°.	Normal:	Peak gradually increases with increasing directional shear and decreases more dramatically with increasing speed shear.
	Conflagration:	Peak decreases with increasing directional shear and increases with increasing speed shear (due to increase in mean speed).	Conflagration:	Same as normal launch.
	Deflagration:	Same as normal launch.	Deflagration:	Same as normal launch.

approximately linearly with wind speed in the ACTA study. For a conflagration, REEDM uses a bent-over-plume model to compute the stabilization height z_s. The value of z_s for a bent-over plume tends to decrease with increasing wind speed, which explains the behavior of C_{peak}.

Because z_s in a conflagration tends to decrease with increasing wind speed, we would expect from Eq. (R12) that the downwind distance D_{peak} to the peak concentration should decrease as the wind speed increases. This behavior was indeed observed in the ACTA study. However, D_{peak} was also found to decrease with increasing wind speed for the normal launch and the deflagration. We do not understand this result; it is the opposite of what was obtained in our own wind-speed sensitivity tests (Runs F and G in Fig. 2).

For a normal launch and a deflagration, the ACTA study found that the peak dosage was inversely proportional to wind speed. This behavior is expected, since the residence time of the cloud at a particular downwind location decreases as the wind speed increases. The peak dosage for a conflagration was found to be less sensitive to the wind speed, because the effect of the wind speed on the cloud residence time was partly offset by the change in z_s with wind speed.

The ACTA study examined the variation in peak concentration and dosage over a range of vertical temperature profiles. These results are questionable, however, because it appears that the temperature gradient was confused with the potential-temperature gradient. The latter is given by

$$\frac{\partial \theta}{\partial z} = \frac{\partial T}{\partial z} + \Gamma \,, \qquad \text{(R15)}$$

where θ is the potential temperature, T is the dry-bulb temperature, and Γ is the adiabatic lapse rate of $9.77°\mathrm{C\,km^{-1}}$. In a neutral atmosphere, $\partial\theta/\partial z = 0$, and $\partial T/\partial z = -9.77°\mathrm{C\,km^{-1}}$. However, it appears that $\partial T/\partial z = 0$ was taken to indicate a neutral lapse rate when in fact it is stable. As a result of this confusion, REEDM was tested only for stable conditions with $\partial T/\partial z$ between about $-6.6°\mathrm{C\,km^{-1}}$ and $+23.0°\mathrm{C\,km^{-1}}$.

In the temperature-profile tests, the wind speed was held constant at about $3.6\,\mathrm{m\,s^{-1}}$. All three of the launch modes showed an increase in peak concentration and dosage as $\partial T/\partial z$ increased. As the temperature gradient increases, the stabilization height z_s decreases. Thus, from Eq. (R10) we would expect the peak concentration (and dosage) to increase. The downwind distances to the peak concentration and dosage were found to decrease with increasing temperature gradient, which can also be explained by the dependence of these downwind distances on z_s [e.g., Eq. (R12) with $h \approx z_s$].

The effect of wind-direction shear was considered in the ACTA study by holding the wind speed fixed at $3.6\,\mathrm{m\,s^{-1}}$ and allowing the wind direction to vary linearly by up to 180° in the first 3048 m of the atmosphere. During the buoyant-rise phase, directional shear causes the developing exhaust cloud to fan out as material at different altitudes moves downwind along different bearings. During the passive-diffusion phase, the directional shear increases the rate of crosswind cloud expansion [see Eq. (106) of the UM]. The results of these tests showed that the peak centerline concentration reduces gradually with increasing directional shear. However, the dosage can increase with increasing directional shear, because the residence time of the cloud over a fixed downwind location increases significantly once the total directional shear in the boundary layer exceeds approximately 90°.

6. Conclusions

From a broad perspective, the approach used by REEDM to describe the diffusion of rocket effluents is sound. The model divides the diffusion process into two parts: a buoyant-rise phase and a passive-diffusion phase. In the latter phase, the model splits the stabilized ground cloud into a series of vertical layers that are treated independently. These basic features of REEDM are physically sound and would likely be retained in any upgrade to REEDM or in a future replacement to REEDM.

In the implementation of these basic features, however, we think that REEDM has some shortcomings. Because of the long history of the model, many of its specific features are now becoming obsolete. Its main drawback is that most of the meteorological parameters are averaged over the entire depth of the mixing layer, so that information regarding vertical variability is lost. This loss of vertical variability is a significant drawback in atmospheric conditions such as a sea-breeze circulation, where the winds and turbulence can have strong variations with height.

The procedure that REEDM currently uses to estimate mixing-layer depth does not generally work properly in stable conditions at night. REEDM assumes that the mixing layer is always capped by a temperature inversion. This is a reasonable assumption for unstable daytime boundary layers, but not for stable boundary layers.

The turbulence algorithms used in REEDM are also outdated. In the current version of REEDM, the alongwind diffusion parameter σ_{xL} is not affected by turbulence and is therefore constant unless wind-speed shear is present in the boundary layer. This lack of growth in the alongwind diffusion will lead to overestimates of the concentration in most situations. The crosswind and vertical diffusion in REEDM are formulated better than the alongwind diffusion, but there is still room for improvement. The REEDM climatological algorithms that are currently used for σ'_A and σ'_E at elevations below 100 m are empirical fits largely based on measurements at the White Sands Missile Range in New Mexico and the Round Hill Field Station in Massachusetts. Since the vertical variations of σ'_A and σ'_E are affected by the profiles of both the wind speed $\overline{u}$ and the velocity standard deviations σ_v and σ_w, it is not clear whether the climatological algorithms used in REEDM are applicable to Cape Canaveral and Vandenberg AFB.

We feel that the scientific description of REEDM in the existing UM is not adequate. Little or no explanation is given in the document as to how the major equations in the model are derived, and we found many errors and inconsistencies in the equations. One can argue that we should be commenting on REEDM itself and not the UM. In practice, however, one cannot separate the code from the documentation. Without adequate documentation, a model will remain an enigma to its users, in spite of all the time and effort invested in it.

The sensitivity studies we performed indicate that REEDM generally performs as would be expected from the simple relationships given by Eqs. (R9)–(R15). The peak concentration C_{peak} was found to be highly sensitive to the temperature profile in the boundary layer and to the mixing-layer depth. In REEDM's climatological-turbulence mode, C_{peak} also showed some sensitivity to wind-speed shear. This speed shear could also have a significant effect on the downwind distance D_{peak} to the peak concentration. Since strong temperature gradients and wind-speed shear are often present at night, these results suggest that REEDM may show greater overall sensitivity to input variables at night than during the day.

REEDM was surprisingly insensitive to wind-direction shear in the boundary layer. A closer inspection of the REEDM output files revealed that the amount of wind-direction shear computed by the model (based on the rawinsonde profile) was significantly less than what would be expected from the equations given in the UM. It is possible that an undocumented change was made to the part of the code that computes wind shear.

In some circumstances, the value of D_{peak} was found to be highly sensitive to cloud cover in the climatological-turbulence mode. As the cloud ceiling falls below 2134 m AGL and the fractional cloud cover increases beyond 5/10, a sudden jump in D_{peak} can occur as a result of changes in the net radiation index. This jump can only occur during the day, and it has little effect on the peak concentration C_{peak}. In REEDM's measured-turbulence mode, D_{peak} was most sensitive to the measured values of σ'_A and σ'_E. Higher levels of turbulence tend to decrease D_{peak} while having little effect on C_{peak} itself.

Most of the sensitivity tests showed that C_{avg} and D_{avg} vary in ways similar to C_{peak} and D_{peak}. The main exception was the sensitivity to wind speed. C_{avg} is highly sensitive to wind speed, since the residence time of the cloud at a fixed location is inversely proportional to wind speed.

7. Recommendations

If REEDM is to be retained as the primary model for estimating the diffusion of rocket-vehicle launch clouds, we recommend that a number of changes be made to the model to improve its scientific formulations. These changes are listed according to our estimation of their priority.

1. The extensive vertical averaging of atmospheric variables that takes place in the model should be eliminated, so that the rocket exhaust at a given height is transported and dispersed by winds and turbulence that correspond to this height. The current version of REEDM uses the same bulk-averaged winds and turbulence at all heights within the boundary layer.

2. The algorithm used by REEDM to estimate mixing depth H_m should be modified so that it provides more realistic estimates in stable conditions at night. One approach for estimating H_m in stable conditions is to use the equation $H_m \approx 0.4[u_* L/f]^{1/2}$, where u_* is the friction velocity, L is the Monin-Obukhov length, and f is the Coriolis parameter. It is also possible that H_m can be estimated more directly by using turbulence measurements from towers or Doppler sodars.

3. The assumption of straight-line transport, which is implicit in the equations REEDM uses for dosage and deposition [UM Eqs. (103) and (115)], should be eliminated. An interpolation or diagnostic wind-field model could then be used to provide spatially and temporally variable wind fields based on the meteorological measurements that are already being collected at Cape Canaveral and Vandenberg AFB.

4. For estimating the turbulent diffusion of the ground cloud, we strongly recommend that field measurements of the turbulence parameters σ'_A and σ'_E (or σ_v and σ_w) be used whenever possible. Currently, field measurements are used at Vandenberg AFB but not at Cape Canaveral Air Station. Since an extensive tower network is available at Cape Canaveral, we think that measured turbulence should also be used there. Accurate turbulence data can now be routinely acquired with sonic anemometers, and these could be added to the Cape tower network. If there is an intention to continue relying on REEDM's climatological algorithm to estimate the turbulence at Cape Canaveral, we think that further study is required to determine how well this algorithm compares with the observed turbulence at Cape Canaveral.

5. The alongwind diffusion should be reformulated so that it includes the effect of turbulent mixing in the alongwind direction (see, for example, Appendix A). Currently, the alongwind diffusion in the model is affected by wind-speed shear but not turbulent mixing.

6. Even when near-surface turbulence measurements are available, a climatological turbulence algorithm will still be necessary in REEDM to extrapolate upward to the top of the boundary layer. This extrapolation should be based on the current scientific understanding of how the velocity standard deviations σ_v and σ_w vary with height in the boundary layer. In convective conditions, for example, σ_v is

nearly constant with height at least up to about $0.8H_m$ (Hicks, 1985); hence, upward extrapolation is straightforward. Field observations and large-eddy simulations in convective conditions (Moeng and Wyngaard, 1989) show that σ_w increases with height for $z \leq 0.2H_m$, is roughly constant for $0.2H_m < z \leq 0.6H_m$, and decreases with height for $0.6H_m < z \leq H_m$. For stable conditions, the work by Lenschow *et al.* (1988) indicates that both σ_v and σ_w are proportional to $[1-(z/H_m)]^{7/8}$ through the depth of the boundary layer.

7. The User's Manual should be thoroughly overhauled and rewritten to state clearly the various assumptions, definitions, and units, and to incorporate intermediate steps and details of the derivations of various equations. It is possible that previous studies by other investigators have already accomplished some of this work, and an attempt should be made to collect and incorporate their work into the revision of the REEDM Manual. The manual should be separated into two sections: the first consisting only of details of model formulations and assumptions, algorithms, and related technical discussions; the second consisting of the computer code User's Guide, which includes the tables for the I/O variables (clearly identifying the related equations) and all other information that would explain the model implementation and assist the model users. The revised report then should be peer-reviewed by other scientists and model users to ensure its accuracy and clarity of presentation.

Sections 3 and 4 of this report discussed many other problems or potential problems in REEDM that have somewhat lower priorities than those listed above. These include the problems associated with averaging the wind vector in polar coordinates instead of rectangular coordinates (Section 3.1), our inability to fully derive the REEDM equations for dosage and deposition (Sections 3.2.9 and 3.2.10), and REEDM's lack of sensitivity to wind-direction shear (Section 4.3.2). If continued use is to be made of REEDM, these problems should also be addressed.

One alternative to performing extensive modifications to REEDM and the User's Manual would be to develop an improved model which combines the best features of REEDM (Version 7) with current understanding of atmospheric turbulence, diffusion, and deposition. A great deal of progress has been made in atmospheric dispersion modeling and meteorological measurements over the past two decades or so, and the successor model can incorporate many of these up-to-date techniques and knowledge. Development of such a model can also benefit strongly from the large amounts of data becoming available from ongoing field experiments at the test ranges, including tracer releases.

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References

Baron, T., E. R. Gerhard, and H. F. Johnstone, 1949: Dissemination of aerosol particles dispersed from stacks. *Ind. Chem. Eng.*, **41**, 2403–2408.

Berkowicz, R. and L. P. Prahm, 1982: Evaluation of the profile method for estimation of surface fluxes of momentum and heat. *Atmos. Environ.*, **16**, 2809–2819.

Bjorklund, J. R., 1990: User's manual for the REEDM Version 7 (Rocket Exhaust Effluent Diffusion Model) computer program. Report No. TR-90-157-01, H. E. Cramer Company, Inc., prepared for Eastern Space and Missile Center, Patrick Air Force Base, FL, 279 pp.

Bjorklund, J. R. and R. K. Dumbauld, 1981: User's instructions for the volume source diffusion models computer program and the volume/line source graphics computer program. Report No. TR-81-321-08, H. E. Cramer Company, Inc., prepared for U.S. Army Dugway Proving Ground, Dugway, UT.

Briggs, G.A., 1969: *Plume Rise.* TID-25075, U.S. Atomic Energy Commission, Division of Technical Information, 81 pp.

Briggs, G.A., 1970: Some recent analysis of plume rise observations. Paper ME-8E, Second International Clean Air Congress, 6-11 December 1970, Washington, D.C., also published as NOAA Atmospheric Turbulence and Diffusion Laboratory Contribution No. 38, 35 pp.

Briggs, G. A., 1972: Chimney plumes in neutral and stable surroundings. *Atmos. Environ.*, **6**, 507–510.

Briggs, G. A., 1975: Plume rise predictions. In *Lectures on Air Pollution and Environmental Impact Analyses*, D. A. Haugen (Ed.), American Meteorological Society, Boston, MA, 59-111.

Cadle, R. D., 1975: *The Measurement of Airborne Particles.* John Wiley & Sons, New York, 342 pp.

Chatwin, P. C., 1982: The use of statistics in describing and predicting the effects of dispersing gas clouds. *J. Haz. Mat.*, **6**, 213–230.

Csanady, G. T., 1955: Dispersal of dust particles from elevated sources. *Aust. J. Phys.*, **8**, 545–550.

Davidson, G. A., 1989: Simultaneous trajectory and dilution predictions from a simple integral plume model. *Atmos. Environ.*, **23**, 341–349.

Drivas, P. J. and F. H. Shair, 1974: Dispersion of an instantaneous crosswind line source of tracer released from an urban highway. *Atmos. Environ.*, **8**, 475–485.

Dumbauld, R. K., J. R. Bjorklund, H. E. Cramer, and F. A. Record, 1969: Handbook for estimating toxic fuel hazards. Report No. NASA-CR-61326, NASA George C. Marshall Space Flight Center, Huntsville, AL.

Dumbauld, R. K., J. R. Bjorklund, and J. F. Bowers, 1973: NASA/MSFC multi-layer diffusion models and computer programs for operational prediction of toxic fuel hazards. Report No. NASA-CR-129006, George C. Marshall Space Flight Center, Huntsville, AL.

Dumbauld, R. K. and J. F. Bowers, 1983: Functional methodologies for characterizing wind-speed and turbulence profiles and turbulent diffusion coefficients within and above vegetative canopies and urban domains. Report No. TR-83-341-01, H. E. Cramer Company, Inc., prepared for U.S. Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM.

Eckman, R. M., 1994: Influence of the sampling time on the kinematics of turbulent diffusion from a continuous source. *J. Fluid Mech.*, **270**, 349–375.

Hanna, S. R., 1984: Concentration fluctuations in a smoke plume. *Atmos. Environ.*, **18**, 1091–1106.

Healy, J. W., 1968: Radioactive cloud dose calculations. In *Meteorology and Atomic Energy 1968*, D. H. Slade (Ed.), U.S. Atomic Energy Commission, Available from NTIS as TID-24190, 304-377.

Herdan, G., 1960: *Small Particle Statistics.* Academic Press, New York, 418 pp.

Hicks, B.B., 1985: Behavior of turbulence statistics in the convective boundary layer. *J. Clim. Appl. Meteor.*, **24**, 607–614.

Hudson, J. M., R. L. Nyman, L. L. Philipson, A. M. See, and D. P. Stapleton, 1991: Hot spill risk model development. ACTA Report No. 91-250/05-01, ACTA, Inc., Torrance, CA.

Knight, R. W. and S. P. Prince, 1988: Atmospheric dispersion of solid and liquid rocket propellants. Report No. MCR-87-052, Martin Marietta Astronautics Group, prepared under U. S. Air Force Contract F04701-86-C-0074.

Lenschow, D. L., X. S. Li, C. J. Zhu, and B. B. Stankov, 1988: The stably stratified boundary layer over the Great Plains. *Boundary-Layer Meteor.*, **42**, 95–121.

Moeng, C.-H. and J. C. Wyngaard, 1989: Evaluation of turbulent transport and dissipation closures in second-order modeling. *J. Atmos. Sci.*, **46**, 2311–2330.

Morton, B. R., G. I. Taylor, and J. S. Turner, 1956: Turbulent gravitational convection from maintained and instantaneous sources. *Proc. Roy. Soc., Ser. A*, **234**, 1–23.

Nickola, P. W., 1971: Measurements of the movement, concentration and dimensions of clouds resulting from instantaneous point sources. *J. Appl. Meteor.*, **8**, 962–973.

Overcamp, T. J., 1976: A general Gaussian diffusion-deposition model for elevated point sources. *J. Appl. Meteor.*, **15**, 1167–1171.

Panofsky, H. A. and J. A. Dutton, 1984: *Atmospheric Turbulence.* John Wiley & Sons, New York, 397 pp.

Panwar, T. S., I. R. Cowan, and R. E. Britter, 1994: Concentration fluctuation models: a comparative study. Report No. CUED/A-AERO/TR 24, Dept. of Engineering, Cambridge, University, U. K., 42 pp.

Pasquill, F. and F. B. Smith, 1983: *Atmospheric Diffusion,* 3rd edition. John Wiley & Sons, New York, 437 pp.

Peng, M. S., S.-W. Li, S. W. Chang, and R. T. Williams, 1995: Flow over mountains: Coriolis force, transient troughs, and three dimensionality. *Quart. J. R. Meteor. Soc.*, **121**, 593–613.

Rao, K. S., 1981: Analytical Solutions of a gradient-transfer model for plume deposition and sedimentation. EPA-600/3-82-079, U.S. Environmental Protection Agency, Research Triangle Park, NC, available from NTIS as PB 82-215 153, 75 pp.

Rao, K. S. and L. Satterfield, 1983: A study of the probable environmental impact of fugitive coal dust emissions at the Ravenswood Power Plant, New York. NOAA Tech. Memo. ERL ARL-123, available from NTIS as PB 84-119 908, 83 pp.

Saffman, P. G., 1962: The effect of wind shear on horizontal spread from an instantaneous ground source. *Quart. J. R. Meteor. Soc.*, **88**, 382–393.

Smith, F. B., 1965: The role of wind shear in horizontal diffusion of ambient particles. *Quart. J. R. Meteor. Soc.*, **91**, 318–329.

Stull, R. B., 1988: *An Introduction to Boundary Layer Meteorology.* Kluwer Academic Publishers, Dordrecht, The Netherlands, 666 pp.

Teske, M. E., J. F. Bowers, J. E. Rafferty, and J. W. Barry, 1993: FSCBG: An aerial spray dispersion model for predicting the fate of released material behind aircraft. *Environ. Toxicol. Chem.*, **12**, 453–464.

Tyldesley, J. B. and C. E. Wallington, 1965: The effect of wind shear and vertical diffusion on horizontal dispersion. *Quart. J. R. Meteor. Soc.*, **91**, 158–174.

van Ulden, A. P. and A. A. M. Holtslag, 1985: Estimation of atmospheric boundary layer parameters for diffusion applications. *J. Clim. Appl. Meteor.*, **24**, 1196–1207.

Walpole, R. E. and R. H. Myers, 1978: *Probability and Statistics for Engineers and Scientists,* 2nd edition. Macmillan Publishing Co., New York, 580 pp.

Womack, J. M., 1995: Rocket exhaust effluent diffusion model sensitivity study. Aerospace Rept. No. TOR-95(5448)-3, Aerospace Corp., El Segundo, CA, 15 pp.

Zilitinkevich, S. S., 1972: On the determination of the height of the Ekman boundary layer. *Boundary-Layer Meteor.*, **3**, 141-145.

Appendix A: Comments on the REEDM Alongwind Dispersion Coefficient Algorithm

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The Rocket Exhaust Effluent Diffusion Model (REEDM) (Bjorklund, 1990) is the most recent version of a model originally developed for NASA in the late 1960s (Dumbauld *et al.*, 1969) and early 1970s (Dumbauld *et al.*, 1973). As shown in Eq. (111) of Bjorklund (1990), REEDM computes the alongwind (longitudinal) Gaussian dispersion coefficient σ_x from

$$\sigma_x = \left[\left(\frac{L(x)}{4.3} \right)^2 + \sigma_{xo}^2 \right]^{1/2} , \tag{R16}$$

$$L(x) = \begin{cases} 0.28 \dfrac{\Delta \overline{u}_L}{\overline{u}_L} x \, ; & \Delta \overline{u}_L \geq 0 \\ 0.28 \dfrac{|\Delta \overline{u}_L|}{\overline{u}_L} x \, ; & \Delta \overline{u}_L < 0 \text{ and } \partial\theta/\partial z < 0 \\ 0 & \Delta \overline{u}_L < 0 \text{ and } \partial\theta/\partial z \geq 0 \end{cases} \tag{R17}$$

where σ_{xo} is the initial source dimension (standard deviation of the alongwind concentration distribution), $L(x)$ is the alongwind length of an instantaneous point source at downwind distance x, $\Delta \overline{u}_L$ is the difference in wind speed through the layer containing the cloud, $\overline{u}_L$ is the mean wind speed through the layer containing the cloud, and $\partial\theta/\partial z$ is the vertical potential temperature gradient.

The origins of Eqs. (R16) and (R17) are not well known by current REEDM users because they have not been discussed in any model documentation since Dumbauld *et al.* (1973). The expression for $L(x)$ comes from a model by Tyldesley and Wallington (1965) for the alongwind growth of an instantaneous source due to vertical diffusion and wind shear. It should be noted that this model is strictly applicable only to surface releases. The coefficient 0.28 is theoretical, but Tyldesley and Wallington conclude that it is consistent with limited measurements downwind from instantaneous line source releases if the normalized wind shear $\Delta \overline{u}_L/\overline{u}_L$ is assumed to be unity. The factor of 4.3 in Eq. (R16) is the nondimensional distance between the points on a Gaussian cloud at which the concentration is equal to 10% of the peak concentration. REEDM is principally intended for application within the surface mixing layer where the model's authors assumed that $\Delta \overline{u}_L$ is greater than zero by definition (at least for averaging times of more than a few minutes). Thus, the case of $\Delta \overline{u}_L$ less than zero was not considered to be a problem. However, subsequent experience in using the model with actual radiosonde soundings showed that $\Delta \overline{u}_L$ less than zero occurred on occasion in unstable mixing layers, and the second line of Eq. (R17) was added to the algorithm. The third line of Eq. (R17) was assumed by REEDM's authors to apply only within elevated stable layers because, as noted above, they assumed $\Delta\overline{u}_L$ greater than zero within a stable mixing layer.

One of the principal weaknesses of the σ_x algorithm defined by Eqs. (R16) and (R17) is that it assumes that alongwind puff growth due to atmospheric turbulence is negligible in comparison with that due to wind shear. The limitations of Eqs. (R16) and (R17) became apparent in work that REEDM's authors performed for Dugway Proving Ground (DPG) in the mid 1970s. A comparison of predicted and observed cloud arrival times and durations for four series of crosswind line source releases (three military tests that are still classified and Drivas and Shair, 1974) and one series of instantaneous point source releases (Nickola, 1971) showed that the actual clouds systematically arrived sooner and remained longer over downwind receptors than predicted by Eqs. (R16) and (R17). It was empirically determined that good overall agreement between predictions and measurements could be obtained for all data sets by changing the coefficient in Eq. (R17) from 0.28 to about 0.6. This larger coefficient was interpreted as being needed to account for the effects of atmospheric turbulence on alongwind growth, effects that are not explicitly included in Eqs. (R16) and (R17). The coefficient of 0.6 was used in the next generation DPG diffusion model VSDM (Bjorklund and Dumbauld, 1981), and it is still used in several models including the widely used DPG/USDA Forest Service FSCBG aerial spray model (Teske *et al.*, 1993). It is not clear why this coefficient was never updated in REEDM.

The σ_x algorithm given by Eqs. (R16) and (R17) with the revised coefficient of 0.6 generally has appeared to work well for low-level releases. However, the algorithm does not work well for elevated releases because the release height strongly affects the magnitude of σ_x until the cloud has become uniformly mixed in the surface mixing layer. For example, near the release point, σ_x for a cloud released in the upper part of the mixing layer can be much smaller than σ_x for a cloud released near the surface under the same meteorological conditions. This result is explained by the fact that the greatest changes in wind speed with height occur near the surface. Thus, for the same shallow cloud depth, $\Delta\overline{u}_L$ is smaller and $\overline{u}_L$ is larger for a cloud released at high levels than for one released near the surface. The rapid growth required for the elevated cloud σ_x to reach the release-height-independent values as the downwind distance approaches the distance at which the cloud fills the mixing layer can cause an anomalous dip or flattening in the calculated profile of peak concentration versus distance, a problem that may not be readily apparent in REEDM predictions because of the large initial source dimensions. Because of this problem, DPG diffusion models now use a σ_x algorithm from Dumbauld and Bowers (1983).

Dumbauld and Bowers (1983) suggested a generalized σ_x algorithm of the form

$$\sigma_x = \left[\sigma_{xt}^2 + \sigma_{xs}^2\right]^{1/2} \qquad \text{(R18)}$$

$$\sigma_{xt} = aI_x(x + x_x) \qquad \text{(R19)}$$

$$x_x = \left(\frac{\sigma_{xo}}{aI_x}\right)^{1/b} \qquad \text{(R20)}$$

$$\sigma_{xs} = E_s\left(\frac{\Delta\overline{u}_L}{\overline{u}_L}\right)x \qquad \text{(R21)}$$

where I_x is the longitudinal turbulence intensity; a, b, and E_s are empirical constants; and the other terms are as defined above. In the absence of I_x measurements, Dumbauld and Bowers assumed that I_x can be approximated by

$$I_x \approx 1.33 I_y \approx 1.33\sigma'_A \,, \qquad \text{(R22)}$$

where I_y is the lateral turbulence intensity and σ'_A is the standard deviation of the wind azimuth angle in radians, adjusted from the reference time to the cloud formation time using the $t^{0.2}$ law (see Eq. (92) of Bjorklund, 1990). Under the assumption that the coefficients a and b are both unity, Dumbauld and Bowers (1983) used the Nickola (1971) data to estimate that E_s is approximately 0.06. The resulting algorithm yields σ_x values for near-surface releases that are very similar to those obtained using Eqs. (R16) and (R17) with the coefficient of 0.6. However, because it reduces the strength of the release height dependence, it avoids the rapid acceleration in σ_x for elevated releases.

As an example of the performance of the σ_x algorithm given by Eqs. (R18) through (R22), Fig. 5 (from Dumbauld and Bowers, 1983) compares predicted and observed σ_x values for the Drivas and Shair (1974) crosswind line source sulfur hexafluoride (SF_6) releases in the Los Angeles urban area. The sampling distances ranged from 0.4 to 3.2 km downwind from the release line. Although wind direction standard deviations were available for use in Eq. (R22), wind profiles were not available to determine $\Delta\overline{u}_L/\overline{u}_L$. Based on the predictions of their urban wind profile methodology, Dumbauld and Bowers assumed $\Delta\overline{u}_L/\overline{u}_L$ equal to 2 within the urban roughness layer in order to compute the wind shear term of Eq. (R21).

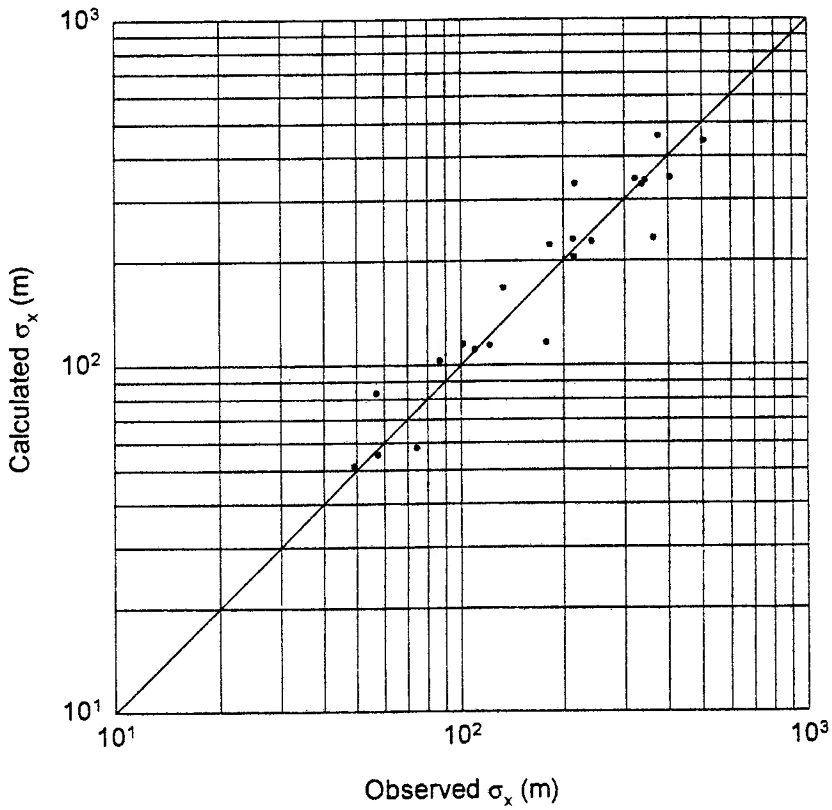

Fig. 5. Comparison of calculated and observed alongwind dispersion coefficients for the Drivas and Shair (1974) tracer releases (from Dumbauld and Bowers, 1983)

Appendix B: Comments on Specific Aspects of REEDM Physics

During a February 1995 meeting in Salt Lake City, Utah, a representative from the 30th Space Wing at Vandenberg Air Force Base put forward nine questions about REEDM that they hoped would be addressed in a model verification. Representatives from other organizations, such as the 45th Space Wing at the Cape Canaveral Air Station, were also present at the Utah meeting, and their concerns regarding REEDM were sometimes different from those of the 30th Space Wing. Because of time and funding limitations, we were unable to pursue all the various proposals that were put forth at the Utah meeting. We therefore found it necessary to limit the scope of our research while still accounting for the varying concerns of each organization.

A majority of the nine questions put forward by the 30th Space Wing are addressed in the main body of this report. However, the 30th Space Wing would still like to see a point-by-point discussion of each question. We have therefore compiled a set of responses to the nine questions in this appendix.

1. *How should REEDM be applied in conditions where exhaust material is wholly or partially contained in a stable layer? In particular, how should the mixing layer and turbulence parameters be defined when a surface-based inversion is present?*

The impetus for this question seems to be some confusion in how to specify REEDM's mixing-layer depth H_m in stable conditions. As was discussed in Section 2.2.2 of this report, REEDM assumes that the boundary layer is always capped by a stable layer. This assumption does not generally work at night when the lowest stable layer is based at the surface. Section 2.2.2 discusses some alternative techniques for estimating the mixing-layer depth in stable conditions.

To estimate REEDM's turbulence parameters in stable conditions, the best approach is to use tower and sodar measurements directly. If only near-surface measurements are available, it can be assumed that the velocity standard deviations σ_v and σ_w are proportional to $[1 - (z/H_m)]^{7/8}$, as suggested by Lenschow *et al.* (1988). When no turbulence measurements are available, the full equations suggested by Lenschow *et al.* (1988) can be used:

$$\frac{\sigma_v^2}{u_*^2} = 4.5\left[1 - \frac{z}{H_m}\right]^{7/4} ; \qquad \text{(R23)}$$

$$\frac{\sigma_w^2}{u_*^2} = 3.1\left[1 - \frac{z}{H_m}\right]^{7/4} . \qquad \text{(R24)}$$

An estimate of the friction velocity u_* can be obtained using either mean profiles (Berkowicz and Prahm, 1982) or surface energy budgets (van Ulden and Holtslag, 1985).

2. *The climatological turbulence model in REEDM is based on empirical data from Round Hill, Massachusetts. How applicable are these data to Cape Canaveral and Vandenberg AFB?*

As stated in Section 2.2.8 of this report, we believe that it is questionable whether the climatological turbulence algorithm used by REEDM is applicable to Cape Canaveral and Vandenberg AFB. These locations are affected by coastal phenomena that are not accounted for in REEDM's climatological turbulence algorithm. The best way to resolve this issue is to compare the algorithm with field measurements taken at the two locations. A series of field experiments at Cape Canaveral and Vandenberg AFB was started in July 1995, and the turbulence data from these experiments will be useful in addressing this issue.

3. *The dispersion algorithm used in REEDM uses mixing-layer-averaged values of the mean wind and turbulence parameters along with empirical adjustments for wind shear. How good is this approach?*

The vertical averaging used by REEDM is probably a reasonable assumption during sunny afternoons when the boundary layer is strongly convective. Under these conditions, the mean wind speed and direction as well as the horizontal turbulence parameters σ_u and σ_v are more or less constant with height through much of the boundary layer. The one problem would be the vertical-velocity standard deviation σ_w, which increases with height near the ground, reaches a maximum near the middle of the boundary layer, and then decreases with height in the upper parts of the boundary layer (Moeng and Wyngaard, 1989). The layer-averaged value of σ'_E used by REEDM will likely overestimate the vertical mixing near the top and bottom of the boundary layer, and underestimate the mixing near the center of the boundary layer.

In the stable boundary layer, the layer averaging performed by REEDM can produce considerable error. In these conditions, the wind speed tends to increase with height, and the turbulence parameters tend to decrease with height. The wind direction can also show significant variation with height. REEDM has some empirical adjustments to account for wind speed and direction shear, but these adjustments rely on the assumption that the shear effects are rapidly mixed in the vertical. The shear adjustment for σ_{yL} assumes that the effects of wind-direction shear are rapidly mixed throughout the depth of the boundary layer, whereas the adjustment to σ_{xL} assumes that the wind-speed shear is rapidly mixed through each layer of depth Δz_k. Of course, the assumption of rapid vertical mixing is not realistic in a stable boundary layer.

In stable conditions, the layer-average wind speed used in REEDM will generally cause the part of the effluent cloud near the ground to advect downwind too quickly and the part of the cloud near the top of the mixing layer to advect too slowly. As a result, the cloud may reach downwind surface receptors too quickly. The rapid mixing that is implicitly assumed in REEDM's wind-shear adjustments will cause the modeled cloud to mix too rapidly. Hence, these adjustments will tend to cause underestimates in the ground-level concentration. In contrast, the layer-average turbulence values σ'_{AL} and σ'_{EL} used by REEDM are likely to underestimate the turbulent mixing near the surface and overestimate it near the top of the mixing layer. The effluent near the surface will therefore be diffused too slowly, whereas the effluent in the upper portions of the mixing layer will be diffused too quickly; the overall effect is to increase the calculated ground-level concentration. The net effect of all these factors on the estimated ground-level concentration is difficult to determine, since it will depend on specific aspects of the wind, turbulence, and concentration profiles.

4. *What averaging time should be used to compute the turbulence parameters* σ'_A *and* σ'_E*?*

The stabilized ground cloud produced by a Titan IV rocket can have an initial radius of about 1 km. Further diffusion by ambient turbulence over a downwind distance of 30 km can increase the horizontal size of the cloud to something on the order of 5–10 km. This means that atmospheric eddies having horizontal length scales up to 5–10 km can be effective in diffusing the cloud over a 30 km downwind distance. The averaging time used for σ'_A and σ'_E should therefore be long enough to include the effects of these large eddies. A rough estimate of the required averaging time can be obtained by dividing the horizontal length scales of the large eddies by the mean wind speed. For a length scale of 10 km and a wind speed of $5\,\mathrm{m\,s^{-1}}$, it would be necessary to use an averaging time of about 30 min.

5. *REEDM uses reflection coefficients to account for the behavior of the effluent cloud at the surface and top of the mixing layer. What strength and depth of thermal inversion is required to stop effluent from mixing through the top of the mixing layer? How should the ground reflection coefficient be set to account for surface chemistry and wet/dry deposition?*

The partial-reflection approach has been used for a long time to account for the dry deposition of pollutants from a Gaussian plume. Baron *et al.* (1949) developed a dispersion model that includes both the real and image source contributions, and suggested that the removal of airborne particles by deposition can be treated by adjusting the image source strength to be a fraction γ of the real source strength. Csanady (1955) derived an analytical solution for this image source strength fraction, usually referred to as the reflection coefficient. Overcamp (1976) extended Csanady's theory and gave an analytical expression for the concentration of gases and small particles when the deposition velocity v_d does not equal the gravitational settling velocity v_g. In this approach, an equation for the reflection coefficient γ was derived by setting the deposition flux equal to the difference in fluxes from the real and image sources, and its value was determined by solving this equation together with an implicit relation based on considerations of the streamlines from the real and image sources. Note that $\gamma = 1$ for a perfectly reflecting surface, and $\gamma = 0$ for a perfect sink. In general, $0 < \gamma < 1$ for realistic surface and atmospheric conditions.

Using a gradient-transfer model and a radiation boundary condition for deposition, Rao (1981) derived an explicit relation for the reflection coefficient for a Gaussian plume in terms of the downwind and vertical coordinates (x, z), effective plume height h, wind speed $\overline{u}$, vertical dispersion parameter σ_z, and the pollutant deposition and settling velocities v_d and v_g, which were assumed to be constant and specified as inputs to the model. This approach can be adapted to estimate or specify the reflection coefficients that account for the deposition and/or chemical loss at the lower boundary in the REEDM model. The current practice for γ specification in REEDM is *ad hoc* and does not account for the deposition of gases and small droplets by turbulent transfer.

Though the approach outlined above can be extended to the upper boundary (*i.e.*, inversion base) as well, one needs to specify the ventilation or entrainment rates at the top of the boundary layer as inputs, and these parameters are generally less well-known than the deposition velocities. Given the level of sophistication of REEDM and the other uncertainties associated with modeling a rocket-effluent cloud, the entrainment of passive effluent through the top of the mixing layer is a secondary issue. It is therefore reasonable to assume that total reflection occurs at the top of the mixing layer, as is done in most Gaussian diffusion models.

6. *REEDM accounts for the vertical variations of atmospheric parameters during the buoyant-rise phase of the effluent cloud, but then uses mixing-layer-average parameters during the passive-diffusion phase. Could REEDM be modified so that the passive-diffusion phase also accounts for the vertical variations of atmospheric parameters? Would it be easier to abandon the REEDM dispersion algorithms and use a puff model or particle-in-cell model?*

The modifications required in REEDM to account for the vertical variations of atmospheric parameters are in concept easy to implement. One would simply modify the diffusion algorithm so that the effluent in each of REEDM's sublayers is transported and diffused by the winds and turbulence at its own height instead of the mixing-layer-average winds and turbulence. However, we are not familiar enough with the detailed structure of REEDM's FORTRAN source code to say whether these modifications would be easy to implement in practice. It should be noted that REEDM is already a type of puff model. It differs from other puff models mainly in that the initial shape of the puffs are somewhat different and that the puffs all move with the same speed and direction.

7. *The ranges must now respond to toxicological concentration thresholds that are not to be exceeded even for short durations. How can REEDM be matched to such a requirement given that Gaussian models provide only mean concentrations? Can we empirically define a relationship between peak concentrations and the mean concentration produced by REEDM?*

Chatwin (1982) discussed the question of modeling the environmental effects of toxic contaminants from either routine or accidental releases, and concluded that the long-term (typically 1-hr) average concentration predictions are irrelevant. It is not enough to be able to predict the mean concentration, which has been the sole emphasis of most of the current models such as REEDM, because the standard deviation can be at least as large as the mean. Therefore, it is necessary to predict the probability density function of the concentrations, especially at the upper end of the distribution, in order to respond to toxicological concentration criteria. The stochastic uncertainty in air quality models such as REEDM can be estimated by assuming that the concentration distribution is completely determined by the mean ($\overline{C}$) and the standard deviation (σ_c).

The concentration fluctuations at a fixed receptor include contributions both from in-plume fluctuations (relative diffusion) and from plume meandering. The latter dominates the fluctuations from small sources at downwind travel times t less than one Lagrangian time scale (τ_L). The in-plume component dominates the fluctuations from small sources at large travel times or from broad sources (such as the nearly instantaneous, large exhaust clouds from rocket launches modeled by REEDM) at all travel times.

Hanna (1984) reviewed the methods for estimating concentration fluctuations. For the internal fluctuations (for $t > \tau_L$), he recommended a simple expression for $\sigma_c/\overline{C}$ in terms of the ratios of horizontal and vertical coordinates to the corresponding dispersion parameters, and the ratios of Eulerian length and time scales to the standard deviations of the initial source distribution and the concentration averaging time, respectively. These equations may be used to estimate the concentration probability distributions based on REEDM model predictions of mean concentrations. However, this method should be carefully evaluated with suitable data before it can be adopted for routine use.

The problem of modeling concentration fluctuations is an active topic of current research. Although this modeling ability has improved in the past fifteen years or so, it is presently not at a stage whereby reliable assessments can be made for general atmospheric conditions (*e.g.*, different stabilities, wind speeds, *etc.*) and for arbitrary sources (Panwar *et al.*, 1994). Currently, one of the primary limiting factors in concentration-fluctuation research is a lack of field data. Past field experiments have focused almost exclusively on average concentrations, in part because the technology for measuring concentration fluctuations was not generally available until recently. The current lack of suitable data would make it difficult to test any concentration-fluctuation algorithm that is added to REEDM.

8. *REEDM uses a linear cloud-growth model with constant entrainment coefficients during the buoyant-rise phase of cloud development. Can a more physically based model be devised?*

The assumption of linear cloud growth actually has a somewhat stronger physical basis than is immediately apparent. For a buoyant cloud, Morton *et al.* (1956) used an entrainment velocity u_e to represent the rate at which ambient air is entrained along the outer edge of the cloud. They then assumed that u_e is proportional to the vertical velocity $\overline{w}$ of the cloud:

$$u_e = \gamma_e |\overline{w}| \, . \qquad \text{(R25)}$$

This is a reasonable assumption, since the main source of energy for the development of turbulence is the velocity shear at the cloud's outer edge (neglecting ambient turbulence). For a spherical cloud, it is easy to show that Eq. (R25) is equivalent to requiring that the cloud radius r grows linearly with height above the ground.

The assumption of linear cloud growth with height will of course be in error if Eq. (R25) is a poor assumption. It is possible to develop a more complicated entrainment hypothesis, but, as noted by Davidson (1989), these more complicated hypotheses have never been shown to produce results that are significantly better than those obtained with Eq. (R25). The value of the entrainment coefficient γ_e is another possible source of error. REEDM uses values based on relatively small clouds that may not be representative of the large, hot clouds produced during rocket launches. Since γ_e is an empirical parameter, the best way to estimate it is to use data from actual rocket launches. The ongoing analysis by Aerospace Corporation of infrared images from launch clouds may be helpful in providing refined estimates of γ_e.

There has been some discussion in the REEDM community that the model concentrations are highly sensitive to small changes in the entrainment coefficient γ_e. Given our understanding of the REEDM physics, we do not see why the model should exhibit such strong sensitivity to γ_e, and we therefore regard this result to be suspect. Informal tests at ATDD did not show a strong sensitivity of the REEDM peak concentrations to γ_e.

9. *During the buoyant-rise phase, REEDM treats conflagrations as continuous sources and other releases as instantaneous sources. After stabilization, all releases are treated as instantaneous sources. How significant is this lack of consistency in cloud treatment?*

This particular problem was mentioned in Section 2.1 of this report. For a conflagration, REEDM uses a plume-rise equation valid for bent-over plumes. With a source burn time of 10 minutes, the bent-over plume can stretch for several kilometers in the along-wind direction. During the passive-diffusion phase, however, REEDM assumes that the effluent cloud is a nearly spherical instantaneous cloud. This spherical cloud will have higher initial concentrations than the bent-over plume, since the along-wind dimension of the spherical cloud is smaller.

One way to correct the inconsistent treatment of conflagrations is to represent the stabilized cloud as a series of puffs that are released sequentially at the stabilization height z_s over a period corresponding to the burn time of the solid rocket propellant. This is the usual way that finite-duration releases are treated in traditional puff models.